



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:38 am BST

PDB ID : 4M57  
Title : Crystal structure of the pentatricopeptide repeat protein PPR10 from maize  
Authors : Yin, P.; Li, Q.; Yan, C.; Liu, Y.; Yan, N.  
Deposited on : 2013-08-08  
Resolution : 2.86 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

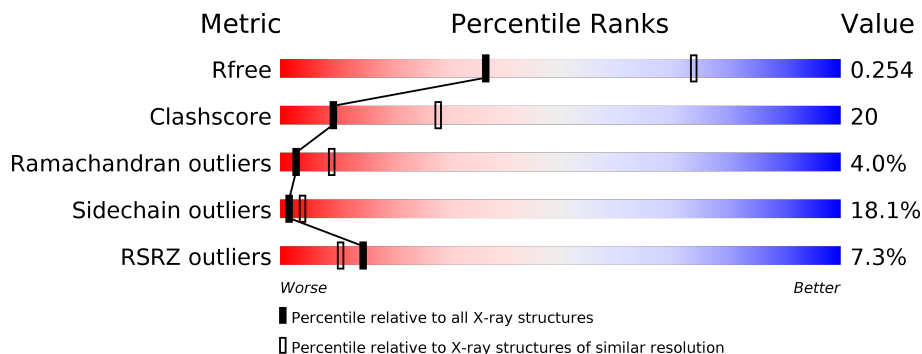
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

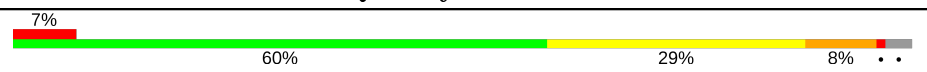
The reported resolution of this entry is 2.86 Å.

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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	A	726	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5326 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 Chloroplast pentatricopeptide repeat protein 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	702	5326	3367	910	1007	14	28	0	0	0

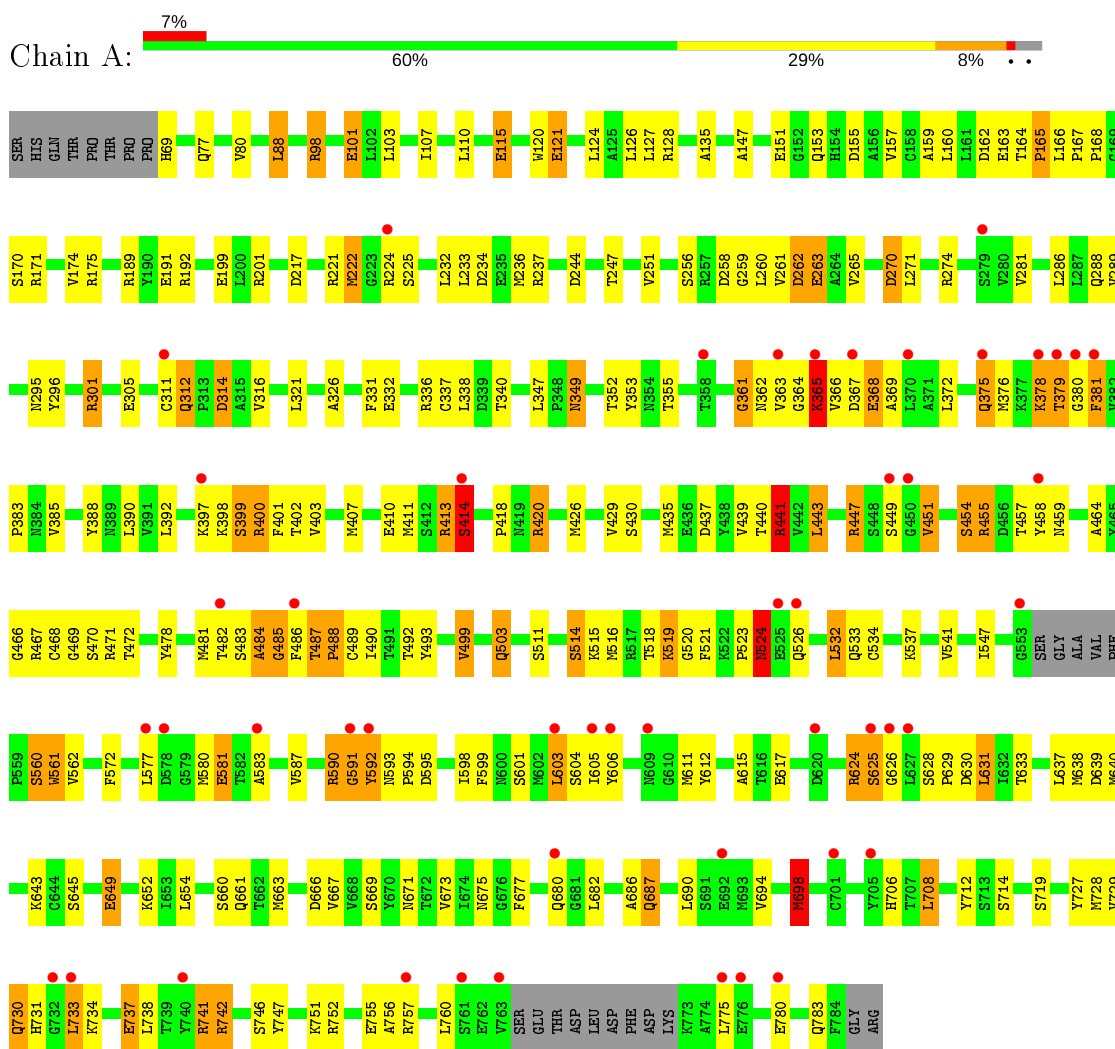
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
A	279	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
A	430	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
A	449	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Chloroplast pentatricopeptide repeat protein 10



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.37Å 176.54Å 64.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.08 – 2.86 37.08 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.08-2.86) 99.5 (37.08-2.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.88 (at 2.85Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.240 , 0.254 0.242 , 0.254	Depositor DCC
$R_{free}$ test set	952 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.4	Xtrriage
Anisotropy	0.448	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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	A	0.63	5/5395 (0.1%)	0.64	3/7269 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	N-CD	5.30	1.55	1.47
1	A	167	PRO	N-CD	5.29	1.55	1.47
1	A	407	MSE	CG-SE	-5.11	1.78	1.95
1	A	222	MSE	CG-SE	-5.03	1.78	1.95
1	A	698	MSE	CG-SE	-5.03	1.78	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	167	PRO	C-N-CD	5.67	140.31	128.40
1	A	603	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5326	0	5228	207	1
All	All	5326	0	5228	207	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 20.

All (207) 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:365:LYS:HE2	1:A:368:GLU:CG	1.67	1.23
1:A:471:ARG:CD	1:A:503:GLN:HE22	1.52	1.23
1:A:471:ARG:HD2	1:A:503:GLN:NE2	1.57	1.19
1:A:455:ARG:HG2	1:A:455:ARG:HH11	1.05	1.11
1:A:455:ARG:CG	1:A:455:ARG:HH11	1.61	1.10
1:A:365:LYS:HE2	1:A:368:GLU:HG2	1.29	1.09
1:A:590:ARG:HG2	1:A:590:ARG:HH21	1.01	1.09
1:A:455:ARG:HB2	1:A:486:PHE:CD2	1.92	1.03
1:A:455:ARG:HB2	1:A:486:PHE:HD2	1.23	1.03
1:A:471:ARG:HD2	1:A:503:GLN:HE22	0.90	1.02
1:A:331:PHE:CE2	1:A:363:VAL:HG21	1.98	0.98
1:A:365:LYS:HE2	1:A:368:GLU:HG3	1.43	0.96
1:A:590:ARG:HH21	1:A:590:ARG:CG	1.78	0.96
1:A:455:ARG:NH2	1:A:489:CYS:SG	2.40	0.94
1:A:727:TYR:O	1:A:731:HIS:CD2	2.23	0.92
1:A:727:TYR:O	1:A:731:HIS:HD2	1.55	0.90
1:A:590:ARG:NH2	1:A:590:ARG:HG2	1.80	0.89
1:A:331:PHE:HE2	1:A:363:VAL:HG21	1.39	0.88
1:A:518:THR:C	1:A:520:GLY:H	1.77	0.87
1:A:455:ARG:HG2	1:A:455:ARG:NH1	1.88	0.87
1:A:485:GLY:O	1:A:486:PHE:CD1	2.30	0.85
1:A:737:GLU:CD	1:A:737:GLU:H	1.80	0.84
1:A:455:ARG:NH1	1:A:455:ARG:CG	2.30	0.84
1:A:103:LEU:HD23	1:A:135:ALA:HB2	1.58	0.83
1:A:365:LYS:CE	1:A:368:GLU:HG3	2.08	0.83
1:A:466:GLY:HA2	1:A:499:VAL:HG13	1.62	0.82
1:A:649:GLU:OE2	1:A:652:LYS:HD3	1.81	0.81
1:A:260:LEU:HB3	1:A:263:GLU:HG3	1.62	0.81
1:A:365:LYS:HD3	1:A:368:GLU:HG3	1.63	0.79
1:A:233:LEU:HA	1:A:236:MSE:HE3	1.65	0.78
1:A:410:GLU:O	1:A:414:SER:HB2	1.85	0.77
1:A:518:THR:O	1:A:520:GLY:N	2.19	0.76
1:A:365:LYS:CE	1:A:368:GLU:CG	2.56	0.75
1:A:590:ARG:HB2	1:A:592:TYR:CD1	2.21	0.75
1:A:365:LYS:CD	1:A:368:GLU:HG3	2.17	0.74
1:A:630:ASP:HA	1:A:663:MSE:HE1	1.68	0.74
1:A:615:ALA:HB3	1:A:640:MSE:HE1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:SER:O	1:A:680:GLN:NE2	2.20	0.73
1:A:441:ARG:HH11	1:A:441:ARG:HG2	1.53	0.73
1:A:349:ASN:HB2	1:A:352:THR:HG23	1.70	0.72
1:A:757:ARG:NH2	1:A:783:GLN:OE1	2.24	0.71
1:A:256:SER:HB3	1:A:289:VAL:HG22	1.73	0.70
1:A:471:ARG:HD3	1:A:503:GLN:HE22	1.54	0.70
1:A:413:ARG:O	1:A:414:SER:C	2.30	0.70
1:A:760:LEU:HD11	1:A:775:LEU:HB3	1.74	0.70
1:A:590:ARG:O	1:A:591:GLY:C	2.29	0.69
1:A:164:THR:HG22	1:A:165:PRO:N	2.07	0.69
1:A:581:GLU:OE2	1:A:606:TYR:OH	2.09	0.69
1:A:727:TYR:CE1	1:A:731:HIS:NE2	2.61	0.68
1:A:486:PHE:O	1:A:488:PRO:HD3	1.94	0.68
1:A:388:TYR:HB3	1:A:411:MSE:SE	2.44	0.68
1:A:429:VAL:O	1:A:467:ARG:NH1	2.27	0.68
1:A:478:TYR:O	1:A:482:THR:HG23	1.93	0.68
1:A:687:GLN:HG2	1:A:708:LEU:CD1	2.24	0.67
1:A:590:ARG:HD3	1:A:592:TYR:CE1	2.30	0.66
1:A:727:TYR:CD1	1:A:731:HIS:NE2	2.64	0.66
1:A:737:GLU:CD	1:A:737:GLU:N	2.49	0.65
1:A:365:LYS:HA	1:A:365:LYS:HE3	1.76	0.65
1:A:514:SER:O	1:A:518:THR:HG23	1.98	0.64
1:A:471:ARG:CD	1:A:503:GLN:NE2	2.35	0.64
1:A:590:ARG:HB2	1:A:592:TYR:HD1	1.64	0.63
1:A:483:SER:C	1:A:485:GLY:H	2.00	0.63
1:A:727:TYR:CE1	1:A:731:HIS:CE1	2.87	0.63
1:A:217:ASP:O	1:A:221:ARG:HG3	2.00	0.62
1:A:115:GLU:OE2	1:A:115:GLU:HA	2.00	0.61
1:A:311:CYS:O	1:A:312:GLN:HB3	1.99	0.61
1:A:455:ARG:HB2	1:A:486:PHE:CE2	2.35	0.61
1:A:455:ARG:NH1	1:A:455:ARG:HG3	2.15	0.61
1:A:594:PRO:HG2	1:A:599:PHE:HE2	1.65	0.61
1:A:314:ASP:HB3	1:A:316:VAL:H	1.66	0.61
1:A:594:PRO:HG2	1:A:599:PHE:CE2	2.37	0.60
1:A:612:TYR:HD1	1:A:640:MSE:HE2	1.66	0.59
1:A:312:GLN:HG3	1:A:312:GLN:O	2.02	0.59
1:A:437:ASP:O	1:A:440:THR:OG1	2.20	0.58
1:A:690:LEU:O	1:A:694:VAL:HG23	2.03	0.58
1:A:262:ASP:OD1	1:A:262:ASP:N	2.31	0.57
1:A:410:GLU:O	1:A:414:SER:CB	2.52	0.57
1:A:435:MSE:O	1:A:439:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASP:OD2	1:A:221:ARG:NH1	2.37	0.57
1:A:103:LEU:CD2	1:A:135:ALA:HB2	2.32	0.56
1:A:435:MSE:HE2	1:A:464:ALA:O	2.05	0.56
1:A:411:MSE:HE2	1:A:418:PRO:HG3	1.88	0.56
1:A:256:SER:HB2	1:A:289:VAL:HA	1.86	0.56
1:A:120:TRP:CD1	1:A:151:GLU:HG2	2.40	0.56
1:A:687:GLN:HG3	1:A:712:TYR:OH	2.04	0.56
1:A:729:VAL:O	1:A:731:HIS:N	2.37	0.56
1:A:560:SER:OG	1:A:561:TRP:N	2.36	0.55
1:A:687:GLN:HG2	1:A:708:LEU:HD11	1.88	0.55
1:A:455:ARG:CB	1:A:486:PHE:CE2	2.90	0.55
1:A:729:VAL:C	1:A:731:HIS:H	2.09	0.55
1:A:524:ASN:HB3	1:A:526:GLN:H	1.72	0.55
1:A:400:ARG:HB3	1:A:403:VAL:CG2	2.37	0.55
1:A:455:ARG:HH21	1:A:489:CYS:CB	2.18	0.55
1:A:728:MSE:HE3	1:A:733:LEU:HD23	1.90	0.54
1:A:296:TYR:CZ	1:A:336:ARG:HD2	2.42	0.54
1:A:455:ARG:CB	1:A:486:PHE:CD2	2.79	0.54
1:A:326:ALA:HB3	1:A:355:THR:HG22	1.90	0.53
1:A:590:ARG:HB2	1:A:592:TYR:CE1	2.42	0.53
1:A:115:GLU:HG2	1:A:147:ALA:HB1	1.91	0.53
1:A:256:SER:HA	1:A:289:VAL:HG13	1.91	0.53
1:A:624:ARG:O	1:A:625:SER:C	2.47	0.52
1:A:115:GLU:HG2	1:A:147:ALA:CB	2.39	0.52
1:A:741:ARG:HG2	1:A:775:LEU:HD11	1.92	0.52
1:A:166:LEU:HD11	1:A:199:GLU:HG3	1.92	0.52
1:A:741:ARG:HA	1:A:775:LEU:HD11	1.92	0.52
1:A:449:SER:O	1:A:451:VAL:HG23	2.10	0.51
1:A:331:PHE:CD2	1:A:363:VAL:HG21	2.44	0.51
1:A:518:THR:C	1:A:520:GLY:N	2.47	0.51
1:A:493:TYR:HB3	1:A:516:MSE:HE2	1.91	0.51
1:A:667:VAL:HG23	1:A:698:MSE:HE2	1.91	0.51
1:A:366:VAL:O	1:A:369:ALA:HB3	2.10	0.51
1:A:88:LEU:HD21	1:A:121:GLU:HB2	1.93	0.50
1:A:376:MSE:O	1:A:381:PHE:HB2	2.12	0.50
1:A:413:ARG:O	1:A:414:SER:O	2.30	0.50
1:A:400:ARG:O	1:A:402:THR:N	2.45	0.50
1:A:469:GLY:O	1:A:471:ARG:N	2.40	0.50
1:A:592:TYR:O	1:A:593:ASN:OD1	2.30	0.50
1:A:80:VAL:HG23	1:A:110:LEU:HD22	1.93	0.49
1:A:487:THR:O	1:A:488:PRO:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:O	1:A:115:GLU:CD	2.50	0.49
1:A:483:SER:C	1:A:485:GLY:N	2.65	0.48
1:A:484:ALA:O	1:A:485:GLY:O	2.30	0.48
1:A:189:ARG:NH2	1:A:192:ARG:HG3	2.27	0.48
1:A:594:PRO:CG	1:A:599:PHE:CE2	2.95	0.48
1:A:365:LYS:CA	1:A:365:LYS:HE3	2.39	0.48
1:A:447:ARG:HB3	1:A:447:ARG:HE	1.50	0.48
1:A:580:MSE:HE1	1:A:605:ILE:HD13	1.95	0.48
1:A:490:ILE:HG13	1:A:521:PHE:HD2	1.79	0.47
1:A:115:GLU:OE2	1:A:115:GLU:CA	2.61	0.47
1:A:392:LEU:HD22	1:A:426:MSE:HE3	1.96	0.47
1:A:631:LEU:HD13	1:A:666:ASP:OD2	2.14	0.47
1:A:680:GLN:O	1:A:680:GLN:HG2	2.14	0.47
1:A:435:MSE:CE	1:A:464:ALA:O	2.62	0.47
1:A:166:LEU:CD1	1:A:199:GLU:HG3	2.44	0.47
1:A:361:GLY:O	1:A:364:GLY:N	2.42	0.47
1:A:451:VAL:O	1:A:451:VAL:HG12	2.15	0.47
1:A:455:ARG:HH21	1:A:489:CYS:HB3	1.80	0.47
1:A:153:GLN:O	1:A:157:VAL:HG23	2.15	0.46
1:A:247:THR:O	1:A:251:VAL:HG23	2.15	0.46
1:A:757:ARG:NH1	1:A:780:GLU:OE2	2.49	0.46
1:A:326:ALA:CB	1:A:355:THR:HG22	2.46	0.46
1:A:518:THR:OG1	1:A:519:LYS:N	2.48	0.45
1:A:728:MSE:O	1:A:733:LEU:HB2	2.16	0.45
1:A:706:HIS:CE1	1:A:742:ARG:HG3	2.52	0.45
1:A:69:HIS:HA	1:A:77:GLN:NE2	2.31	0.45
1:A:366:VAL:HG23	1:A:367:ASP:H	1.81	0.45
1:A:410:GLU:O	1:A:414:SER:N	2.46	0.45
1:A:590:ARG:O	1:A:591:GLY:O	2.35	0.45
1:A:487:THR:O	1:A:487:THR:OG1	2.30	0.45
1:A:443:LEU:O	1:A:447:ARG:HG2	2.17	0.45
1:A:481:MSE:CE	1:A:488:PRO:HA	2.47	0.45
1:A:458:TYR:CG	1:A:481:MSE:HB2	2.52	0.45
1:A:441:ARG:NH1	1:A:441:ARG:HG2	2.23	0.44
1:A:375:GLN:O	1:A:379:THR:HG23	2.16	0.44
1:A:458:TYR:CE2	1:A:481:MSE:HA	2.53	0.44
1:A:730:GLN:O	1:A:731:HIS:CD2	2.70	0.44
1:A:594:PRO:HB2	1:A:599:PHE:CE2	2.52	0.44
1:A:677:PHE:CB	1:A:686:ALA:HB2	2.47	0.44
1:A:727:TYR:HE1	1:A:731:HIS:CE1	2.35	0.44
1:A:639:ASP:OD1	1:A:643:LYS:NZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:LEU:HD23	1:A:637:LEU:HA	1.66	0.43
1:A:261:VAL:O	1:A:265:VAL:HG23	2.18	0.43
1:A:459:ASN:OD1	1:A:492:THR:HG22	2.17	0.43
1:A:583:ALA:O	1:A:587:VAL:HG23	2.17	0.43
1:A:430:SER:HB3	1:A:467:ARG:HD3	1.98	0.43
1:A:429:VAL:HG12	1:A:430:SER:O	2.18	0.43
1:A:598:ILE:O	1:A:601:SER:HB2	2.18	0.43
1:A:738:LEU:HD12	1:A:738:LEU:HA	1.80	0.43
1:A:159:ALA:O	1:A:163:GLU:HG3	2.18	0.43
1:A:590:ARG:NH2	1:A:590:ARG:CG	2.50	0.43
1:A:671:ASN:O	1:A:675:ASN:HB2	2.19	0.43
1:A:677:PHE:HB2	1:A:686:ALA:HB2	2.01	0.43
1:A:483:SER:OG	1:A:484:ALA:N	2.51	0.43
1:A:561:TRP:HB2	1:A:592:TYR:CE2	2.52	0.43
1:A:592:TYR:HB3	1:A:593:ASN:H	1.27	0.42
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.87	0.42
1:A:420:ARG:NH1	1:A:454:SER:OG	2.48	0.42
1:A:164:THR:CG2	1:A:165:PRO:N	2.77	0.42
1:A:628:SER:HA	1:A:629:PRO:HD3	1.78	0.42
1:A:638:MSE:HE2	1:A:673:VAL:CG2	2.50	0.42
1:A:376:MSE:HE2	1:A:383:PRO:HB3	2.01	0.42
1:A:775:LEU:HA	1:A:775:LEU:HD13	1.66	0.42
1:A:485:GLY:O	1:A:486:PHE:HD1	1.96	0.42
1:A:521:PHE:CD1	1:A:521:PHE:N	2.87	0.42
1:A:729:VAL:C	1:A:731:HIS:N	2.73	0.42
1:A:411:MSE:HA	1:A:414:SER:HB2	2.02	0.42
1:A:378:LYS:C	1:A:380:GLY:H	2.23	0.42
1:A:455:ARG:CA	1:A:486:PHE:CE2	3.03	0.42
1:A:338:LEU:HA	1:A:338:LEU:HD23	1.82	0.42
1:A:368:GLU:HG2	1:A:368:GLU:H	1.54	0.41
1:A:532:LEU:HD13	1:A:547:ILE:HD12	2.02	0.41
1:A:572:PHE:HA	1:A:580:MSE:HE2	2.02	0.41
1:A:115:GLU:CD	1:A:115:GLU:C	2.79	0.41
1:A:259:GLY:O	1:A:261:VAL:HG23	2.20	0.41
1:A:747:TYR:HB3	1:A:756:ALA:HB2	2.03	0.41
1:A:301:ARG:HH11	1:A:305:GLU:HG3	1.86	0.41
1:A:481:MSE:HE2	1:A:488:PRO:HA	2.02	0.41
1:A:98:ARG:NH2	1:A:101:GLU:OE1	2.53	0.41
1:A:233:LEU:O	1:A:237:ARG:HG3	2.21	0.41
1:A:471:ARG:HH11	1:A:503:GLN:NE2	2.18	0.41
1:A:577:LEU:HA	1:A:580:MSE:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLU:H	1:A:263:GLU:HG2	1.16	0.41
1:A:443:LEU:HA	1:A:443:LEU:HD23	1.78	0.41
1:A:660:SER:O	1:A:661:GLN:HB2	2.20	0.41
1:A:270:ASP:O	1:A:274:ARG:HG3	2.21	0.41
1:A:312:GLN:CG	1:A:312:GLN:O	2.65	0.40
1:A:361:GLY:O	1:A:362:ASN:C	2.59	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:OD2	1:A:733:LEU:O[2_555]	1.99	0.21

## 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	696/726 (96%)	628 (90%)	40 (6%)	28 (4%)	<b>3</b> <b>9</b>

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	SER
1	A	401	PHE
1	A	519	LYS
1	A	524	ASN
1	A	560	SER
1	A	624	ARG
1	A	625	SER
1	A	470	SER
1	A	485	GLY
1	A	591	GLY

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Mol	Chain	Res	Type
1	A	730	GLN
1	A	165	PRO
1	A	349	ASN
1	A	365	LYS
1	A	398	LYS
1	A	484	ALA
1	A	523	PRO
1	A	682	LEU
1	A	400	ARG
1	A	414	SER
1	A	626	GLY
1	A	734	LYS
1	A	312	GLN
1	A	487	THR
1	A	361	GLY
1	A	379	THR
1	A	451	VAL
1	A	488	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	A	551/567 (97%)	451 (82%)	100 (18%)	<b>1</b> <b>4</b>

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	98	ARG
1	A	101	GLU
1	A	107	ILE
1	A	115	GLU
1	A	121	GLU
1	A	124	LEU
1	A	126	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	127	LEU
1	A	128	ARG
1	A	155	ASP
1	A	160	LEU
1	A	162	ASP
1	A	170	SER
1	A	171	ARG
1	A	174	VAL
1	A	175	ARG
1	A	191	GLU
1	A	201	ARG
1	A	222	MSE
1	A	224	ARG
1	A	225	SER
1	A	232	LEU
1	A	234	ASP
1	A	258	ASP
1	A	262	ASP
1	A	263	GLU
1	A	270	ASP
1	A	271	LEU
1	A	281	VAL
1	A	288	GLN
1	A	295	ASN
1	A	301	ARG
1	A	314	ASP
1	A	321	LEU
1	A	332	GLU
1	A	337	CYS
1	A	340	THR
1	A	347	LEU
1	A	353	TYR
1	A	365	LYS
1	A	368	GLU
1	A	372	LEU
1	A	375	GLN
1	A	378	LYS
1	A	381	PHE
1	A	385	VAL
1	A	390	LEU
1	A	397	LYS
1	A	399	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	413	ARG
1	A	414	SER
1	A	420	ARG
1	A	441	ARG
1	A	443	LEU
1	A	447	ARG
1	A	454	SER
1	A	455	ARG
1	A	457	THR
1	A	468	CYS
1	A	472	THR
1	A	499	VAL
1	A	503	GLN
1	A	511	SER
1	A	514	SER
1	A	515	LYS
1	A	524	ASN
1	A	532	LEU
1	A	533	GLN
1	A	534	CYS
1	A	537	LYS
1	A	541	VAL
1	A	561	TRP
1	A	562	VAL
1	A	581	GLU
1	A	590	ARG
1	A	592	TYR
1	A	595	ASP
1	A	603	LEU
1	A	604	SER
1	A	611	MSE
1	A	617	GLU
1	A	631	LEU
1	A	633	THR
1	A	649	GLU
1	A	654	LEU
1	A	669	SER
1	A	687	GLN
1	A	698	MSE
1	A	708	LEU
1	A	714	SER
1	A	719	SER

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Mol	Chain	Res	Type
1	A	733	LEU
1	A	737	GLU
1	A	741	ARG
1	A	742	ARG
1	A	746	SER
1	A	751	LYS
1	A	752	ARG
1	A	755	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	503	GLN
1	A	680	GLN
1	A	687	GLN
1	A	731	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 carbohydrates 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

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, 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	A	674/726 (92%)	0.47	49 (7%) <b>15</b> <b>11</b>	39, 71, 113, 199	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	625	SER	5.7
1	A	525	GLU	4.6
1	A	763	VAL	4.4
1	A	381	PHE	3.8
1	A	591	GLY	3.6
1	A	603	LEU	3.3
1	A	761	SER	3.2
1	A	776	GLU	3.1
1	A	414	SER	3.1
1	A	553	GLY	3.1
1	A	449	SER	3.1
1	A	486	PHE	3.0
1	A	458	TYR	3.0
1	A	733	LEU	3.0
1	A	380	GLY	3.0
1	A	311	CYS	2.9
1	A	775	LEU	2.9
1	A	627	LEU	2.8
1	A	482	THR	2.8
1	A	692	GLU	2.7
1	A	363	VAL	2.6
1	A	367	ASP	2.6
1	A	606	TYR	2.6
1	A	583	ALA	2.5
1	A	605	ILE	2.5
1	A	701	CYS	2.5
1	A	609	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	780	GLU	2.4
1	A	375	GLN	2.4
1	A	680	GLN	2.4
1	A	620	ASP	2.4
1	A	365	LYS	2.4
1	A	378	LYS	2.3
1	A	705	TYR	2.3
1	A	577	LEU	2.3
1	A	279	SER	2.3
1	A	732	GLY	2.3
1	A	526	GLN	2.3
1	A	592	TYR	2.2
1	A	450	GLY	2.2
1	A	370	LEU	2.2
1	A	740	TYR	2.2
1	A	757	ARG	2.2
1	A	578	ASP	2.2
1	A	224	ARG	2.1
1	A	626	GLY	2.1
1	A	358	THR	2.0
1	A	397	LYS	2.0
1	A	379	THR	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 carbohydrates 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.