



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:06 am GMT

PDB ID : 1XM9
Title : Structure of the armadillo repeat domain of plakophilin 1
Authors : Choi, H.J.; Weis, W.I.
Deposited on : 2004-10-01
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

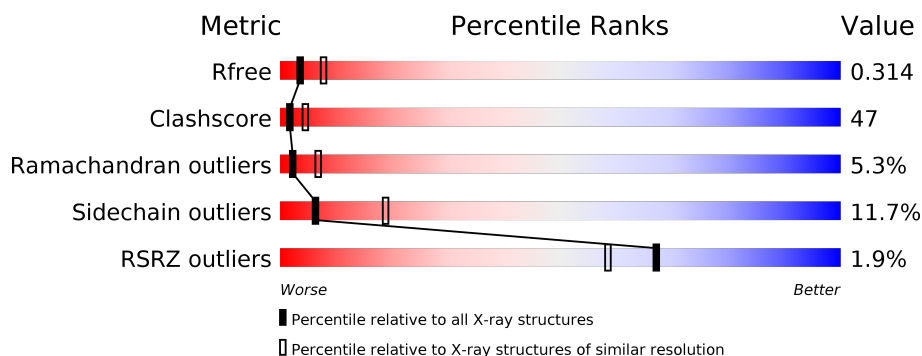
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	457	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3237 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.

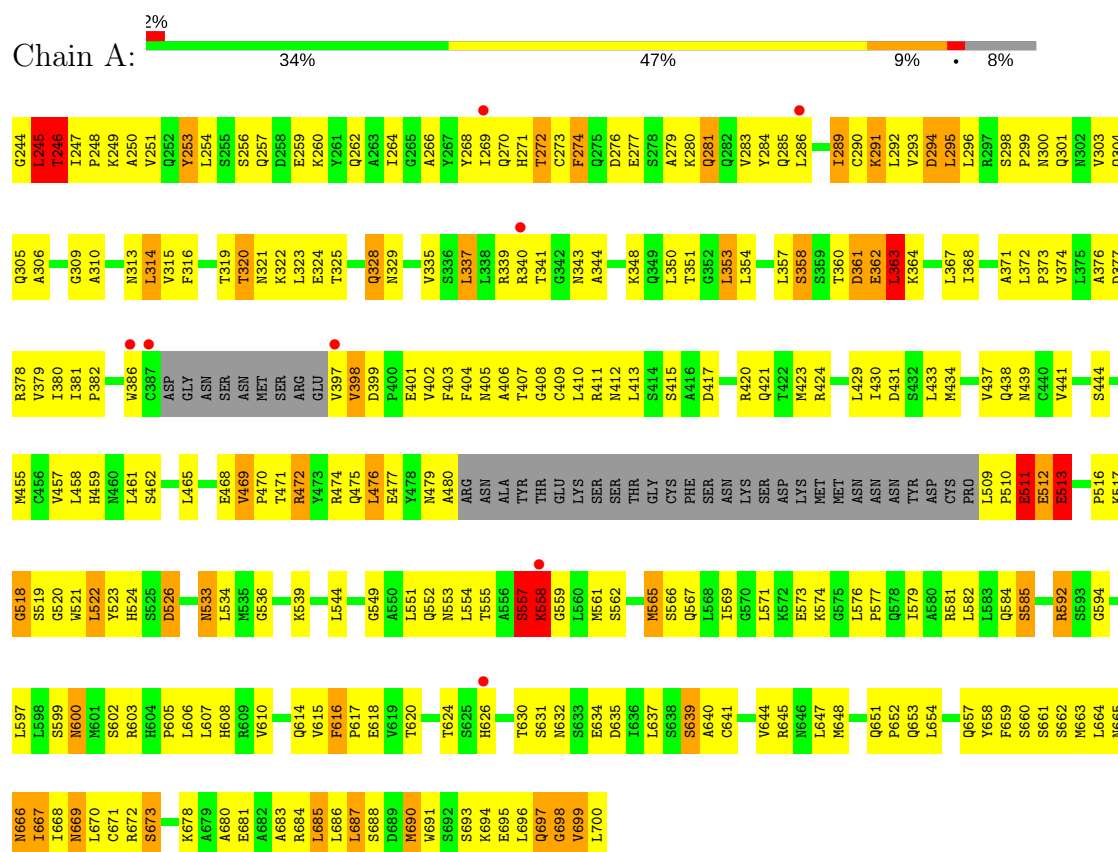
- Molecule 1 is a protein called plakophilin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3237	2007	581	627	22	0	0	0

3 Residue-property plots

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: plakophilin 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	53.35Å 131.98Å 142.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.80 48.34 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.9 (29.92-2.80) 86.6 (48.34-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.324 0.252 , 0.314	Depositor DCC
R_{free} test set	1142 reflections (9.97%)	DCC
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.9	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	0.92	EDS
Total number of atoms	3237	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/3282	0.73	3/4434 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	246	THR	N-CA-C	5.43	125.66	111.00
1	A	557	SER	N-CA-C	5.06	124.67	111.00

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	3237	0	3249	308	0
All	All	3237	0	3249	308	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 47.

All (308) 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:244:GLY:HA3	1:A:249:LYS:HZ3	1.21	1.01
1:A:693:SER:OG	1:A:696:LEU:HD23	1.66	0.94
1:A:551:LEU:O	1:A:555:THR:HG22	1.68	0.93
1:A:455:MET:HE1	1:A:458:LEU:HD12	1.51	0.90
1:A:354:LEU:HA	1:A:357:LEU:HD12	1.53	0.89
1:A:279:ALA:O	1:A:283:VAL:HG23	1.73	0.89
1:A:660:SER:O	1:A:664:LEU:HG	1.73	0.89
1:A:289:ILE:H	1:A:289:ILE:HD12	1.38	0.87
1:A:539:LYS:HA	1:A:539:LYS:HE2	1.55	0.87
1:A:600:ASN:HD22	1:A:600:ASN:N	1.68	0.87
1:A:600:ASN:H	1:A:600:ASN:HD22	1.20	0.86
1:A:644:VAL:O	1:A:648:MET:HG2	1.75	0.86
1:A:653:GLN:O	1:A:657:GLN:HG3	1.76	0.86
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.39	0.85
1:A:291:LYS:HE3	1:A:291:LYS:HA	1.57	0.84
1:A:471:THR:HG22	1:A:472:ARG:H	1.43	0.84
1:A:471:THR:HG22	1:A:472:ARG:HD2	1.61	0.83
1:A:295:LEU:O	1:A:298:SER:HB3	1.80	0.82
1:A:645:ARG:NH1	1:A:685:LEU:HD22	1.96	0.81
1:A:244:GLY:HA3	1:A:249:LYS:NZ	1.95	0.81
1:A:289:ILE:O	1:A:293:VAL:HG23	1.81	0.80
1:A:273:CYS:SG	1:A:280:LYS:HG2	2.22	0.78
1:A:247:ILE:HB	1:A:248:PRO:HD3	1.66	0.77
1:A:576:LEU:HD12	1:A:614:GLN:HE21	1.48	0.76
1:A:455:MET:CE	1:A:458:LEU:HD12	2.15	0.76
1:A:244:GLY:CA	1:A:249:LYS:HZ3	1.99	0.75
1:A:600:ASN:H	1:A:600:ASN:ND2	1.85	0.75
1:A:281:GLN:O	1:A:285:GLN:HG2	1.87	0.74
1:A:254:LEU:HD23	1:A:291:LYS:HB3	1.67	0.74
1:A:630:THR:HG22	1:A:632:ASN:H	1.52	0.74
1:A:472:ARG:NH1	1:A:511:GLU:HG3	2.02	0.74
1:A:557:SER:OG	1:A:562:SER:HB2	1.87	0.74
1:A:376:ALA:O	1:A:381:ILE:HG13	1.87	0.74
1:A:360:THR:HG23	1:A:360:THR:O	1.88	0.73
1:A:254:LEU:CD2	1:A:291:LYS:HB3	2.18	0.73
1:A:634:GLU:HG2	1:A:678:LYS:HB3	1.72	0.72
1:A:557:SER:O	1:A:559:GLY:N	2.23	0.72
1:A:617:PRO:HB3	1:A:658:TYR:HE2	1.54	0.71
1:A:294:ASP:O	1:A:296:LEU:N	2.22	0.71
1:A:353:LEU:HD22	1:A:357:LEU:HD11	1.71	0.71
1:A:455:MET:CE	1:A:455:MET:HA	2.21	0.71
1:A:291:LYS:O	1:A:295:LEU:HD13	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ARG:HH12	1:A:511:GLU:HG3	1.56	0.71
1:A:357:LEU:O	1:A:360:THR:HG22	1.90	0.70
1:A:244:GLY:O	1:A:245:LEU:HB2	1.90	0.70
1:A:337:LEU:HD13	1:A:350:LEU:HD11	1.74	0.69
1:A:270:GLN:HG2	1:A:313:ASN:HD22	1.58	0.69
1:A:664:LEU:HD11	1:A:699:VAL:HG11	1.74	0.68
1:A:686:LEU:HD23	1:A:686:LEU:O	1.94	0.68
1:A:681:GLU:O	1:A:685:LEU:HB2	1.94	0.68
1:A:351:THR:HG23	1:A:405:ASN:HB2	1.74	0.67
1:A:472:ARG:HG2	1:A:472:ARG:NH1	2.07	0.67
1:A:472:ARG:HD2	1:A:472:ARG:H	1.60	0.67
1:A:558:LYS:HA	1:A:603:ARG:NH1	2.10	0.66
1:A:470:PRO:HG3	1:A:474:ARG:HH22	1.61	0.66
1:A:291:LYS:HE3	1:A:291:LYS:CA	2.26	0.65
1:A:271:HIS:O	1:A:274:PHE:N	2.29	0.65
1:A:291:LYS:HA	1:A:291:LYS:CE	2.26	0.65
1:A:351:THR:HG23	1:A:405:ASN:CB	2.26	0.65
1:A:671:CYS:SG	1:A:684:ARG:HB3	2.36	0.65
1:A:246:THR:OG1	1:A:248:PRO:HD2	1.97	0.65
1:A:335:VAL:HG23	1:A:374:VAL:HG21	1.79	0.64
1:A:423:MET:HB3	1:A:429:LEU:HD23	1.80	0.64
1:A:368:ILE:HG22	1:A:413:LEU:HD13	1.78	0.64
1:A:251:VAL:HA	1:A:254:LEU:HD13	1.78	0.64
1:A:576:LEU:HD11	1:A:610:VAL:HG13	1.81	0.63
1:A:254:LEU:HD21	1:A:292:LEU:HG	1.80	0.62
1:A:511:GLU:O	1:A:512:GLU:HB2	1.99	0.62
1:A:665:ASN:O	1:A:668:ILE:HD12	1.99	0.62
1:A:472:ARG:HH12	1:A:511:GLU:CG	2.13	0.62
1:A:245:LEU:H	1:A:249:LYS:NZ	1.97	0.62
1:A:301:GLN:O	1:A:304:GLN:HB2	1.99	0.62
1:A:372:LEU:O	1:A:372:LEU:HD12	1.99	0.62
1:A:348:LYS:O	1:A:351:THR:HG22	2.00	0.62
1:A:462:SER:O	1:A:553:ASN:HB3	1.99	0.62
1:A:605:PRO:HA	1:A:608:HIS:CD2	2.35	0.62
1:A:690:MET:O	1:A:696:LEU:HB3	2.00	0.61
1:A:617:PRO:HB3	1:A:658:TYR:CE2	2.35	0.61
1:A:397:VAL:O	1:A:398:VAL:HB	2.01	0.61
1:A:632:ASN:O	1:A:635:ASP:N	2.30	0.61
1:A:360:THR:CG2	1:A:363:LEU:HG	2.31	0.60
1:A:645:ARG:HD2	1:A:686:LEU:HA	1.83	0.60
1:A:367:LEU:O	1:A:371:ALA:HB3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:MET:O	1:A:438:GLN:HG3	2.01	0.60
1:A:669:ASN:O	1:A:672:ARG:N	2.34	0.60
1:A:360:THR:HG21	1:A:363:LEU:HG	1.84	0.60
1:A:372:LEU:HB3	1:A:373:PRO:HD3	1.82	0.60
1:A:471:THR:HG22	1:A:472:ARG:N	2.15	0.60
1:A:386:TRP:CE2	1:A:431:ASP:HB3	2.36	0.59
1:A:244:GLY:O	1:A:245:LEU:HD23	2.02	0.59
1:A:472:ARG:NH2	1:A:513:GLU:N	2.51	0.59
1:A:360:THR:CG2	1:A:360:THR:O	2.50	0.58
1:A:558:LYS:HA	1:A:603:ARG:HH11	1.67	0.58
1:A:620:THR:O	1:A:624:THR:HG23	2.03	0.58
1:A:651:GLN:HG3	1:A:654:LEU:HD23	1.84	0.58
1:A:315:VAL:HG13	1:A:322:LYS:HG2	1.84	0.57
1:A:322:LYS:HD3	1:A:360:THR:HB	1.85	0.57
1:A:688:SER:C	1:A:690:MET:H	2.06	0.57
1:A:372:LEU:C	1:A:372:LEU:HD12	2.25	0.57
1:A:660:SER:C	1:A:664:LEU:HG	2.25	0.57
1:A:284:TYR:HA	1:A:289:ILE:HD11	1.87	0.57
1:A:630:THR:HG22	1:A:631:SER:N	2.20	0.57
1:A:687:LEU:O	1:A:687:LEU:HD22	2.05	0.56
1:A:249:LYS:HG3	1:A:250:ALA:N	2.19	0.56
1:A:315:VAL:HG13	1:A:322:LYS:CG	2.35	0.56
1:A:283:VAL:HG11	1:A:314:LEU:HD11	1.87	0.56
1:A:632:ASN:O	1:A:635:ASP:HB2	2.05	0.56
1:A:524:HIS:ND1	1:A:526:ASP:HB2	2.21	0.55
1:A:657:GLN:HB2	1:A:658:TYR:CD1	2.41	0.55
1:A:270:GLN:CG	1:A:313:ASN:HD22	2.20	0.55
1:A:554:LEU:HB3	1:A:565:MET:HG2	1.88	0.55
1:A:247:ILE:HD11	1:A:279:ALA:HB1	1.88	0.55
1:A:430:ILE:O	1:A:434:MET:HB2	2.06	0.55
1:A:270:GLN:HG2	1:A:313:ASN:ND2	2.22	0.55
1:A:476:LEU:O	1:A:480:ALA:HB3	2.07	0.55
1:A:472:ARG:NH2	1:A:513:GLU:H	2.06	0.54
1:A:610:VAL:O	1:A:614:GLN:HG2	2.07	0.54
1:A:472:ARG:HH12	1:A:511:GLU:CD	2.10	0.54
1:A:600:ASN:ND2	1:A:600:ASN:N	2.41	0.54
1:A:476:LEU:HD11	1:A:509:LEU:HD23	1.88	0.54
1:A:470:PRO:HA	1:A:474:ARG:NH2	2.22	0.54
1:A:520:GLY:HA2	1:A:523:TYR:CE2	2.43	0.54
1:A:661:SER:O	1:A:664:LEU:HB2	2.07	0.54
1:A:399:ASP:HB3	1:A:402:VAL:HG23	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:TRP:O	1:A:386:TRP:CG	2.61	0.54
1:A:511:GLU:O	1:A:512:GLU:CB	2.56	0.53
1:A:557:SER:C	1:A:559:GLY:N	2.62	0.53
1:A:558:LYS:H	1:A:603:ARG:HH12	1.56	0.53
1:A:472:ARG:NH1	1:A:511:GLU:OE2	2.38	0.53
1:A:664:LEU:CD1	1:A:699:VAL:HG11	2.37	0.53
1:A:687:LEU:C	1:A:687:LEU:HD22	2.30	0.53
1:A:413:LEU:C	1:A:415:SER:H	2.11	0.52
1:A:269:ILE:O	1:A:273:CYS:HB3	2.09	0.52
1:A:290:CYS:HB2	1:A:328:GLN:CD	2.29	0.52
1:A:557:SER:C	1:A:559:GLY:H	2.12	0.52
1:A:681:GLU:HG2	1:A:685:LEU:HD12	1.92	0.52
1:A:271:HIS:O	1:A:272:THR:C	2.49	0.52
1:A:251:VAL:CA	1:A:254:LEU:HD13	2.40	0.52
1:A:381:ILE:HB	1:A:382:PRO:HD3	1.92	0.51
1:A:667:ILE:O	1:A:670:LEU:HB2	2.10	0.51
1:A:377:ASP:O	1:A:382:PRO:HD3	2.10	0.51
1:A:699:VAL:O	1:A:700:LEU:C	2.49	0.51
1:A:321:ASN:O	1:A:325:THR:OG1	2.22	0.51
1:A:250:ALA:HA	1:A:253:TYR:HB2	1.92	0.51
1:A:339:ARG:HE	1:A:374:VAL:CG1	2.24	0.51
1:A:509:LEU:N	1:A:510:PRO:CD	2.74	0.51
1:A:512:GLU:O	1:A:513:GLU:C	2.49	0.51
1:A:539:LYS:CA	1:A:539:LYS:HE2	2.34	0.51
1:A:686:LEU:O	1:A:690:MET:HB2	2.11	0.51
1:A:536:GLY:HA2	1:A:581:ARG:HH22	1.75	0.51
1:A:254:LEU:HB3	1:A:291:LYS:HD3	1.93	0.51
1:A:290:CYS:HB2	1:A:328:GLN:OE1	2.11	0.50
1:A:344:ALA:O	1:A:348:LYS:HG3	2.10	0.50
1:A:364:LYS:O	1:A:367:LEU:HB2	2.11	0.50
1:A:690:MET:O	1:A:691:TRP:HD1	1.94	0.50
1:A:245:LEU:H	1:A:249:LYS:HZ3	1.57	0.50
1:A:289:ILE:HD12	1:A:289:ILE:N	2.18	0.50
1:A:697:GLN:O	1:A:698:GLY:C	2.50	0.50
1:A:351:THR:CG2	1:A:405:ASN:HB2	2.41	0.50
1:A:640:ALA:O	1:A:644:VAL:HG23	2.12	0.50
1:A:276:ASP:O	1:A:277:GLU:HB2	2.10	0.50
1:A:403:PHE:CE1	1:A:407:THR:HG21	2.47	0.50
1:A:665:ASN:O	1:A:667:ILE:N	2.45	0.49
1:A:274:PHE:CD1	1:A:274:PHE:C	2.82	0.49
1:A:254:LEU:HD22	1:A:291:LYS:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PRO:CA	1:A:474:ARG:NH2	2.75	0.49
1:A:536:GLY:HA2	1:A:581:ARG:NH2	2.28	0.49
1:A:600:ASN:O	1:A:603:ARG:HB3	2.14	0.48
1:A:328:GLN:O	1:A:329:ASN:HB2	2.12	0.48
1:A:361:ASP:HA	1:A:364:LYS:HE3	1.95	0.48
1:A:592:ARG:HB3	1:A:592:ARG:CZ	2.42	0.48
1:A:315:VAL:CG1	1:A:322:LYS:HG2	2.43	0.48
1:A:475:GLN:C	1:A:477:GLU:N	2.67	0.48
1:A:266:ALA:HB3	1:A:306:ALA:HB1	1.94	0.48
1:A:469:VAL:HG11	1:A:519:SER:OG	2.14	0.48
1:A:662:SER:O	1:A:663:MET:C	2.52	0.48
1:A:521:TRP:O	1:A:523:TYR:N	2.47	0.48
1:A:624:THR:HG22	1:A:663:MET:CB	2.44	0.48
1:A:549:GLY:O	1:A:552:GLN:HB3	2.13	0.48
1:A:315:VAL:O	1:A:316:PHE:C	2.51	0.47
1:A:523:TYR:O	1:A:565:MET:CE	2.62	0.47
1:A:470:PRO:HG3	1:A:474:ARG:NH2	2.27	0.47
1:A:536:GLY:CA	1:A:581:ARG:HH22	2.27	0.47
1:A:544:LEU:HD13	1:A:582:LEU:CD2	2.45	0.47
1:A:281:GLN:O	1:A:284:TYR:HB3	2.15	0.47
1:A:592:ARG:NH1	1:A:592:ARG:C	2.68	0.47
1:A:659:PHE:C	1:A:664:LEU:HD21	2.35	0.47
1:A:417:ASP:O	1:A:421:GLN:HG3	2.15	0.47
1:A:475:GLN:C	1:A:477:GLU:H	2.17	0.47
1:A:441:VAL:CG1	1:A:533:ASN:HD22	2.28	0.47
1:A:599:SER:OG	1:A:600:ASN:N	2.48	0.47
1:A:298:SER:HA	1:A:299:PRO:HD3	1.69	0.47
1:A:520:GLY:HA2	1:A:523:TYR:HE2	1.80	0.47
1:A:281:GLN:HE21	1:A:281:GLN:HA	1.80	0.46
1:A:290:CYS:HB2	1:A:328:GLN:NE2	2.30	0.46
1:A:517:LYS:O	1:A:520:GLY:N	2.43	0.46
1:A:576:LEU:HB2	1:A:577:PRO:HD3	1.96	0.46
1:A:668:ILE:O	1:A:669:ASN:C	2.52	0.46
1:A:247:ILE:HB	1:A:248:PRO:CD	2.43	0.46
1:A:283:VAL:CG1	1:A:314:LEU:HD11	2.44	0.46
1:A:413:LEU:C	1:A:415:SER:N	2.68	0.46
1:A:273:CYS:O	1:A:273:CYS:SG	2.73	0.46
1:A:424:ARG:NH1	1:A:461:LEU:O	2.49	0.46
1:A:433:LEU:O	1:A:437:VAL:HG23	2.16	0.46
1:A:341:THR:HG22	1:A:343:ASN:H	1.81	0.46
1:A:616:PHE:N	1:A:617:PRO:HD2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:OD2	1:A:277:GLU:N	2.49	0.46
1:A:472:ARG:NH1	1:A:472:ARG:CG	2.75	0.46
1:A:301:GLN:O	1:A:305:GLN:HG3	2.16	0.45
1:A:270:GLN:HA	1:A:310:ALA:HA	1.98	0.45
1:A:567:GLN:O	1:A:571:LEU:HB2	2.16	0.45
1:A:244:GLY:O	1:A:245:LEU:CB	2.63	0.45
1:A:424:ARG:NH2	1:A:468:GLU:OE1	2.48	0.45
1:A:337:LEU:HD22	1:A:341:THR:OG1	2.16	0.45
1:A:576:LEU:N	1:A:577:PRO:CD	2.79	0.45
1:A:567:GLN:HA	1:A:607:LEU:HD21	1.99	0.45
1:A:666:ASN:O	1:A:670:LEU:HD23	2.16	0.45
1:A:479:ASN:O	1:A:480:ALA:HB2	2.16	0.45
1:A:606:LEU:HD22	1:A:606:LEU:N	2.32	0.45
1:A:659:PHE:HB3	1:A:664:LEU:HD21	1.98	0.45
1:A:401:GLU:O	1:A:404:PHE:HB3	2.16	0.45
1:A:457:VAL:O	1:A:461:LEU:HG	2.17	0.45
1:A:513:GLU:OE1	1:A:516:PRO:HA	2.16	0.45
1:A:300:ASN:O	1:A:304:GLN:HG3	2.17	0.45
1:A:351:THR:HG23	1:A:405:ASN:HD22	1.82	0.44
1:A:379:VAL:HG11	1:A:402:VAL:HG12	1.99	0.44
1:A:599:SER:OG	1:A:600:ASN:ND2	2.49	0.44
1:A:626:HIS:O	1:A:637:LEU:HD11	2.16	0.44
1:A:641:CYS:CA	1:A:686:LEU:HD12	2.47	0.44
1:A:659:PHE:HB3	1:A:664:LEU:CD2	2.48	0.44
1:A:690:MET:SD	1:A:696:LEU:HD12	2.57	0.44
1:A:284:TYR:C	1:A:286:LEU:H	2.20	0.44
1:A:669:ASN:O	1:A:670:LEU:C	2.55	0.44
1:A:260:LYS:O	1:A:264:ILE:HG13	2.18	0.44
1:A:245:LEU:HD12	1:A:268:TYR:HE2	1.83	0.44
1:A:303:VAL:HG12	1:A:303:VAL:O	2.18	0.44
1:A:271:HIS:O	1:A:273:CYS:N	2.51	0.44
1:A:295:LEU:H	1:A:295:LEU:CD1	2.30	0.44
1:A:602:SER:O	1:A:608:HIS:HE1	2.01	0.44
1:A:350:LEU:O	1:A:354:LEU:HG	2.18	0.44
1:A:351:THR:CG2	1:A:405:ASN:HD22	2.31	0.44
1:A:465:LEU:CD1	1:A:469:VAL:HG21	2.48	0.44
1:A:594:GLY:O	1:A:597:LEU:HB3	2.18	0.44
1:A:518:GLY:O	1:A:520:GLY:N	2.51	0.43
1:A:661:SER:CA	1:A:664:LEU:HG	2.48	0.43
1:A:669:ASN:N	1:A:669:ASN:OD1	2.49	0.43
1:A:291:LYS:HE3	1:A:291:LYS:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ILE:HD13	1:A:597:LEU:CD2	2.48	0.43
1:A:637:LEU:C	1:A:639:SER:N	2.72	0.43
1:A:294:ASP:N	1:A:294:ASP:OD2	2.51	0.43
1:A:377:ASP:O	1:A:382:PRO:CD	2.67	0.43
1:A:386:TRP:CD2	1:A:386:TRP:O	2.71	0.43
1:A:455:MET:HA	1:A:455:MET:HE1	1.97	0.43
1:A:688:SER:C	1:A:690:MET:N	2.70	0.43
1:A:517:LYS:O	1:A:518:GLY:C	2.57	0.43
1:A:592:ARG:C	1:A:592:ARG:HH11	2.22	0.43
1:A:617:PRO:HG2	1:A:618:GLU:H	1.84	0.43
1:A:341:THR:H	1:A:378:ARG:HH12	1.66	0.43
1:A:522:LEU:O	1:A:554:LEU:HD21	2.19	0.43
1:A:667:ILE:C	1:A:667:ILE:HD13	2.39	0.42
1:A:408:GLY:O	1:A:411:ARG:HB3	2.19	0.42
1:A:592:ARG:NH1	1:A:592:ARG:HB3	2.35	0.42
1:A:251:VAL:O	1:A:254:LEU:HB2	2.20	0.42
1:A:648:MET:CE	1:A:690:MET:HG2	2.49	0.42
1:A:672:ARG:O	1:A:673:SER:C	2.57	0.42
1:A:250:ALA:O	1:A:253:TYR:HB2	2.19	0.42
1:A:663:MET:O	1:A:667:ILE:HG22	2.20	0.42
1:A:360:THR:O	1:A:362:GLU:N	2.52	0.42
1:A:363:LEU:HD12	1:A:363:LEU:C	2.40	0.42
1:A:523:TYR:O	1:A:565:MET:HE1	2.20	0.42
1:A:668:ILE:HD12	1:A:668:ILE:H	1.84	0.42
1:A:266:ALA:HB2	1:A:292:LEU:CD2	2.50	0.42
1:A:565:MET:O	1:A:569:ILE:HG13	2.19	0.42
1:A:310:ALA:O	1:A:314:LEU:HB2	2.20	0.42
1:A:245:LEU:N	1:A:249:LYS:HZ3	2.16	0.41
1:A:465:LEU:HD12	1:A:469:VAL:CG2	2.50	0.41
1:A:295:LEU:H	1:A:295:LEU:HD12	1.85	0.41
1:A:651:GLN:O	1:A:652:PRO:C	2.59	0.41
1:A:671:CYS:SG	1:A:684:ARG:CB	3.07	0.41
1:A:319:THR:O	1:A:323:LEU:HG	2.20	0.41
1:A:289:ILE:HG21	1:A:324:GLU:HG3	2.02	0.41
1:A:573:GLU:O	1:A:574:LYS:C	2.57	0.41
1:A:397:VAL:O	1:A:398:VAL:CB	2.68	0.41
1:A:455:MET:HG3	1:A:534:LEU:HD13	2.02	0.41
1:A:648:MET:HE3	1:A:690:MET:HG2	2.02	0.41
1:A:358:SER:HB2	1:A:412:ASN:HB2	2.02	0.41
1:A:695:GLU:C	1:A:696:LEU:HD22	2.40	0.41
1:A:420:ARG:NH1	1:A:468:GLU:OE2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:THR:CG2	1:A:631:SER:N	2.84	0.41
1:A:680:ALA:O	1:A:683:ALA:HB3	2.21	0.41
1:A:584:GLN:O	1:A:585:SER:C	2.58	0.41
1:A:615:VAL:C	1:A:617:PRO:HD2	2.41	0.41
1:A:371:ALA:O	1:A:374:VAL:HG22	2.20	0.41
1:A:315:VAL:HG13	1:A:322:LYS:HG3	2.03	0.41
1:A:309:GLY:O	1:A:310:ALA:C	2.59	0.41
1:A:358:SER:HB2	1:A:412:ASN:CB	2.51	0.41
1:A:406:ALA:O	1:A:409:CYS:HB3	2.21	0.41
1:A:566:SER:HB3	1:A:607:LEU:HD11	2.03	0.41
1:A:259:GLU:HA	1:A:262:GLN:HB2	2.03	0.40
1:A:289:ILE:H	1:A:289:ILE:CD1	2.08	0.40
1:A:380:ILE:CD1	1:A:410:LEU:HD12	2.51	0.40
1:A:270:GLN:HG3	1:A:310:ALA:N	2.36	0.40
1:A:372:LEU:CB	1:A:373:PRO:HD3	2.49	0.40
1:A:471:THR:HG23	1:A:523:TYR:CE1	2.57	0.40
1:A:696:LEU:HA	1:A:696:LEU:HD13	1.84	0.40
1:A:518:GLY:C	1:A:520:GLY:N	2.74	0.40
1:A:661:SER:HA	1:A:664:LEU:HD12	2.04	0.40
1:A:624:THR:HG22	1:A:663:MET:CG	2.51	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	414/457 (91%)	317 (77%)	75 (18%)	22 (5%)	2 7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	246	THR
1	A	295	LEU
1	A	361	ASP
1	A	512	GLU
1	A	557	SER
1	A	558	LYS
1	A	666	ASN
1	A	673	SER
1	A	697	GLN
1	A	699	VAL
1	A	257	GLN
1	A	320	THR
1	A	513	GLU
1	A	518	GLY
1	A	522	LEU
1	A	698	GLY
1	A	272	THR
1	A	585	SER
1	A	363	LEU
1	A	398	VAL
1	A	511	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	358/392 (91%)	316 (88%)	42 (12%)	6 19

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LEU
1	A	246	THR
1	A	253	TYR
1	A	256	SER
1	A	274	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	281	GLN
1	A	289	ILE
1	A	291	LYS
1	A	294	ASP
1	A	314	LEU
1	A	320	THR
1	A	328	GLN
1	A	337	LEU
1	A	340	ARG
1	A	353	LEU
1	A	358	SER
1	A	362	GLU
1	A	363	LEU
1	A	439	ASN
1	A	444	SER
1	A	459	HIS
1	A	469	VAL
1	A	472	ARG
1	A	476	LEU
1	A	511	GLU
1	A	513	GLU
1	A	526	ASP
1	A	533	ASN
1	A	558	LYS
1	A	561	MET
1	A	565	MET
1	A	592	ARG
1	A	600	ASN
1	A	616	PHE
1	A	639	SER
1	A	647	LEU
1	A	667	ILE
1	A	669	ASN
1	A	685	LEU
1	A	687	LEU
1	A	690	MET
1	A	694	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	262	GLN
1	A	271	HIS
1	A	281	GLN
1	A	313	ASN
1	A	328	GLN
1	A	405	ASN
1	A	412	ASN
1	A	421	GLN
1	A	425	ASN
1	A	533	ASN
1	A	553	ASN
1	A	600	ASN
1	A	604	HIS
1	A	608	HIS
1	A	614	GLN

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 [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, 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	420/457 (91%)	0.06	8 (1%) 67 58	35, 69, 98, 109	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	ARG	3.2
1	A	269	ILE	2.9
1	A	397	VAL	2.7
1	A	558	LYS	2.6
1	A	286	LEU	2.5
1	A	387	CYS	2.2
1	A	386	TRP	2.2
1	A	626	HIS	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 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.