Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 11:20 PM EST

PDB ID	:	4DJ3
Title	:	Unwinding the Differences of the Mammalian PERIOD Clock Proteins from Crystal Structure to Cellular Function
Authors	:	Wolf, E.; Kucera, N.; Hennig, S.
Deposited on	:	2012-02-01
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

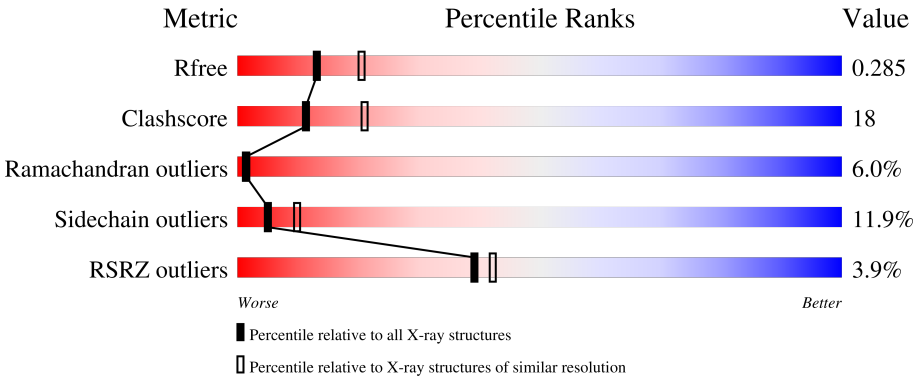
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	317	3% 61% 25% 8% • 6%
1	B	317	4% 46% 30% 7% • 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4468 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2274	1470	390	407	7			
1	B	265	Total	C	N	O	S	0	0	0
			2033	1314	353	360	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	-	expression tag	UNP O70361
A	96	PRO	-	expression tag	UNP O70361
A	97	LEU	-	expression tag	UNP O70361
A	98	GLY	-	expression tag	UNP O70361
A	99	SER	-	expression tag	UNP O70361
A	100	PRO	-	expression tag	UNP O70361
A	101	GLU	-	expression tag	UNP O70361
A	102	PHE	-	expression tag	UNP O70361
A	103	PRO	-	expression tag	UNP O70361
A	104	GLY	-	expression tag	UNP O70361
A	105	ARG	-	expression tag	UNP O70361
A	106	LEU	-	expression tag	UNP O70361
A	107	GLU	-	expression tag	UNP O70361
B	95	GLY	-	expression tag	UNP O70361
B	96	PRO	-	expression tag	UNP O70361
B	97	LEU	-	expression tag	UNP O70361
B	98	GLY	-	expression tag	UNP O70361
B	99	SER	-	expression tag	UNP O70361
B	100	PRO	-	expression tag	UNP O70361
B	101	GLU	-	expression tag	UNP O70361
B	102	PHE	-	expression tag	UNP O70361
B	103	PRO	-	expression tag	UNP O70361
B	104	GLY	-	expression tag	UNP O70361
B	105	ARG	-	expression tag	UNP O70361
B	106	LEU	-	expression tag	UNP O70361

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	107	GLU	-	expression tag	UNP O70361

- Molecule 2 is water.

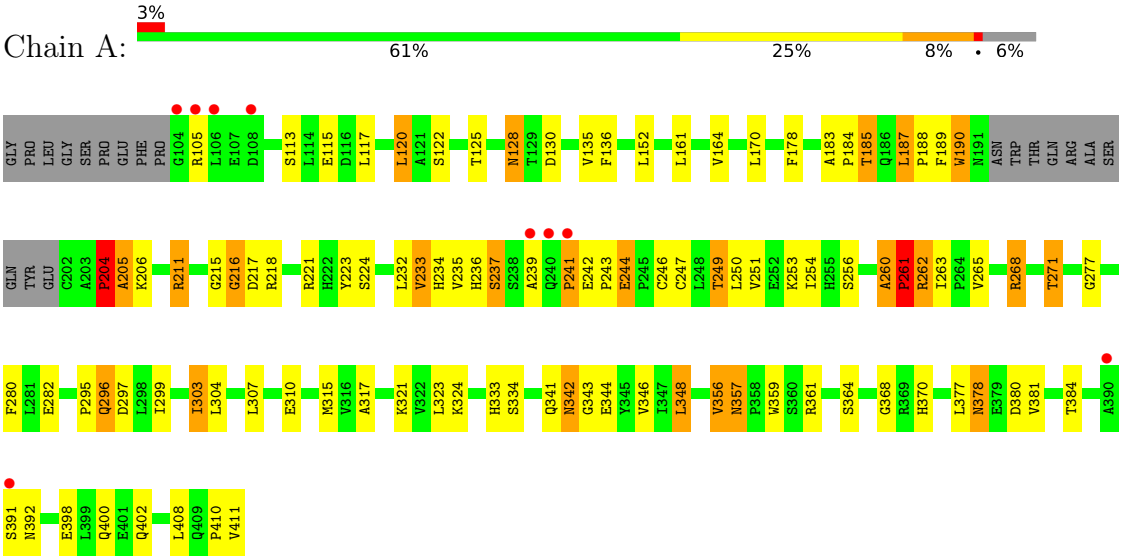
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	115	Total O 115 115	0	0
2	B	46	Total O 46 46	0	0

3 Residue-property plots (i)

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

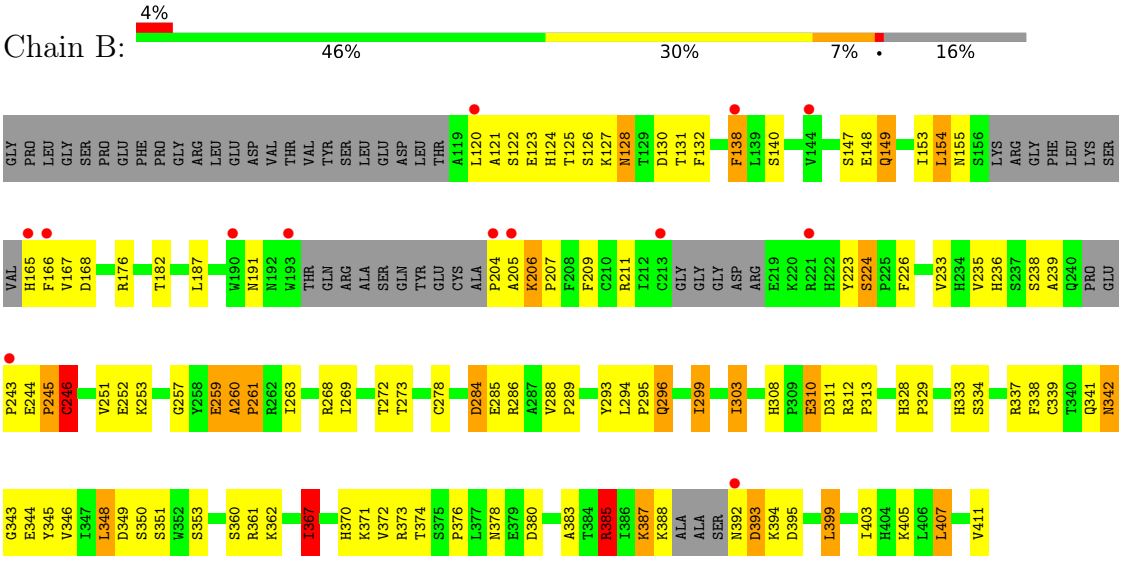
• Molecule 1: Period circadian protein homolog 3

Chain A:



• Molecule 1: Period circadian protein homolog 3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.65Å 78.64Å 67.17Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	48.73 – 2.50 48.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.73-2.50) 99.6 (48.73-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.289 0.211 , 0.285	Depositor DCC
R_{free} test set	1121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4468	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.82	1/2338 (0.0%)	0.88	5/3195 (0.2%)
1	B	0.71	0/2087	0.87	6/2844 (0.2%)
All	All	0.77	1/4425 (0.0%)	0.87	11/6039 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	GLU	CG-CD	5.25	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	261	PRO	N-CA-CB	6.81	111.47	103.30
1	A	152	LEU	CB-CG-CD2	-6.61	99.76	111.00
1	B	243	PRO	N-CA-CB	6.49	111.09	103.30
1	A	410	PRO	N-CA-CB	6.38	110.95	103.30
1	B	245	PRO	N-CA-CB	5.98	110.47	103.30
1	A	241	PRO	N-CA-CB	5.84	110.30	103.30
1	B	204	PRO	N-CA-CB	5.69	110.13	103.30
1	A	211	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	204	PRO	N-CA-CB	5.27	109.63	103.30
1	B	246	CYS	N-CA-C	5.25	125.17	111.00
1	B	367	ILE	CB-CA-C	-5.06	101.48	111.60

There are no chirality outliers.

There are no planarity outliers.

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	A	2274	0	2172	77	0
1	B	2033	0	1932	73	0
2	A	115	0	0	5	0
2	B	46	0	0	7	0
All	All	4468	0	4104	150	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 18.

All (150) 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:128:ASN:HD22	1:A:130:ASP:H	1.01	1.01
1:B:124:HIS:HB3	2:B:543:HOH:O	1.64	0.97
1:B:387:LYS:HE3	1:B:387:LYS:HA	1.43	0.96
1:B:149:GLN:HE21	1:B:149:GLN:H	1.16	0.91
1:A:128:ASN:ND2	1:A:130:ASP:H	1.69	0.90
1:B:333:HIS:CD2	1:B:334:SER:H	1.91	0.88
1:A:296:GLN:H	1:A:296:GLN:HE21	1.27	0.83
1:B:149:GLN:H	1:B:149:GLN:NE2	1.78	0.82
1:B:236:HIS:HB3	2:B:538:HOH:O	1.80	0.79
1:A:260:ALA:CB	1:A:261:PRO:CD	2.63	0.77
1:A:304:LEU:HD12	1:A:400:GLN:HG3	1.66	0.76
1:A:260:ALA:HB1	1:A:261:PRO:CD	2.15	0.76
1:B:360:SER:O	1:B:360:SER:OG	2.04	0.74
1:B:308:HIS:CD2	1:B:310:GLU:HB2	2.22	0.74
1:B:165:HIS:O	1:B:168:ASP:HB2	1.88	0.73
1:B:211:ARG:HA	1:B:224:SER:O	1.89	0.72
1:A:260:ALA:CB	1:A:261:PRO:HD2	2.19	0.71
1:A:261:PRO:O	1:A:262:ARG:HB2	1.90	0.71
1:A:304:LEU:HD12	1:A:400:GLN:CG	2.21	0.70
1:B:273:THR:HG22	1:B:367:ILE:HG23	1.74	0.70
1:A:296:GLN:H	1:A:296:GLN:NE2	1.89	0.69
1:A:122:SER:HA	1:A:125:THR:OG1	1.95	0.66
1:B:125:THR:HA	2:B:536:HOH:O	1.95	0.66
1:A:117:LEU:HD22	1:A:120:LEU:HD12	1.78	0.65
1:B:278:CYS:SG	1:B:303:ILE:HD11	2.37	0.65
1:A:361:ARG:O	1:A:411:VAL:N	2.23	0.64
1:A:189:PHE:O	1:A:190:TRP:CB	2.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:H	1:A:221:ARG:HG3	1.62	0.64
1:A:260:ALA:HB3	1:A:261:PRO:HD2	1.78	0.64
1:B:123:GLU:HB2	2:B:545:HOH:O	1.99	0.62
1:B:353:SER:HB3	1:B:367:ILE:HD12	1.80	0.62
1:A:211:ARG:HB3	1:A:223:TYR:HB3	1.82	0.62
1:A:342:ASN:HD22	1:A:342:ASN:C	2.03	0.61
1:B:149:GLN:HE21	1:B:149:GLN:N	1.95	0.61
1:B:333:HIS:CD2	1:B:334:SER:N	2.66	0.61
1:B:328:HIS:HB3	1:B:329:PRO:HD2	1.82	0.61
1:B:399:LEU:O	1:B:403:ILE:HG12	2.00	0.61
1:B:342:ASN:C	1:B:342:ASN:HD22	2.04	0.60
1:B:349:ASP:OD1	1:B:373:ARG:HD3	2.02	0.59
1:B:338:PHE:HB2	1:B:348:LEU:HD22	1.83	0.59
1:B:130:ASP:HB3	1:B:253:LYS:HB3	1.83	0.59
1:B:308:HIS:HD2	1:B:310:GLU:HB2	1.65	0.58
1:A:117:LEU:CD2	1:A:120:LEU:HD12	2.34	0.58
1:A:204:PRO:O	1:A:205:ALA:CB	2.53	0.56
1:A:304:LEU:CD1	1:A:400:GLN:HG3	2.34	0.56
1:B:342:ASN:ND2	1:B:344:GLU:H	2.02	0.56
1:B:342:ASN:HD22	1:B:343:GLY:N	2.03	0.56
1:A:128:ASN:HD22	1:A:130:ASP:N	1.86	0.56
1:A:204:PRO:O	1:A:205:ALA:HB3	2.04	0.55
1:B:296:GLN:HE21	1:B:296:GLN:H	1.54	0.55
1:A:344:GLU:HB3	2:A:511:HOH:O	2.06	0.55
1:A:234:HIS:HA	1:A:244:GLU:O	2.06	0.54
1:B:308:HIS:HD2	1:B:310:GLU:H	1.55	0.54
1:A:333:HIS:CG	1:A:334:SER:H	2.25	0.54
1:A:260:ALA:HB1	1:A:261:PRO:HD3	1.90	0.53
1:A:189:PHE:O	1:A:190:TRP:HB3	2.09	0.53
1:B:272:THR:OG1	1:B:370:HIS:HE1	1.92	0.53
1:B:131:THR:HA	1:B:251:VAL:O	2.09	0.52
1:A:296:GLN:HE21	1:A:296:GLN:N	2.02	0.52
1:B:268:ARG:HB3	1:B:372:VAL:HG12	1.90	0.52
1:A:280:PHE:CZ	1:A:303:ILE:HG23	2.43	0.52
1:B:126:SER:HA	2:B:535:HOH:O	2.09	0.51
1:A:211:ARG:NH2	1:A:297:ASP:OD2	2.43	0.51
1:B:209:PHE:HB3	1:B:294:LEU:HD13	1.93	0.51
1:A:136:PHE:CZ	1:A:178:PHE:HZ	2.29	0.50
1:A:271:THR:HA	1:A:368:GLY:O	2.11	0.50
1:B:312:ARG:HB2	1:B:313:PRO:HD3	1.94	0.50
1:A:304:LEU:CD1	1:A:400:GLN:CG	2.88	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLY:O	1:A:400:GLN:NE2	2.44	0.50
1:A:161:LEU:HA	1:A:164:VAL:HG22	1.94	0.50
1:A:295:PRO:O	1:A:299:ILE:HG12	2.12	0.50
1:B:295:PRO:O	1:B:299:ILE:HG12	2.13	0.49
1:B:350:SER:OG	1:B:370:HIS:HD2	1.95	0.49
1:B:121:ALA:O	1:B:235:VAL:HA	2.12	0.49
1:B:235:VAL:HG22	1:B:246:CYS:SG	2.52	0.49
1:A:183:ALA:O	1:A:187:LEU:HD22	2.12	0.49
1:B:346:VAL:HB	1:B:372:VAL:HG23	1.94	0.49
1:B:233:VAL:O	1:B:246:CYS:HB2	2.12	0.49
1:A:215:GLY:O	1:A:216:GLY:O	2.31	0.49
1:B:268:ARG:O	1:B:371:LYS:HA	2.13	0.48
1:A:378:ASN:HD22	1:A:380:ASP:H	1.60	0.48
1:A:357:ASN:ND2	1:A:359:TRP:H	2.11	0.48
1:B:353:SER:HB3	1:B:367:ILE:CD1	2.44	0.47
1:B:154:LEU:HG	1:B:155:ASN:N	2.30	0.47
1:A:317:ALA:O	1:A:321:LYS:HG3	2.14	0.47
1:A:218:ARG:N	1:A:221:ARG:HG3	2.28	0.47
1:A:249:THR:CG2	1:A:251:VAL:HG23	2.44	0.47
1:A:378:ASN:HD22	1:A:378:ASN:C	2.17	0.47
1:A:249:THR:HG22	1:A:251:VAL:HG23	1.97	0.46
1:A:253:LYS:NZ	2:A:524:HOH:O	2.47	0.46
1:A:342:ASN:C	1:A:342:ASN:ND2	2.69	0.46
1:B:394:LYS:O	1:B:395:ASP:HB2	2.15	0.46
1:B:360:SER:O	1:B:362:LYS:N	2.38	0.46
1:B:380:ASP:HB3	1:B:383:ALA:HB2	1.98	0.46
1:B:209:PHE:HE2	1:B:285:GLU:HG2	1.81	0.46
1:A:265:VAL:HA	1:A:268:ARG:HG3	1.97	0.45
1:B:147:SER:HB3	1:B:149:GLN:HE22	1.82	0.45
1:B:311:ASP:OD2	1:B:337:ARG:NE	2.50	0.45
1:B:339:CYS:HB2	1:B:345:TYR:CE1	2.52	0.45
1:A:342:ASN:HD22	1:A:343:GLY:N	2.15	0.45
1:B:182:THR:HA	1:B:187:LEU:HD21	1.98	0.45
1:B:403:ILE:HG22	1:B:407:LEU:HD22	1.99	0.45
1:B:392:ASN:O	1:B:393:ASP:HB2	2.16	0.45
1:A:356:VAL:HG21	1:A:361:ARG:NH2	2.32	0.45
1:A:361:ARG:HE	1:A:411:VAL:HG13	1.82	0.45
1:A:187:LEU:HA	1:A:188:PRO:HD2	1.70	0.45
1:A:234:HIS:HB3	1:A:243:PRO:O	2.17	0.45
1:A:221:ARG:HA	2:A:548:HOH:O	2.17	0.44
1:A:183:ALA:C	1:A:185:THR:H	2.20	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLU:O	1:B:260:ALA:C	2.55	0.44
1:B:284:ASP:OD2	1:B:286:ARG:N	2.43	0.44
1:A:348:LEU:HG	1:A:370:HIS:HB3	1.99	0.44
1:B:259:GLU:HB3	1:B:260:ALA:H	1.62	0.44
1:B:131:THR:HG22	1:B:252:GLU:HB2	2.00	0.43
1:A:233:VAL:O	1:A:246:CYS:N	2.36	0.43
1:A:232:LEU:HD12	1:A:233:VAL:H	1.84	0.43
1:A:303:ILE:HD13	1:A:315:MET:HE2	2.00	0.43
1:B:166:PHE:C	1:B:168:ASP:N	2.69	0.43
1:A:189:PHE:O	1:A:232:LEU:O	2.37	0.43
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.86	0.43
1:A:135:VAL:HA	1:A:247:CYS:O	2.19	0.42
1:A:136:PHE:CZ	1:A:178:PHE:CZ	3.06	0.42
1:B:372:VAL:HG22	1:B:374:THR:H	1.83	0.42
1:B:293:TYR:CZ	1:B:341:GLN:HA	2.54	0.42
1:A:211:ARG:HA	1:A:224:SER:O	2.19	0.42
1:A:242:GLU:CB	1:A:243:PRO:HD2	2.49	0.42
1:B:333:HIS:HD2	1:B:334:SER:H	1.57	0.42
1:A:236:HIS:O	1:A:237:SER:CB	2.68	0.42
1:A:256:SER:OG	1:A:381:VAL:HG22	2.20	0.42
1:B:122:SER:HB2	2:B:540:HOH:O	2.19	0.42
1:A:323:LEU:O	1:A:324:LYS:C	2.56	0.42
1:B:342:ASN:HA	1:B:385:ARG:HB2	2.01	0.42
1:A:128:ASN:ND2	1:A:130:ASP:N	2.51	0.42
1:B:342:ASN:HD22	1:B:344:GLU:H	1.68	0.42
1:B:127:LYS:HB3	1:B:128:ASN:H	1.66	0.41
1:B:269:ILE:HA	1:B:370:HIS:O	2.20	0.41
1:B:257:GLY:HA3	1:B:263:ILE:HD12	2.01	0.41
1:B:226:PHE:CD1	1:B:251:VAL:HG12	2.56	0.41
1:A:398:GLU:O	1:A:402:GLN:HG2	2.21	0.41
1:B:206:LYS:HA	1:B:207:PRO:HD3	1.92	0.41
1:A:128:ASN:ND2	1:A:130:ASP:HB2	2.36	0.41
1:A:217:ASP:HA	2:A:553:HOH:O	2.21	0.41
1:B:376:PRO:HG2	1:B:378:ASN:O	2.21	0.41
1:A:364:SER:HB2	2:A:556:HOH:O	2.21	0.41
1:B:132:PHE:HB2	1:B:147:SER:HB2	2.03	0.40
1:B:288:VAL:HB	1:B:289:PRO:CD	2.50	0.40
1:A:303:ILE:H	1:A:303:ILE:HG13	1.65	0.40
1:A:333:HIS:CG	1:A:334:SER:N	2.89	0.40
1:A:262:ARG:O	1:A:263:ILE:C	2.59	0.40
1:B:167:VAL:CG2	2:B:522:HOH:O	2.70	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	294/317 (93%)	255 (87%)	23 (8%)	16 (5%)	2	2
1	B	253/317 (80%)	214 (85%)	22 (9%)	17 (7%)	1	1
All	All	547/634 (86%)	469 (86%)	45 (8%)	33 (6%)	1	1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	190	TRP
1	A	204	PRO
1	A	205	ALA
1	A	216	GLY
1	A	237	SER
1	A	241	PRO
1	A	260	ALA
1	A	392	ASN
1	B	140	SER
1	B	239	ALA
1	B	244	GLU
1	B	245	PRO
1	B	260	ALA
1	A	239	ALA
1	A	244	GLU
1	A	391	SER
1	B	153	ILE
1	B	246	CYS
1	B	393	ASP
1	A	261	PRO
1	A	262	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	120	LEU
1	B	191	ASN
1	B	205	ALA
1	B	361	ARG
1	B	223	TYR
1	B	385	ARG
1	A	235	VAL
1	B	138	PHE
1	B	259	GLU
1	A	184	PRO
1	B	261	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	235/280 (84%)	207 (88%)	28 (12%)	5 10
1	B	210/280 (75%)	185 (88%)	25 (12%)	5 10
All	All	445/560 (80%)	392 (88%)	53 (12%)	5 10

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	A	115	GLU
1	A	120	LEU
1	A	128	ASN
1	A	170	LEU
1	A	185	THR
1	A	187	LEU
1	A	206	LYS
1	A	233	VAL
1	A	249	THR
1	A	250	LEU
1	A	254	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	PRO
1	A	268	ARG
1	A	271	THR
1	A	282	GLU
1	A	296	GLN
1	A	303	ILE
1	A	307	LEU
1	A	341	GLN
1	A	342	ASN
1	A	346	VAL
1	A	348	LEU
1	A	356	VAL
1	A	357	ASN
1	A	378	ASN
1	A	384	THR
1	A	408	LEU
1	B	128	ASN
1	B	138	PHE
1	B	148	GLU
1	B	149	GLN
1	B	154	LEU
1	B	176	ARG
1	B	206	LYS
1	B	224	SER
1	B	238	SER
1	B	284	ASP
1	B	296	GLN
1	B	299	ILE
1	B	303	ILE
1	B	310	GLU
1	B	342	ASN
1	B	348	LEU
1	B	351	SER
1	B	367	ILE
1	B	385	ARG
1	B	387	LYS
1	B	388	LYS
1	B	399	LEU
1	B	405	LYS
1	B	407	LEU
1	B	411	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	173	GLN
1	A	181	HIS
1	A	296	GLN
1	A	319	HIS
1	A	342	ASN
1	A	357	ASN
1	A	378	ASN
1	A	400	GLN
1	B	124	HIS
1	B	149	GLN
1	B	296	GLN
1	B	308	HIS
1	B	333	HIS
1	B	342	ASN
1	B	370	HIS
1	B	404	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

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^{th} 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	298/317 (94%)	-0.09	9 (3%) 50 53	23, 38, 72, 92	0
1	B	265/317 (83%)	0.10	13 (4%) 29 31	31, 53, 82, 88	0
All	All	563/634 (88%)	-0.00	22 (3%) 39 42	23, 46, 78, 92	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	PHE	6.2
1	A	106	LEU	5.3
1	A	105	ARG	4.4
1	A	240	GLN	4.3
1	B	205	ALA	4.0
1	B	392	ASN	3.5
1	A	108	ASP	3.3
1	B	193	TRP	3.2
1	B	190	TRP	3.2
1	A	104	GLY	3.2
1	B	204	PRO	3.1
1	A	390	ALA	3.0
1	B	213	CYS	2.9
1	A	241	PRO	2.8
1	B	165	HIS	2.7
1	B	120	LEU	2.4
1	A	239	ALA	2.4
1	B	144	VAL	2.3
1	A	391	SER	2.2
1	B	221	ARG	2.1
1	B	138	PHE	2.1
1	B	243	PRO	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.