Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 09:28 PM EST

PDB ID	:	4DJ2
Title	:	Unwinding the Differences of the Mammalian PERIOD Clock Proteins from Crystal Structure to Cellular Function
Authors	:	Kucera, N.; Schmalen, I.; Hennig, S.; Oellinger, R.; Strauss, H.M.; Grudziecki, A.; Wieczorek, C.; Kramer, A.; Wolf, E.
Deposited on	:	2012-02-01
Resolution	:	2.75 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:

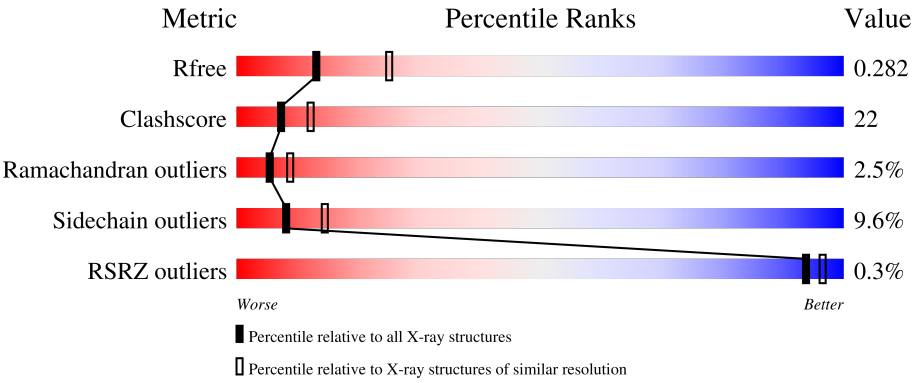
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	320	54% 28% · 14%
1	B	320	51% 32% · 13%
1	C	320	44% 32% 6% 18%
1	D	320	46% 27% · 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8170 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2105	1359	367	370	9			
1	B	279	Total	C	N	O	S	0	0	0
			2112	1360	368	375	9			
1	C	264	Total	C	N	O	S	0	0	0
			2024	1297	365	355	7			
1	D	246	Total	C	N	O	S	0	0	0
			1852	1194	328	324	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLY	-	expression tag	UNP O35973
A	184	PRO	-	expression tag	UNP O35973
A	185	LEU	-	expression tag	UNP O35973
A	186	GLY	-	expression tag	UNP O35973
A	187	SER	-	expression tag	UNP O35973
A	188	PRO	-	expression tag	UNP O35973
A	189	GLU	-	expression tag	UNP O35973
A	190	PHE	-	expression tag	UNP O35973
B	183	GLY	-	expression tag	UNP O35973
B	184	PRO	-	expression tag	UNP O35973
B	185	LEU	-	expression tag	UNP O35973
B	186	GLY	-	expression tag	UNP O35973
B	187	SER	-	expression tag	UNP O35973
B	188	PRO	-	expression tag	UNP O35973
B	189	GLU	-	expression tag	UNP O35973
B	190	PHE	-	expression tag	UNP O35973
C	183	GLY	-	expression tag	UNP O35973
C	184	PRO	-	expression tag	UNP O35973
C	185	LEU	-	expression tag	UNP O35973
C	186	GLY	-	expression tag	UNP O35973
C	187	SER	-	expression tag	UNP O35973

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Chain	Residue	Modelled	Actual	Comment	Reference
C	188	PRO	-	expression tag	UNP O35973
C	189	GLU	-	expression tag	UNP O35973
C	190	PHE	-	expression tag	UNP O35973
D	183	GLY	-	expression tag	UNP O35973
D	184	PRO	-	expression tag	UNP O35973
D	185	LEU	-	expression tag	UNP O35973
D	186	GLY	-	expression tag	UNP O35973
D	187	SER	-	expression tag	UNP O35973
D	188	PRO	-	expression tag	UNP O35973
D	189	GLU	-	expression tag	UNP O35973
D	190	PHE	-	expression tag	UNP O35973

- Molecule 2 is water.

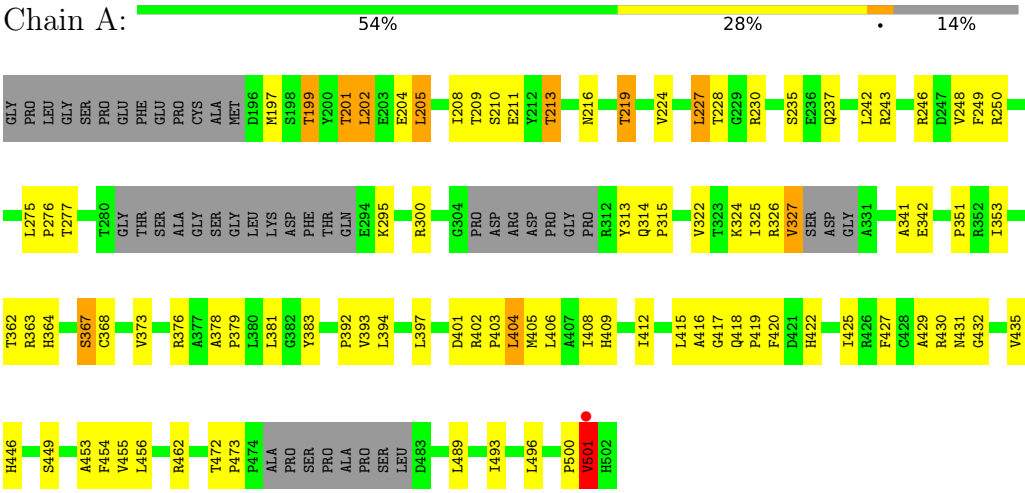
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	21	Total O 21 21	0	0
2	B	30	Total O 30 30	0	0
2	C	14	Total O 14 14	0	0
2	D	12	Total O 12 12	0	0

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.

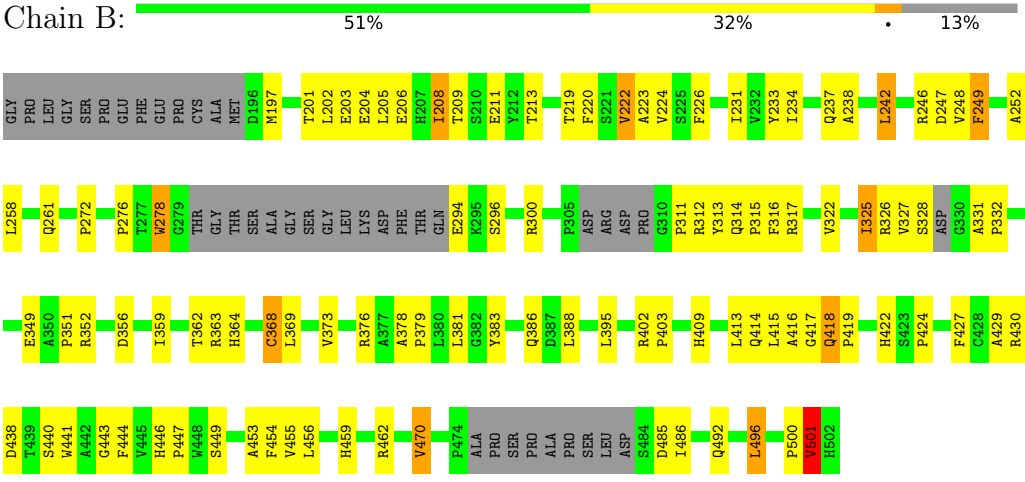
• Molecule 1: Period circadian protein homolog 1

Chain A:



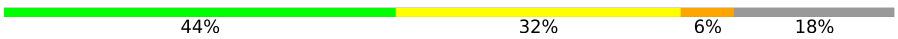
• Molecule 1: Period circadian protein homolog 1

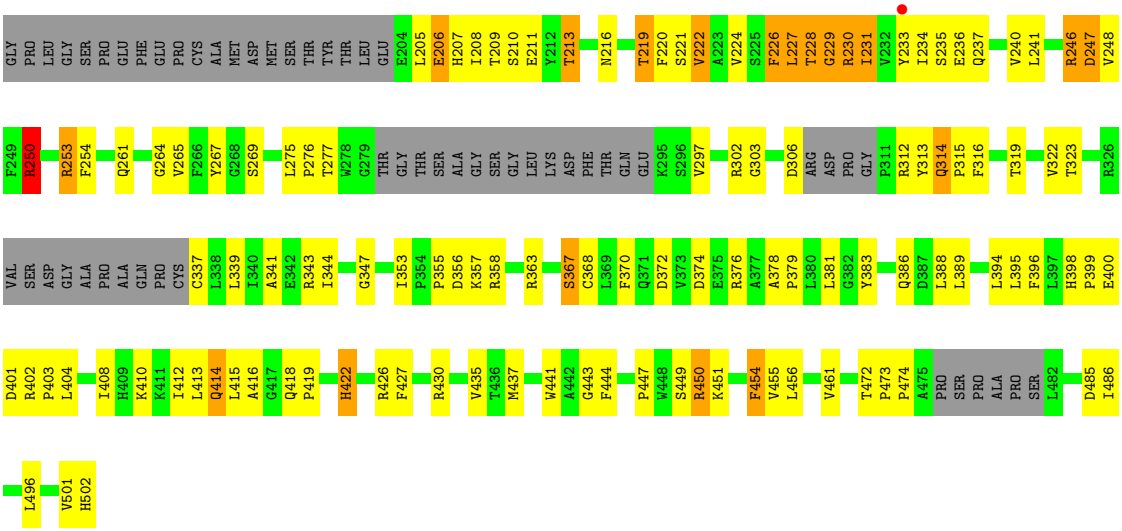
Chain B:



• Molecule 1: Period circadian protein homolog 1

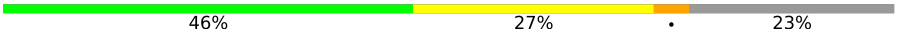
Chain C:

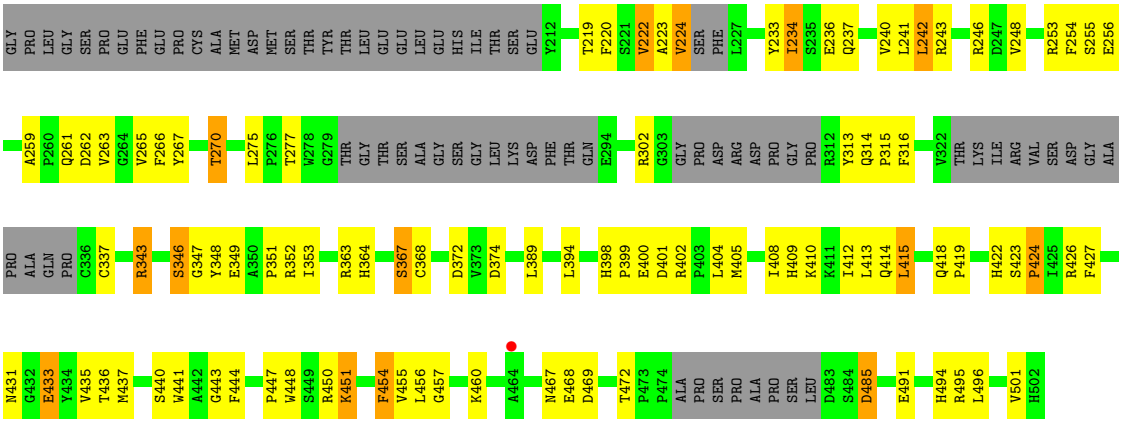




• Molecule 1: Period circadian protein homolog 1

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.34Å 56.87Å 100.95Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	49.55 – 2.75 49.55 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.55-2.75) 98.8 (49.55-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.208 , 0.282 0.207 , 0.282	Depositor DCC
R_{free} test set	1997 reflections (6.71%)	wwPDB-VP
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,k,-h 0.477 for h,-k,-l 0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8170	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.32% 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	0.47	0/2161	0.64	0/2951
1	B	0.48	1/2167 (0.0%)	0.63	0/2959
1	C	0.44	0/2076	0.64	0/2830
1	D	0.45	0/1902	0.63	0/2598
All	All	0.46	1/8306 (0.0%)	0.63	0/11338

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	CYS	CB-SG	-5.09	1.73	1.81

There are no bond angle outliers.

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	2105	0	2029	77	0
1	B	2112	0	2012	85	0
1	C	2024	0	1955	117	0
1	D	1852	0	1741	89	0
2	A	21	0	0	2	0
2	B	30	0	0	1	0
2	C	14	0	0	3	0
2	D	12	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8170	0	7737	355	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 22.

All (355) 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:C:236:GLU:HA	1:C:246:ARG:HH12	1.12	1.10
1:C:230:ARG:HG2	1:C:254:PHE:H	1.15	1.09
1:D:236:GLU:HA	1:D:246:ARG:HH12	1.35	0.91
1:C:230:ARG:CG	1:C:254:PHE:H	1.85	0.90
1:C:399:PRO:HG3	1:C:402:ARG:HH21	1.37	0.90
1:B:208:ILE:HG21	1:B:278:TRP:HH2	1.37	0.90
1:C:230:ARG:HG2	1:C:254:PHE:N	1.87	0.90
1:D:399:PRO:HG3	1:D:402:ARG:NH2	1.88	0.87
1:C:236:GLU:HA	1:C:246:ARG:NH1	1.91	0.85
1:C:399:PRO:HG3	1:C:402:ARG:NH2	1.92	0.84
1:D:410:LYS:O	1:D:414:GLN:HG3	1.78	0.83
1:C:222:VAL:HG12	1:C:231:ILE:HD11	1.59	0.83
1:A:454:PHE:HZ	1:C:454:PHE:HZ	1.28	0.82
1:C:213:THR:HG21	1:C:237:GLN:NE2	1.93	0.82
1:A:246:ARG:HA	1:A:249:PHE:HD2	1.43	0.81
1:A:431:ASN:N	1:A:432:GLY:HA2	1.95	0.81
1:A:500:PRO:O	1:A:501:VAL:HB	1.79	0.81
1:B:500:PRO:O	1:B:501:VAL:HB	1.85	0.77
1:B:254:PHE:HA	1:B:257:LEU:HD23	1.65	0.77
1:D:413:LEU:HD22	1:D:496:LEU:HD23	1.65	0.76
1:C:222:VAL:CG1	1:C:231:ILE:HD11	2.16	0.75
1:C:410:LYS:O	1:C:414:GLN:HG3	1.85	0.75
1:C:343:ARG:NH1	1:C:344:ILE:O	2.19	0.75
1:C:427:PHE:CD1	1:C:437:MET:HG3	2.21	0.75
1:C:398:HIS:CD2	1:C:399:PRO:HD2	2.22	0.74
1:C:230:ARG:HG2	1:C:253:ARG:HA	1.68	0.74
1:A:431:ASN:H	1:A:432:GLY:HA2	1.52	0.73
1:A:401:ASP:O	1:A:404:LEU:HB2	1.89	0.73
1:D:398:HIS:ND1	1:D:399:PRO:HD2	2.06	0.71
1:C:213:THR:HG21	1:C:237:GLN:HE21	1.55	0.71
1:A:406:LEU:HD13	1:A:489:LEU:HD22	1.72	0.70
1:C:435:VAL:HG22	1:C:437:MET:HE3	1.73	0.70
1:A:359:ILE:O	1:A:376:ARG:HD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:HIS:HB2	1:A:453:ALA:HB2	1.73	0.69
1:A:454:PHE:CZ	1:C:454:PHE:HZ	2.09	0.69
1:D:427:PHE:CE1	1:D:437:MET:HG3	2.27	0.69
1:C:395:LEU:HD12	1:C:395:LEU:O	1.93	0.69
1:D:236:GLU:HA	1:D:246:ARG:NH1	2.07	0.69
1:A:417:GLY:HA2	2:A:618:HOH:O	1.93	0.68
1:C:209:THR:HG21	1:C:233:TYR:HE2	1.57	0.68
1:D:372:ASP:HA	1:D:389:LEU:HD21	1.76	0.68
1:C:435:VAL:HG22	1:C:437:MET:CE	2.23	0.68
1:C:427:PHE:CE1	1:C:437:MET:HG3	2.29	0.68
1:D:491:GLU:O	1:D:495:ARG:HG3	1.94	0.67
1:C:415:LEU:HB3	1:C:418:GLN:HB2	1.76	0.67
1:D:263:VAL:HG13	1:D:267:TYR:HE2	1.60	0.67
1:B:427:PHE:CD1	1:B:437:MET:HG3	2.30	0.66
1:B:419:PRO:HG3	1:D:447:PRO:HB3	1.78	0.65
1:C:404:LEU:O	1:C:408:ILE:HG13	1.95	0.65
1:A:199:THR:HB	1:A:324:LYS:HB3	1.78	0.65
1:C:314:GLN:HB2	1:C:316:PHE:HE2	1.62	0.65
1:A:404:LEU:O	1:A:408:ILE:HD12	1.95	0.65
1:C:408:ILE:O	1:C:412:ILE:HD12	1.97	0.64
1:B:208:ILE:HG21	1:B:278:TRP:CH2	2.26	0.64
1:D:427:PHE:CD1	1:D:437:MET:HG3	2.32	0.64
1:A:427:PHE:CD1	1:A:437:MET:HG3	2.32	0.64
1:D:343:ARG:HD2	2:D:607:HOH:O	1.96	0.64
1:C:315:PRO:HD2	1:C:343:ARG:NH1	2.13	0.64
1:C:208:ILE:O	1:C:211:GLU:HB2	1.97	0.63
1:C:316:PHE:CE1	1:C:343:ARG:HB2	2.34	0.63
1:D:267:TYR:HA	1:D:270:THR:HG23	1.81	0.63
1:A:268:GLY:HA2	1:C:264:GLY:HA3	1.81	0.62
1:C:209:THR:C	1:C:211:GLU:H	2.02	0.62
1:C:302:ARG:HG3	1:C:313:TYR:CE1	2.35	0.62
1:D:237:GLN:HA	1:D:240:VAL:HG23	1.80	0.62
1:D:408:ILE:HD11	1:D:422:HIS:CD2	2.35	0.62
1:D:399:PRO:HG3	1:D:402:ARG:HH21	1.63	0.61
1:D:440:SER:O	1:D:457:GLY:HA2	2.01	0.61
1:A:381:LEU:HD21	1:A:437:MET:HE3	1.83	0.61
1:C:276:PRO:O	1:C:322:VAL:HG12	2.01	0.61
1:B:414:GLN:C	1:B:416:ALA:H	2.03	0.61
1:D:363:ARG:NH1	2:D:605:HOH:O	2.34	0.60
1:B:237:GLN:HE22	1:C:357:LYS:NZ	1.99	0.60
1:C:226:PHE:CE2	1:C:337:CYS:HB2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TYR:CE2	1:A:430:ARG:HG3	2.37	0.60
1:B:257:LEU:N	1:B:257:LEU:HD22	2.17	0.59
1:D:253:ARG:HE	1:D:256:GLU:CB	2.16	0.59
1:A:446:HIS:HB3	1:A:449:SER:HB2	1.83	0.59
1:C:415:LEU:O	1:C:418:GLN:HG2	2.02	0.59
1:D:266:PHE:O	1:D:270:THR:HG22	2.03	0.59
1:C:209:THR:HG21	1:C:233:TYR:CE2	2.38	0.58
1:A:235:SER:HB2	2:A:619:HOH:O	2.02	0.58
1:B:373:VAL:HG11	1:B:388:LEU:HD12	1.85	0.58
1:D:316:PHE:CE1	1:D:343:ARG:HB2	2.39	0.58
1:C:502:HIS:HE1	2:C:605:HOH:O	1.87	0.58
1:C:419:PRO:HA	1:C:441:TRP:O	2.04	0.57
1:B:362:THR:HG22	1:B:373:VAL:HG23	1.86	0.57
1:A:246:ARG:HA	1:A:249:PHE:CD2	2.32	0.57
1:D:259:ALA:HB3	1:D:262:ASP:OD2	2.04	0.57
1:D:266:PHE:O	1:D:270:THR:CG2	2.53	0.57
1:D:220:PHE:HD1	1:D:241:LEU:HD12	1.70	0.57
1:D:419:PRO:HA	1:D:441:TRP:O	2.05	0.57
1:C:370:PHE:HB2	1:C:388:LEU:O	2.05	0.57
1:C:220:PHE:HD1	1:C:241:LEU:HD12	1.70	0.56
1:C:206:GLU:H	1:C:208:ILE:HD11	1.69	0.56
1:A:394:LEU:HD23	1:A:397:LEU:HD12	1.87	0.56
1:B:201:THR:OG1	1:B:204:GLU:HG3	2.06	0.56
1:C:437:MET:HE2	1:C:461:VAL:HA	1.87	0.56
1:B:202:LEU:HG	1:B:327:VAL:HA	1.87	0.56
1:B:238:ALA:O	1:B:242:LEU:HB2	2.06	0.56
1:B:246:ARG:HA	1:B:249:PHE:HD2	1.70	0.56
1:B:363:ARG:HG3	1:B:456:LEU:HD13	1.86	0.56
1:C:414:GLN:O	1:C:415:LEU:HB2	2.04	0.56
1:A:415:LEU:HD21	1:A:418:GLN:CB	2.35	0.56
1:D:472:THR:HG23	1:D:472:THR:O	2.06	0.56
1:B:429:ALA:HB1	1:B:470:VAL:HG22	1.88	0.56
1:B:444:PHE:CD1	1:D:444:PHE:CD1	2.93	0.56
1:A:462:ARG:HG2	1:A:462:ARG:HH11	1.71	0.55
1:B:446:HIS:HB2	1:B:453:ALA:HB2	1.89	0.55
1:C:250:ARG:HA	1:C:250:ARG:NH1	2.22	0.55
1:B:446:HIS:HB3	1:B:449:SER:HB2	1.89	0.54
1:D:431:ASN:HD22	1:D:467:ASN:ND2	2.06	0.54
1:C:237:GLN:OE1	1:C:237:GLN:N	2.37	0.54
1:D:405:MET:O	1:D:409:HIS:HD2	1.91	0.54
1:D:270:THR:O	1:D:270:THR:OG1	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:PRO:O	1:B:501:VAL:CB	2.56	0.54
1:C:213:THR:HA	1:C:216:ASN:O	2.08	0.54
1:C:302:ARG:NH1	1:C:306:ASP:H	2.06	0.54
1:C:367:SER:O	1:C:368:CYS:HB2	2.08	0.54
1:D:364:HIS:NE2	1:D:409:HIS:HE1	2.05	0.53
1:C:347:GLY:HA2	1:C:353:ILE:HG13	1.90	0.53
1:C:363:ARG:NH1	2:C:604:HOH:O	2.41	0.53
1:A:213:THR:HA	1:A:216:ASN:O	2.09	0.53
1:B:326:ARG:HD3	1:B:331:ALA:O	2.09	0.53
1:B:454:PHE:CZ	1:D:454:PHE:HZ	2.27	0.53
1:C:398:HIS:HD2	1:C:400:GLU:H	1.56	0.53
1:B:222:VAL:HG13	1:B:234:ILE:HD12	1.90	0.53
1:A:408:ILE:O	1:A:412:ILE:HG13	2.09	0.53
1:D:367:SER:O	1:D:368:CYS:HB2	2.08	0.53
1:D:248:VAL:HG13	1:D:248:VAL:O	2.09	0.52
1:D:415:LEU:HD12	1:D:418:GLN:HB2	1.91	0.52
1:A:409:HIS:CE1	1:A:455:VAL:HG21	2.45	0.52
1:B:349:GLU:O	1:B:352:ARG:N	2.43	0.52
1:C:386:GLN:H	1:C:386:GLN:NE2	2.06	0.52
1:C:383:TYR:CD2	1:C:430:ARG:HD2	2.44	0.52
1:B:204:GLU:O	1:B:208:ILE:HB	2.09	0.52
1:D:314:GLN:NE2	1:D:343:ARG:NH2	2.58	0.52
1:B:226:PHE:HE2	1:B:322:VAL:HG23	1.74	0.52
1:B:224:VAL:HG22	1:B:337:CYS:HB3	1.92	0.52
1:D:418:GLN:N	2:D:608:HOH:O	2.43	0.52
1:D:485:ASP:N	1:D:485:ASP:OD1	2.43	0.52
1:A:202:LEU:HG	1:A:327:VAL:HA	1.92	0.52
1:A:435:VAL:HB	1:A:437:MET:HE2	1.92	0.52
1:C:408:ILE:HD11	1:C:422:HIS:CD2	2.45	0.52
1:D:233:TYR:CG	1:D:234:ILE:N	2.78	0.52
1:B:300:ARG:HB3	1:B:313:TYR:HB3	1.91	0.51
1:D:408:ILE:HD11	1:D:422:HIS:HD2	1.75	0.51
1:B:256:GLU:O	1:B:256:GLU:HG3	2.10	0.51
1:A:209:THR:O	1:A:213:THR:HG23	2.11	0.51
1:C:209:THR:C	1:C:211:GLU:N	2.64	0.51
1:D:408:ILE:O	1:D:412:ILE:HD12	2.11	0.51
1:B:246:ARG:HA	1:B:249:PHE:CD2	2.44	0.51
1:B:414:GLN:C	1:B:416:ALA:N	2.65	0.51
1:A:415:LEU:O	1:A:417:GLY:N	2.44	0.51
1:B:205:LEU:HD21	1:B:325:ILE:HD11	1.93	0.50
1:B:213:THR:HG23	1:B:237:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ASP:OD1	1:B:485:ASP:N	2.43	0.50
1:A:353:ILE:O	1:A:358:ARG:NE	2.43	0.50
1:C:443:GLY:HA2	1:C:455:VAL:HA	1.93	0.50
1:A:409:HIS:HE1	1:A:455:VAL:HG21	1.75	0.50
1:A:381:LEU:HD21	1:A:437:MET:CE	2.42	0.50
1:B:383:TYR:CD2	1:B:430:ARG:HD2	2.46	0.50
1:D:413:LEU:HD22	1:D:496:LEU:CD2	2.37	0.50
1:C:206:GLU:HA	1:C:233:TYR:OH	2.12	0.50
1:C:208:ILE:HD12	1:C:209:THR:N	2.27	0.50
1:C:372:ASP:HA	1:C:389:LEU:HD21	1.93	0.49
1:B:206:GLU:HA	1:B:233:TYR:OH	2.12	0.49
1:B:427:PHE:CE1	1:B:437:MET:HG3	2.47	0.49
1:A:300:ARG:HB3	1:A:313:TYR:HB3	1.93	0.49
1:A:364:HIS:CE1	1:A:455:VAL:HB	2.47	0.49
1:A:402:ARG:HB2	1:A:403:PRO:HD3	1.95	0.49
1:B:359:ILE:O	1:B:376:ARG:HD2	2.11	0.49
1:A:202:LEU:HD11	1:A:327:VAL:HG23	1.93	0.49
1:C:230:ARG:HG2	1:C:253:ARG:CA	2.38	0.49
1:A:327:VAL:O	1:A:327:VAL:HG13	2.12	0.49
1:B:386:GLN:H	1:B:386:GLN:NE2	2.10	0.49
1:D:348:TYR:C	1:D:352:ARG:HD3	2.32	0.49
1:D:398:HIS:ND1	1:D:399:PRO:CD	2.75	0.49
1:B:222:VAL:HG23	1:B:339:LEU:HB2	1.94	0.49
1:C:233:TYR:CG	1:C:234:ILE:N	2.81	0.49
1:A:213:THR:HB	1:A:237:GLN:HG3	1.94	0.49
1:A:444:PHE:CD1	1:C:444:PHE:CD1	3.01	0.49
1:C:205:LEU:O	1:C:206:GLU:CB	2.60	0.49
1:B:431:ASN:OD1	1:B:433:GLU:HB3	2.13	0.48
1:B:381:LEU:O	1:B:429:ALA:O	2.30	0.48
1:C:209:THR:O	1:C:211:GLU:N	2.38	0.48
1:A:394:LEU:CD2	1:A:405:MET:HG3	2.43	0.48
1:A:422:HIS:O	1:A:422:HIS:CG	2.65	0.48
1:B:237:GLN:HB2	2:B:630:HOH:O	2.14	0.48
1:D:431:ASN:HA	1:D:472:THR:O	2.12	0.48
1:A:378:ALA:HB3	1:A:379:PRO:CD	2.43	0.48
1:C:386:GLN:H	1:C:386:GLN:CD	2.17	0.48
1:B:276:PRO:HG3	1:B:294:GLU:CB	2.44	0.48
1:C:302:ARG:HG2	1:C:312:ARG:O	2.14	0.48
1:D:254:PHE:HE2	1:D:266:PHE:CE2	2.32	0.48
1:A:205:LEU:HA	1:A:208:ILE:HG22	1.95	0.47
1:A:431:ASN:N	1:A:432:GLY:CA	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:LYS:O	1:D:414:GLN:CG	2.56	0.47
1:A:201:THR:HG23	1:A:204:GLU:CD	2.34	0.47
1:A:209:THR:C	1:A:211:GLU:H	2.17	0.47
1:C:237:GLN:HA	1:C:240:VAL:HG23	1.96	0.47
1:C:394:LEU:HD22	1:C:402:ARG:HG2	1.95	0.47
1:D:254:PHE:C	1:D:256:GLU:N	2.66	0.47
1:B:409:HIS:CE1	1:B:455:VAL:HG21	2.49	0.47
1:C:206:GLU:H	1:C:208:ILE:CD1	2.27	0.47
1:C:322:VAL:O	1:C:323:THR:HG23	2.14	0.47
1:C:416:ALA:HB2	1:C:501:VAL:HG11	1.96	0.47
1:B:247:ASP:C	1:B:249:PHE:H	2.16	0.47
1:C:398:HIS:CD2	1:C:399:PRO:CD	2.93	0.47
1:B:237:GLN:HE22	1:C:357:LYS:HZ2	1.63	0.47
1:D:472:THR:O	1:D:472:THR:CG2	2.63	0.47
1:A:493:ILE:O	1:A:496:LEU:HB2	2.14	0.47
1:C:398:HIS:CD2	1:C:400:GLU:H	2.32	0.47
1:D:346:SER:OG	1:D:468:GLU:O	2.25	0.47
1:D:443:GLY:HA2	1:D:455:VAL:HA	1.97	0.47
1:B:386:GLN:H	1:B:386:GLN:CD	2.18	0.47
1:A:363:ARG:NH1	2:C:604:HOH:O	2.48	0.47
1:A:394:LEU:HD21	1:A:405:MET:HG3	1.97	0.47
1:B:444:PHE:CZ	1:B:447:PRO:HD3	2.50	0.47
1:D:253:ARG:HH21	1:D:256:GLU:CB	2.27	0.47
1:D:394:LEU:HA	1:D:394:LEU:HD23	1.74	0.47
1:B:402:ARG:HB2	1:B:403:PRO:HD3	1.96	0.46
1:C:414:GLN:C	1:C:416:ALA:H	2.17	0.46
1:C:247:ASP:O	1:C:250:ARG:HD2	2.15	0.46
1:C:228:THR:O	1:C:229:GLY:O	2.33	0.46
1:D:469:ASP:OD2	1:D:472:THR:CG2	2.63	0.46
1:A:362:THR:HG22	1:A:373:VAL:HG13	1.97	0.46
1:C:400:GLU:HB3	1:C:426:ARG:NH2	2.30	0.46
1:C:413:LEU:HD22	1:C:496:LEU:HG	1.98	0.46
1:D:408:ILE:CD1	1:D:422:HIS:HD2	2.29	0.46
1:C:231:ILE:O	1:C:231:ILE:CG2	2.63	0.46
1:D:253:ARG:NH2	1:D:256:GLU:HA	2.31	0.46
1:A:219:THR:HA	1:A:341:ALA:O	2.16	0.46
1:B:456:LEU:N	1:B:456:LEU:HD22	2.31	0.46
1:C:222:VAL:HG12	1:C:231:ILE:CD1	2.37	0.46
1:B:447:PRO:HB3	1:D:419:PRO:HG3	1.97	0.45
1:D:302:ARG:HB2	1:D:313:TYR:CE1	2.51	0.45
1:B:201:THR:C	1:B:203:GLU:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PHE:CE1	1:A:437:MET:HG3	2.51	0.45
1:D:263:VAL:HG13	1:D:267:TYR:CE2	2.46	0.45
1:C:213:THR:HG21	1:C:237:GLN:HE22	1.80	0.45
1:C:231:ILE:O	1:C:231:ILE:HG22	2.15	0.45
1:C:314:GLN:HB2	1:C:316:PHE:CE2	2.47	0.45
1:D:248:VAL:O	1:D:248:VAL:CG1	2.64	0.45
1:A:314:GLN:HA	1:A:315:PRO:HD3	1.66	0.45
1:B:231:ILE:HD12	1:B:252:ALA:HB3	1.98	0.45
1:B:429:ALA:HB1	1:B:470:VAL:CG2	2.47	0.45
1:C:401:ASP:O	1:C:404:LEU:HB2	2.16	0.45
1:C:441:TRP:HA	1:C:456:LEU:O	2.16	0.45
1:D:401:ASP:HB3	1:D:404:LEU:HD12	1.98	0.45
1:A:454:PHE:CE2	1:A:456:LEU:HD21	2.52	0.45
1:C:402:ARG:N	1:C:403:PRO:CD	2.79	0.45
1:A:363:ARG:HG3	1:A:456:LEU:HD13	1.99	0.45
1:B:383:TYR:CE2	1:B:430:ARG:HB2	2.51	0.45
1:D:401:ASP:O	1:D:404:LEU:HB2	2.17	0.45
1:A:367:SER:O	1:A:368:CYS:HB2	2.17	0.45
1:B:417:GLY:O	1:B:418:GLN:C	2.55	0.45
1:C:231:ILE:HD13	1:C:231:ILE:HA	1.78	0.45
1:A:472:THR:HA	1:A:473:PRO:HD3	1.68	0.44
1:B:328:SER:C	1:B:331:ALA:HB2	2.37	0.44
1:B:395:LEU:HB2	1:B:486:ILE:HD13	1.99	0.44
1:A:454:PHE:HE2	1:A:456:LEU:HD21	1.82	0.44
1:B:417:GLY:O	1:B:418:GLN:O	2.36	0.44
1:A:415:LEU:HD11	1:A:418:GLN:CB	2.47	0.44
1:B:315:PRO:HB2	1:B:344:ILE:HB	2.00	0.44
1:B:413:LEU:HD11	1:B:496:LEU:O	2.18	0.44
1:B:419:PRO:HA	1:B:441:TRP:O	2.18	0.44
1:B:359:ILE:HG23	1:B:459:HIS:O	2.18	0.44
1:B:414:GLN:O	1:B:416:ALA:N	2.50	0.44
1:B:378:ALA:HB3	1:B:379:PRO:CD	2.47	0.44
1:C:437:MET:CE	1:C:461:VAL:HG22	2.48	0.44
1:B:381:LEU:HD21	1:B:437:MET:CE	2.47	0.44
1:B:438:ASP:OD2	1:B:462:ARG:HD2	2.18	0.44
1:D:413:LEU:HD12	1:D:413:LEU:HA	1.79	0.43
1:B:364:HIS:CE1	1:B:455:VAL:HB	2.52	0.43
1:B:454:PHE:HZ	1:D:454:PHE:HZ	1.64	0.43
1:A:381:LEU:O	1:A:429:ALA:O	2.36	0.43
1:D:405:MET:O	1:D:409:HIS:CD2	2.71	0.43
1:D:424:PRO:HB2	1:D:436:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:TRP:HA	1:D:456:LEU:O	2.17	0.43
1:B:220:PHE:HE1	1:B:316:PHE:CE1	2.37	0.43
1:B:255:SER:O	1:B:258:LEU:HB2	2.17	0.43
1:C:235:SER:HB3	1:C:237:GLN:OE1	2.18	0.43
1:A:249:PHE:O	1:A:250:ARG:C	2.57	0.43
1:C:220:PHE:HB2	1:C:235:SER:HB2	2.01	0.43
1:D:349:GLU:O	1:D:351:PRO:C	2.57	0.43
1:A:202:LEU:CD1	1:A:327:VAL:HG23	2.49	0.43
1:C:205:LEU:CB	1:C:208:ILE:HD11	2.49	0.43
1:C:449:SER:O	1:C:450:ARG:HB2	2.18	0.43
1:D:347:GLY:HA2	1:D:353:ILE:HG13	2.00	0.43
1:D:275:LEU:HD23	1:D:275:LEU:HA	1.87	0.43
1:A:326:ARG:O	1:A:327:VAL:HG12	2.19	0.43
1:A:415:LEU:C	1:A:417:GLY:H	2.22	0.43
1:B:209:THR:C	1:B:211:GLU:H	2.22	0.43
1:B:440:SER:HG	1:D:448:TRP:HZ2	1.63	0.43
1:C:224:VAL:HG22	1:C:337:CYS:HB3	2.00	0.43
1:D:423:SER:HA	1:D:424:PRO:HA	1.84	0.43
1:C:355:PRO:HA	1:C:358:ARG:HD2	2.01	0.43
1:A:228:THR:OG1	1:A:230:ARG:HG2	2.18	0.42
1:D:242:LEU:H	1:D:242:LEU:HG	1.61	0.42
1:D:460:LYS:NZ	2:D:603:HOH:O	2.49	0.42
1:C:246:ARG:C	1:C:248:VAL:N	2.72	0.42
1:D:451:LYS:HB2	1:D:451:LYS:HE3	1.61	0.42
1:A:419:PRO:HG3	1:C:447:PRO:HB3	2.00	0.42
1:B:314:GLN:HA	1:B:315:PRO:HD3	1.74	0.42
1:B:443:GLY:HA2	1:B:454:PHE:O	2.19	0.42
1:C:374:ASP:OD1	1:C:376:ARG:NH2	2.36	0.42
1:D:400:GLU:HB3	1:D:426:ARG:NH2	2.35	0.42
1:A:257:LEU:HD12	1:A:257:LEU:N	2.34	0.42
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.79	0.42
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.87	0.42
1:A:412:ILE:O	1:A:415:LEU:O	2.38	0.42
1:B:326:ARG:HG2	1:B:332:PRO:O	2.20	0.42
1:C:246:ARG:C	1:C:248:VAL:H	2.23	0.42
1:D:219:THR:HG22	1:D:220:PHE:N	2.35	0.42
1:D:263:VAL:O	1:D:267:TYR:HD2	2.02	0.42
1:A:275:LEU:HA	1:A:276:PRO:HD3	1.94	0.42
1:C:415:LEU:O	1:C:416:ALA:C	2.57	0.42
1:D:220:PHE:HE2	1:D:222:VAL:HG22	1.83	0.42
1:A:277:THR:HA	1:A:322:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LEU:N	1:B:257:LEU:CD2	2.83	0.42
1:C:378:ALA:HB3	1:C:379:PRO:CD	2.50	0.42
1:C:410:LYS:HA	1:C:496:LEU:HD21	2.00	0.42
1:C:408:ILE:CD1	1:C:422:HIS:HD2	2.33	0.41
1:D:433:GLU:OE1	1:D:467:ASN:HB3	2.20	0.41
1:A:364:HIS:NE2	1:A:455:VAL:HB	2.35	0.41
1:B:317:ARG:HB2	1:B:344:ILE:HD11	2.03	0.41
1:B:201:THR:O	1:B:205:LEU:HB2	2.20	0.41
1:D:496:LEU:HD23	1:D:496:LEU:C	2.41	0.41
1:D:253:ARG:O	1:D:254:PHE:HB3	2.21	0.41
1:D:431:ASN:ND2	1:D:467:ASN:ND2	2.67	0.41
1:A:242:LEU:O	1:A:243:ARG:C	2.59	0.41
1:C:269:SER:OG	1:C:297:VAL:HG11	2.20	0.41
1:A:392:PRO:O	1:A:393:VAL:C	2.59	0.41
1:B:223:ALA:HA	1:B:337:CYS:O	2.21	0.41
1:D:314:GLN:HA	1:D:315:PRO:HD3	1.89	0.41
1:C:230:ARG:CG	1:C:253:ARG:HA	2.45	0.41
1:A:412:ILE:HG12	1:A:420:PHE:HE2	1.85	0.41
1:C:219:THR:HA	1:C:341:ALA:O	2.21	0.41
1:C:302:ARG:HA	1:C:303:GLY:HA3	1.83	0.41
1:C:381:LEU:HD23	1:C:435:VAL:HG11	2.03	0.41
1:C:388:LEU:CD2	1:C:396:PHE:CZ	3.04	0.41
1:C:472:THR:HA	1:C:473:PRO:HD3	1.85	0.41
1:D:224:VAL:HG22	1:D:337:CYS:CB	2.51	0.41
1:B:422:HIS:O	1:B:422:HIS:CG	2.72	0.41
1:C:221:SER:O	1:C:234:ILE:HG13	2.20	0.40
1:C:208:ILE:HD12	1:C:209:THR:H	1.85	0.40
1:C:226:PHE:HA	1:C:227:LEU:HA	1.48	0.40
1:C:227:LEU:HD11	1:C:267:TYR:CE1	2.55	0.40
1:D:220:PHE:CD2	1:D:220:PHE:C	2.93	0.40
1:D:223:ALA:HA	1:D:337:CYS:O	2.21	0.40
1:A:300:ARG:HA	1:A:314:GLN:O	2.22	0.40
1:B:300:ARG:HA	1:B:314:GLN:O	2.21	0.40
1:B:368:CYS:O	1:B:369:LEU:HD23	2.21	0.40
1:D:314:GLN:HE21	1:D:343:ARG:NH2	2.19	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	266/320 (83%)	239 (90%)	21 (8%)	6 (2%)	6 10
1	B	269/320 (84%)	239 (89%)	20 (7%)	10 (4%)	3 4
1	C	254/320 (79%)	216 (85%)	31 (12%)	7 (3%)	5 7
1	D	234/320 (73%)	210 (90%)	21 (9%)	3 (1%)	12 21
All	All	1023/1280 (80%)	904 (88%)	93 (9%)	26 (2%)	5 9

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	VAL
1	B	311	PRO
1	B	418	GLN
1	B	501	VAL
1	C	250	ARG
1	C	474	PRO
1	A	416	ALA
1	B	248	VAL
1	B	312	ARG
1	C	206	GLU
1	C	210	SER
1	C	228	THR
1	D	234	ILE
1	D	243	ARG
1	A	295	LYS
1	B	278	TRP
1	A	210	SER
1	B	351	PRO
1	B	415	LEU
1	C	229	GLY
1	A	248	VAL
1	C	486	ILE

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Mol	Chain	Res	Type
1	B	272	PRO
1	D	424	PRO
1	A	351	PRO
1	B	424	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	217/277 (78%)	199 (92%)	18 (8%)	11 20
1	B	214/277 (77%)	200 (94%)	14 (6%)	17 30
1	C	209/277 (76%)	183 (88%)	26 (12%)	4 7
1	D	184/277 (66%)	163 (89%)	21 (11%)	5 9
All	All	824/1108 (74%)	745 (90%)	79 (10%)	8 14

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	MET
1	A	199	THR
1	A	201	THR
1	A	202	LEU
1	A	205	LEU
1	A	213	THR
1	A	219	THR
1	A	224	VAL
1	A	227	LEU
1	A	265	VAL
1	A	325	ILE
1	A	327	VAL
1	A	342	GLU
1	A	356	ASP
1	A	367	SER
1	A	404	LEU
1	A	425	ILE

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Mol	Chain	Res	Type
1	A	501	VAL
1	B	197	MET
1	B	208	ILE
1	B	219	THR
1	B	222	VAL
1	B	242	LEU
1	B	249	PHE
1	B	261	GLN
1	B	296	SER
1	B	325	ILE
1	B	356	ASP
1	B	470	VAL
1	B	492	GLN
1	B	496	LEU
1	B	501	VAL
1	C	207	HIS
1	C	213	THR
1	C	219	THR
1	C	222	VAL
1	C	226	PHE
1	C	227	LEU
1	C	230	ARG
1	C	231	ILE
1	C	246	ARG
1	C	247	ASP
1	C	250	ARG
1	C	253	ARG
1	C	261	GLN
1	C	265	VAL
1	C	277	THR
1	C	314	GLN
1	C	319	THR
1	C	339	LEU
1	C	356	ASP
1	C	367	SER
1	C	414	GLN
1	C	422	HIS
1	C	450	ARG
1	C	451	LYS
1	C	454	PHE
1	C	485	ASP
1	D	222	VAL

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Mol	Chain	Res	Type
1	D	224	VAL
1	D	242	LEU
1	D	255	SER
1	D	261	GLN
1	D	265	VAL
1	D	270	THR
1	D	277	THR
1	D	343	ARG
1	D	346	SER
1	D	367	SER
1	D	374	ASP
1	D	415	LEU
1	D	433	GLU
1	D	435	VAL
1	D	450	ARG
1	D	451	LYS
1	D	454	PHE
1	D	485	ASP
1	D	494	HIS
1	D	501	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	HIS
1	B	237	GLN
1	B	409	HIS
1	C	386	GLN
1	C	398	HIS
1	D	409	HIS
1	D	422	HIS
1	D	467	ASN

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	276/320 (86%)	-0.24	1 (0%) 92 95	33, 60, 106, 131	0
1	B	279/320 (87%)	-0.28	0 100 100	32, 59, 107, 160	0
1	C	264/320 (82%)	-0.13	1 (0%) 92 95	37, 69, 122, 159	0
1	D	246/320 (76%)	-0.14	1 (0%) 92 95	34, 67, 108, 124	0
All	All	1065/1280 (83%)	-0.20	3 (0%) 94 96	32, 64, 114, 160	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	464	ALA	4.3
1	C	233	TYR	3.3
1	A	501	VAL	2.9

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.