



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:58 am BST

PDB ID : 3GDI  
Title : Mammalian Clock Protein mPER2 - Crystal Structure of a PAS Domain Fragment  
Authors : Hennig, S.; Wolf, E.  
Deposited on : 2009-02-24  
Resolution : 2.40 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
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

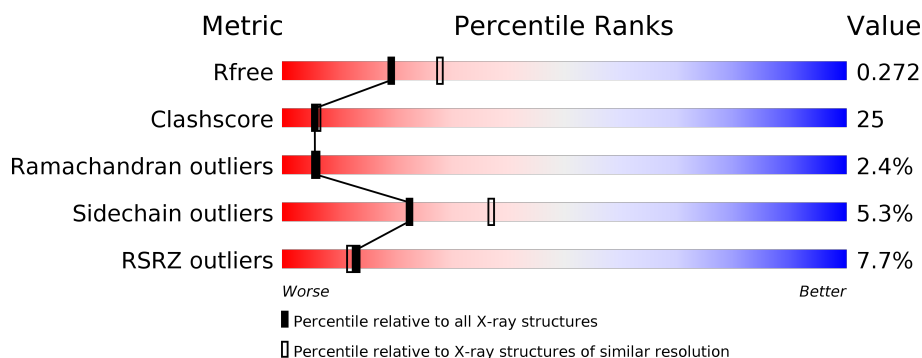
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	309	<div> <div>8%</div> <div> <div></div> <div>49%</div> <div>34%</div> <div>5%</div> <div>13%</div> </div> </div>
1	B	309	<div> <div>5%</div> <div> <div></div> <div>45%</div> <div>32%</div> <div>•</div> <div>19%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4300 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 Period circadian protein homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2148	1389	364	385	10			
1	B	250	Total	C	N	O	S	0	0	0
			1954	1264	335	346	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	GLY	-	EXPRESSION TAG	UNP O54943
A	166	PRO	-	EXPRESSION TAG	UNP O54943
A	167	LEU	-	EXPRESSION TAG	UNP O54943
A	168	GLY	-	EXPRESSION TAG	UNP O54943
A	169	SER	-	EXPRESSION TAG	UNP O54943
B	165	GLY	-	EXPRESSION TAG	UNP O54943
B	166	PRO	-	EXPRESSION TAG	UNP O54943
B	167	LEU	-	EXPRESSION TAG	UNP O54943
B	168	GLY	-	EXPRESSION TAG	UNP O54943
B	169	SER	-	EXPRESSION TAG	UNP O54943

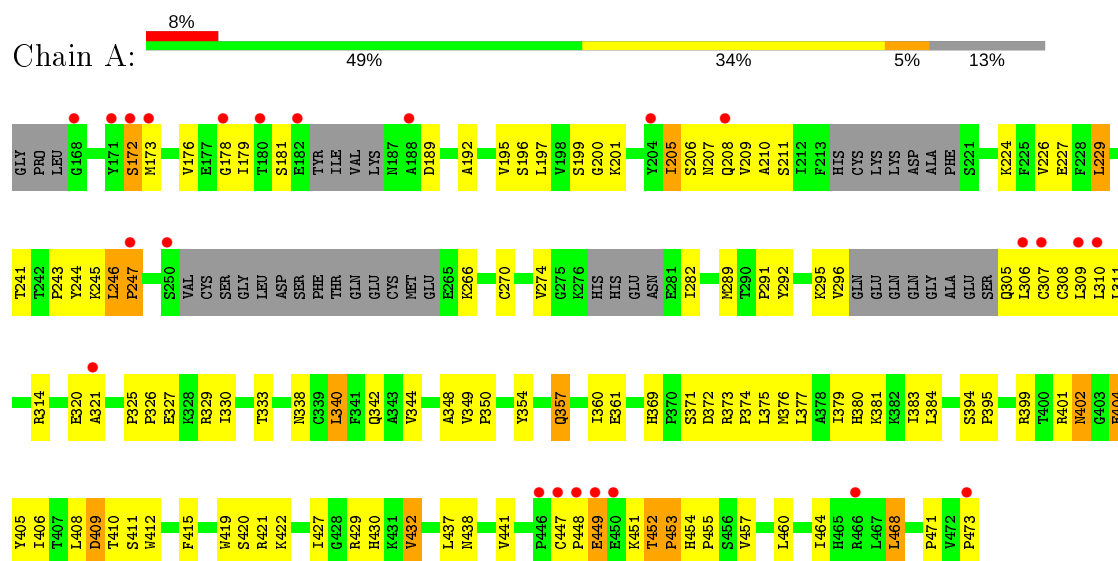
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	109	Total	O	0	0
			109	109		

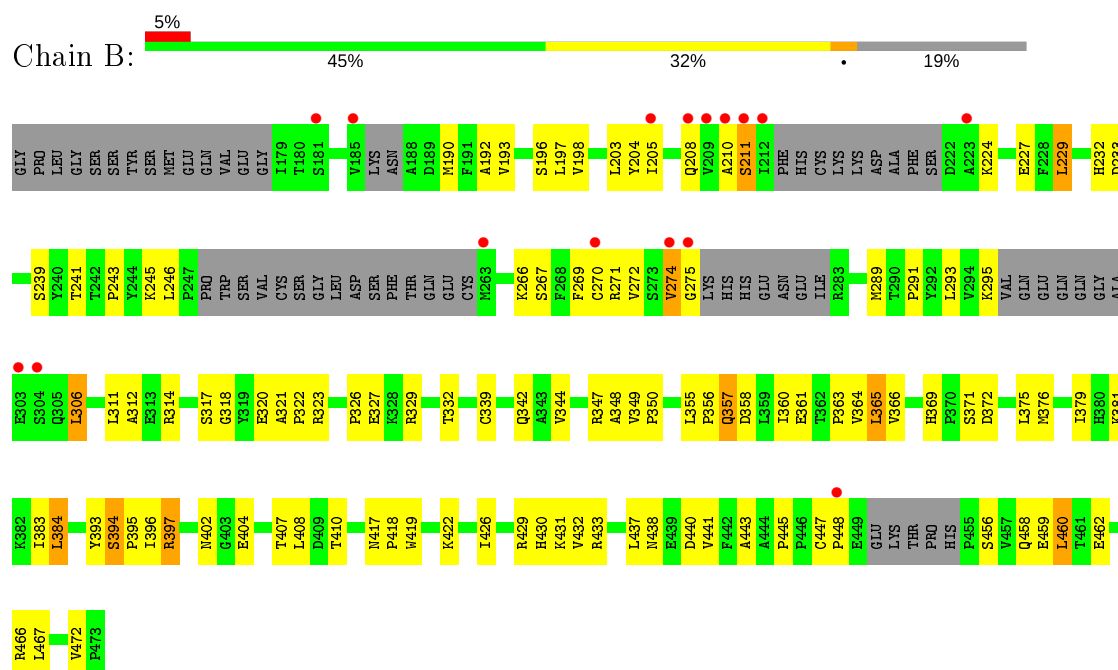
### 3 Residue-property plots

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: Period circadian protein homolog 2



#### • Molecule 1: Period circadian protein homolog 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.67Å 63.38Å 72.51Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	19.92 – 2.40 19.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	57.2 (19.92-2.40) 98.6 (19.92-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.224 , 0.272 0.224 , 0.272	Depositor DCC
$R_{free}$ test set	1199 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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	0.37	0/2208	0.62	1/3002 (0.0%)
1	B	0.36	0/2004	0.65	1/2725 (0.0%)
All	All	0.36	0/4212	0.64	2/5727 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	445	PRO	N-CA-CB	5.47	109.86	103.30
1	A	409	ASP	N-CA-C	-5.06	97.33	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	2148	0	2135	106	0
1	B	1954	0	1923	103	0
2	A	89	0	0	4	0
2	B	109	0	0	11	0
All	All	4300	0	4058	206	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 25.

All (206) 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:B:394:SER:HB2	1:B:395:PRO:HD2	1.42	1.00
1:A:197:LEU:HD21	1:A:243:PRO:HG3	1.46	0.96
1:B:321:ALA:HB3	1:B:322:PRO:HD3	1.49	0.93
1:A:369:HIS:HD2	1:A:371:SER:H	1.10	0.90
1:A:241:THR:HA	1:A:246:LEU:HD21	1.59	0.83
1:B:197:LEU:HD12	1:B:306:LEU:HD12	1.61	0.82
1:B:323:ARG:HD3	2:B:62:HOH:O	1.79	0.82
1:B:320:GLU:HG2	1:B:321:ALA:H	1.43	0.81
1:A:226:VAL:HA	1:A:229:LEU:HD22	1.63	0.81
1:A:326:PRO:HA	1:A:329:ARG:HG3	1.65	0.78
1:B:396:ILE:HD11	1:B:408:LEU:HB2	1.65	0.78
1:A:402:ASN:HD21	1:A:404:GLU:HB2	1.50	0.76
1:A:452:THR:H	1:A:453:PRO:HD2	1.50	0.76
1:A:402:ASN:HD22	1:A:402:ASN:C	1.88	0.76
1:A:402:ASN:ND2	1:A:404:GLU:H	1.83	0.76
1:A:402:ASN:HD22	1:A:404:GLU:H	1.34	0.75
1:B:271:ARG:NH2	1:B:355:LEU:HD23	2.01	0.74
1:A:357:GLN:HE21	1:A:357:GLN:H	1.33	0.74
1:B:375:LEU:HD12	1:B:375:LEU:H	1.53	0.73
1:A:172:SER:HB3	1:A:296:VAL:HA	1.70	0.73
1:A:360:ILE:HG22	1:A:361:GLU:HG2	1.68	0.73
1:B:241:THR:HA	1:B:246:LEU:HD21	1.69	0.73
1:A:452:THR:H	1:A:453:PRO:CD	2.02	0.73
1:B:396:ILE:HD12	1:B:396:ILE:O	1.88	0.73
1:A:306:LEU:HD23	1:A:306:LEU:H	1.52	0.72
1:A:192:ALA:H	1:A:206:SER:HB3	1.55	0.72
1:A:349:VAL:HB	1:A:350:PRO:HD3	1.70	0.72
1:B:372:ASP:HA	1:B:375:LEU:HD13	1.70	0.72
1:B:349:VAL:HB	1:B:350:PRO:HD3	1.72	0.72
1:B:381:LYS:HG3	1:B:467:LEU:HD11	1.72	0.72
1:B:396:ILE:CD1	1:B:408:LEU:HB2	2.20	0.71
1:A:402:ASN:HD21	1:A:404:GLU:CB	2.02	0.71
1:B:295:LYS:HA	1:B:306:LEU:HD22	1.72	0.71
1:A:179:ILE:HD11	1:A:181:SER:HB2	1.72	0.71
1:B:394:SER:HB2	1:B:395:PRO:CD	2.18	0.71
1:A:309:LEU:HD23	1:A:310:LEU:N	2.06	0.70
1:B:274:VAL:HG12	1:B:275:GLY:H	1.56	0.70
1:A:402:ASN:ND2	1:A:404:GLU:HB2	2.07	0.69
1:B:404:GLU:OE2	1:B:438:ASN:HB3	1.92	0.69
1:B:190:MET:HB2	1:B:312:ALA:O	1.93	0.68
1:B:293:LEU:HD11	1:B:306:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:HIS:HB3	1:A:457:VAL:HB	1.75	0.68
1:A:357:GLN:H	1:A:357:GLN:NE2	1.92	0.67
1:A:199:SER:HB3	1:A:201:LYS:HG2	1.75	0.67
1:A:247:PRO:HB3	1:A:266:LYS:NZ	2.08	0.67
1:B:375:LEU:HD23	1:B:393:TYR:OH	1.95	0.66
1:B:369:HIS:HD2	1:B:371:SER:H	1.44	0.66
1:B:269:PHE:CB	1:B:355:LEU:HD12	2.26	0.66
1:B:472:VAL:HG23	2:B:144:HOH:O	1.95	0.65
1:B:375:LEU:HD12	1:B:375:LEU:N	2.11	0.65
1:B:267:SER:HB3	1:B:289:MET:O	1.97	0.64
1:A:208:GLN:O	1:A:211:SER:HB3	1.98	0.64
1:B:357:GLN:H	1:B:357:GLN:HE21	1.43	0.64
1:A:369:HIS:CD2	1:A:371:SER:H	2.03	0.64
1:B:317:SER:HB3	1:B:320:GLU:HB2	1.78	0.64
1:A:451:LYS:HB3	1:A:453:PRO:HD2	1.78	0.63
1:B:271:ARG:CZ	1:B:355:LEU:HD23	2.28	0.63
1:B:375:LEU:CD1	1:B:375:LEU:H	2.12	0.62
1:B:456:SER:HA	1:B:459:GLU:HG2	1.81	0.61
1:A:270:CYS:HB2	1:A:289:MET:CE	2.31	0.60
1:A:406:ILE:HG13	1:A:408:LEU:HD11	1.84	0.60
1:B:320:GLU:HG2	1:B:321:ALA:N	2.13	0.60
1:B:339:CYS:O	1:B:364:VAL:HG12	2.01	0.60
1:A:420:SER:O	1:A:421:ARG:HB2	2.02	0.59
1:B:229:LEU:HD12	1:B:272:VAL:HG22	1.85	0.59
1:B:269:PHE:HB2	1:B:355:LEU:HD12	1.86	0.58
1:A:205:ILE:HD12	1:A:209:VAL:HG11	1.85	0.58
1:A:270:CYS:HB2	1:A:289:MET:HE1	1.84	0.58
1:B:327:GLU:OE2	1:B:327:GLU:HA	2.04	0.58
1:A:394:SER:HB3	1:A:409:ASP:HA	1.85	0.58
1:B:233:ASP:HB3	1:B:270:CYS:HB2	1.85	0.58
1:A:192:ALA:H	1:A:206:SER:CB	2.16	0.57
1:A:247:PRO:HB3	1:A:266:LYS:HZ1	1.68	0.57
1:B:363:PRO:HB2	1:B:366:VAL:HG23	1.86	0.57
1:A:373:ARG:HB2	1:A:374:PRO:HD3	1.86	0.57
1:B:344:VAL:HG13	1:B:348:ALA:CB	2.35	0.57
1:B:447:CYS:SG	1:B:448:PRO:HD2	2.45	0.57
2:A:487:HOH:O	1:B:266:LYS:HG3	2.04	0.57
1:B:410:THR:HG22	1:B:430:HIS:ND1	2.20	0.56
1:B:196:SER:OG	1:B:198:VAL:HG22	2.06	0.56
1:A:452:THR:N	1:A:453:PRO:CD	2.69	0.56
1:A:282:ILE:HD12	1:A:282:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ARG:NH2	1:B:358:ASP:OD2	2.39	0.55
1:B:233:ASP:OD1	1:B:271:ARG:HD2	2.07	0.54
1:A:381:LYS:O	1:A:384:LEU:HD23	2.07	0.54
1:B:458:GLN:O	1:B:462:GLU:HG2	2.08	0.54
1:A:327:GLU:H	1:A:327:GLU:CD	2.11	0.53
1:B:329:ARG:HD3	2:B:61:HOH:O	2.08	0.53
1:A:333:THR:OG1	1:A:430:HIS:HE1	1.92	0.53
1:A:357:GLN:N	1:A:357:GLN:HE21	2.02	0.53
1:A:224:LYS:HB2	1:A:227:GLU:HG3	1.89	0.53
1:A:410:THR:OG1	1:A:430:HIS:HD2	1.92	0.53
1:A:200:GLY:O	1:A:224:LYS:HA	2.09	0.52
1:B:402:ASN:ND2	1:B:441:VAL:HA	2.23	0.52
1:A:406:ILE:HG13	1:A:408:LEU:CD1	2.40	0.52
1:A:199:SER:HB3	1:A:201:LYS:CG	2.39	0.52
1:B:274:VAL:HG12	1:B:275:GLY:N	2.24	0.51
1:B:372:ASP:CA	1:B:375:LEU:HD13	2.39	0.51
1:B:318:GLY:HA2	2:B:60:HOH:O	2.10	0.51
1:A:415:PHE:CZ	1:A:427:ILE:HD13	2.46	0.51
1:B:360:ILE:O	1:B:361:GLU:HB2	2.10	0.51
1:A:410:THR:HG21	1:A:412:TRP:CE2	2.46	0.50
1:A:447:CYS:O	1:A:449:GLU:N	2.44	0.50
1:B:440:ASP:OD2	1:B:443:ALA:HB2	2.12	0.50
1:A:419:TRP:CG	1:B:429:ARG:HD2	2.47	0.50
1:A:429:ARG:HD2	1:B:419:TRP:CG	2.46	0.50
1:A:471:PRO:O	1:A:473:PRO:HD3	2.11	0.50
1:B:394:SER:C	2:B:67:HOH:O	2.50	0.50
1:A:372:ASP:HA	1:A:375:LEU:HD13	1.94	0.50
1:A:274:VAL:HG11	2:A:483:HOH:O	2.12	0.50
1:B:321:ALA:CB	1:B:322:PRO:HD3	2.31	0.50
1:B:357:GLN:NE2	1:B:357:GLN:H	2.08	0.49
1:A:305:GLN:O	1:A:305:GLN:HG3	2.12	0.49
1:B:372:ASP:OD2	1:B:397:ARG:HB2	2.13	0.49
1:A:207:ASN:O	1:A:208:GLN:HB3	2.11	0.49
1:A:243:PRO:C	1:A:245:LYS:H	2.16	0.49
1:A:172:SER:CB	1:A:296:VAL:HG13	2.42	0.49
1:A:189:ASP:HB3	1:A:314:ARG:HB3	1.93	0.49
1:B:192:ALA:O	1:B:193:VAL:HG13	2.11	0.49
1:B:365:LEU:HB2	2:B:138:HOH:O	2.12	0.49
1:B:246:LEU:HD22	1:B:291:PRO:HB2	1.95	0.49
1:B:393:TYR:O	1:B:394:SER:O	2.31	0.49
1:B:431:LYS:HD3	1:B:432:VAL:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LEU:HD11	1:B:376:MET:HG2	1.94	0.49
1:A:307:CYS:SG	1:A:308:CYS:N	2.86	0.48
1:A:432:VAL:O	1:A:432:VAL:HG22	2.12	0.48
1:B:210:ALA:O	1:B:211:SER:HB2	2.13	0.48
1:A:381:LYS:NZ	2:A:129:HOH:O	2.46	0.48
1:B:320:GLU:O	1:B:323:ARG:N	2.46	0.48
1:A:464:ILE:O	1:A:468:LEU:HD22	2.14	0.48
1:B:192:ALA:HB3	1:B:205:ILE:CD1	2.44	0.48
1:A:354:TYR:CD2	1:A:401:ARG:HD3	2.49	0.48
1:B:372:ASP:O	1:B:375:LEU:HD13	2.14	0.47
1:A:454:HIS:N	1:A:455:PRO:HD3	2.29	0.47
1:A:189:ASP:HB3	1:A:314:ARG:CB	2.44	0.47
1:A:195:VAL:O	1:A:307:CYS:HB2	2.15	0.47
1:A:404:GLU:OE2	1:A:437:LEU:HB3	2.14	0.47
1:B:344:VAL:CG1	1:B:348:ALA:HB3	2.45	0.47
1:A:338:ASN:ND2	1:A:340:LEU:HD22	2.30	0.46
1:A:377:LEU:O	1:A:381:LYS:HG3	2.15	0.46
1:B:269:PHE:HB3	1:B:355:LEU:HD12	1.98	0.46
1:B:456:SER:HA	1:B:459:GLU:CG	2.46	0.46
1:A:464:ILE:HG22	1:A:468:LEU:CD2	2.46	0.45
1:A:379:ILE:O	1:A:383:ILE:HG13	2.17	0.45
1:A:173:MET:O	1:A:176:VAL:HG22	2.16	0.45
1:A:197:LEU:HB2	1:A:307:CYS:HA	1.99	0.45
1:B:356:PRO:O	1:B:360:ILE:HG13	2.16	0.45
1:A:410:THR:HG22	1:A:411:SER:N	2.31	0.45
1:B:271:ARG:HH22	1:B:358:ASP:CG	2.19	0.45
1:B:321:ALA:HB3	1:B:322:PRO:CD	2.35	0.45
1:B:432:VAL:CG1	2:B:25:HOH:O	2.65	0.45
1:A:360:ILE:O	1:A:361:GLU:HB2	2.16	0.45
1:A:401:ARG:HB3	1:A:441:VAL:O	2.16	0.45
1:A:402:ASN:C	1:A:402:ASN:ND2	2.60	0.45
1:A:452:THR:HG23	1:B:243:PRO:HB2	1.99	0.44
1:B:355:LEU:HD22	1:B:355:LEU:N	2.32	0.44
1:A:209:VAL:HG23	1:A:210:ALA:H	1.82	0.44
1:A:295:LYS:HA	1:A:306:LEU:HA	1.99	0.44
1:A:172:SER:HB3	1:A:296:VAL:CA	2.44	0.44
1:B:293:LEU:HD11	1:B:306:LEU:CD1	2.46	0.44
1:B:344:VAL:HG13	1:B:348:ALA:HB3	1.99	0.44
1:B:232:HIS:N	1:B:232:HIS:CD2	2.86	0.44
1:A:404:GLU:OE2	1:A:438:ASN:N	2.51	0.43
1:B:432:VAL:HG13	2:B:25:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HB3	1:A:266:LYS:HZ2	1.81	0.43
1:A:172:SER:HB2	1:A:296:VAL:HG13	2.00	0.43
1:A:292:TYR:HE2	1:A:311:LEU:HD12	1.84	0.43
1:A:376:MET:CE	1:A:380:HIS:HE1	2.31	0.43
1:A:399:ARG:HB2	1:A:405:TYR:CE1	2.53	0.43
1:B:384:LEU:HD12	1:B:467:LEU:CD2	2.48	0.43
1:B:379:ILE:O	1:B:383:ILE:HG13	2.18	0.43
1:A:196:SER:HB3	1:A:199:SER:HB2	2.01	0.43
1:B:422:LYS:HD3	2:B:77:HOH:O	2.18	0.43
1:A:270:CYS:HB2	1:A:289:MET:HE2	2.00	0.43
1:A:241:THR:CA	1:A:246:LEU:HD21	2.41	0.43
1:A:330:ILE:HD13	1:A:429:ARG:NH1	2.34	0.43
1:B:372:ASP:C	1:B:375:LEU:HD13	2.38	0.43
1:A:246:LEU:HD23	1:A:291:PRO:HB2	2.01	0.42
1:A:330:ILE:HD13	1:A:429:ARG:HH12	1.84	0.42
1:A:422:LYS:HZ3	1:A:471:PRO:HG3	1.85	0.42
1:B:456:SER:CA	1:B:459:GLU:HG2	2.47	0.42
1:B:407:THR:O	2:B:25:HOH:O	2.22	0.42
1:B:326:PRO:O	1:B:431:LYS:HE2	2.20	0.42
1:B:369:HIS:HB2	1:B:397:ARG:HB3	2.01	0.42
1:A:274:VAL:O	1:A:274:VAL:HG12	2.20	0.42
1:A:344:VAL:HG12	1:A:348:ALA:HB3	2.00	0.42
1:B:332:THR:HG23	1:B:347:ARG:NH2	2.35	0.41
1:B:365:LEU:CD1	1:B:376:MET:HG2	2.49	0.41
1:A:402:ASN:ND2	1:A:404:GLU:N	2.62	0.41
1:B:192:ALA:HB3	1:B:205:ILE:HD11	2.01	0.41
1:B:395:PRO:N	2:B:67:HOH:O	2.53	0.41
1:A:172:SER:HB3	1:A:296:VAL:HG13	2.02	0.41
1:B:224:LYS:HB2	1:B:227:GLU:HG3	2.02	0.41
1:A:243:PRO:O	1:A:245:LYS:N	2.54	0.41
1:B:289:MET:HA	1:B:311:LEU:O	2.21	0.41
1:B:456:SER:O	1:B:460:LEU:HB2	2.21	0.41
1:A:320:GLU:O	1:A:321:ALA:C	2.60	0.40
1:B:203:LEU:HD22	1:B:204:TYR:H	1.86	0.40
1:A:384:LEU:HD21	2:A:490:HOH:O	2.21	0.40
1:A:410:THR:CG2	1:A:411:SER:N	2.84	0.40
1:A:325:PRO:HA	1:A:326:PRO:HD3	1.98	0.40
1:B:417:ASN:HA	1:B:418:PRO:HD3	1.93	0.40
1:B:239:SER:O	1:B:245:LYS:HD2	2.21	0.40
1:B:246:LEU:CB	1:B:293:LEU:HB2	2.52	0.40
1:B:318:GLY:O	1:B:323:ARG:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ILE:HD12	1:B:426:ILE:N	2.37	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	257/309 (83%)	224 (87%)	25 (10%)	8 (3%)	4	3
1	B	236/309 (76%)	203 (86%)	29 (12%)	4 (2%)	9	11
All	All	493/618 (80%)	427 (87%)	54 (11%)	12 (2%)	6	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	449	GLU
1	A	452	THR
1	B	211	SER
1	B	394	SER
1	A	172	SER
1	A	448	PRO
1	A	453	PRO
1	A	178	GLY
1	A	244	TYR
1	B	208	GLN
1	A	247	PRO
1	B	274	VAL

### 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	242/279 (87%)	230 (95%)	12 (5%)	24	40
1	B	213/279 (76%)	201 (94%)	12 (6%)	21	34
All	All	455/558 (82%)	431 (95%)	24 (5%)	22	37

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ILE
1	A	229	LEU
1	A	246	LEU
1	A	340	LEU
1	A	342	GLN
1	A	357	GLN
1	A	395	PRO
1	A	402	ASN
1	A	404	GLU
1	A	432	VAL
1	A	460	LEU
1	A	468	LEU
1	B	229	LEU
1	B	306	LEU
1	B	314	ARG
1	B	342	GLN
1	B	357	GLN
1	B	365	LEU
1	B	384	LEU
1	B	397	ARG
1	B	433	ARG
1	B	437	LEU
1	B	460	LEU
1	B	466	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	342	GLN
1	A	357	GLN
1	A	369	HIS
1	A	385	GLN
1	A	402	ASN
1	A	430	HIS
1	A	438	ASN
1	A	458	GLN
1	A	463	GLN
1	B	232	HIS
1	B	305	GLN
1	B	316	HIS
1	B	342	GLN
1	B	357	GLN
1	B	367	GLN
1	B	369	HIS
1	B	385	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 ⓘ

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	269/309 (87%)	0.27	24 (8%) 9 9	33, 61, 125, 137	0
1	B	250/309 (80%)	0.35	16 (6%) 19 18	35, 62, 115, 129	0
All	All	519/618 (83%)	0.31	40 (7%) 13 12	33, 61, 117, 137	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	5.9
1	B	263	MET	5.6
1	B	208	GLN	5.4
1	B	210	ALA	4.4
1	B	181	SER	4.1
1	A	178	GLY	3.7
1	B	223	ALA	3.5
1	B	211	SER	3.4
1	B	448	PRO	3.4
1	A	171	TYR	3.4
1	B	304	SER	3.3
1	A	247	PRO	3.3
1	B	212	ILE	3.2
1	A	208	GLN	3.2
1	A	250	SER	3.2
1	A	450	GLU	3.2
1	A	306	LEU	3.0
1	A	168	GLY	3.0
1	B	275	GLY	2.9
1	A	188	ALA	2.9
1	A	172	SER	2.8
1	A	180	THR	2.8
1	A	449	GLU	2.7
1	A	173	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	447	CYS	2.6
1	A	321	ALA	2.6
1	A	446	PRO	2.6
1	A	204	TYR	2.6
1	A	309	LEU	2.5
1	B	205	ILE	2.5
1	A	466	ARG	2.4
1	B	270	CYS	2.3
1	A	473	PRO	2.3
1	A	182	GLU	2.2
1	B	303	GLU	2.2
1	A	307	CYS	2.2
1	A	448	PRO	2.2
1	B	274	VAL	2.1
1	B	185	VAL	2.1
1	A	310	LEU	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.