



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:47 AM UTC

PDB ID : 3A2F / pdb_00003a2f
Title : Crystal Structure of Pyrococcus furiosus DNA polymerase/PCNA monomer mutant complex
Authors : Nishida, H.; Ishino, Y.; Morikawa, K.
Deposited on : 2009-05-15
Resolution : 2.67 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

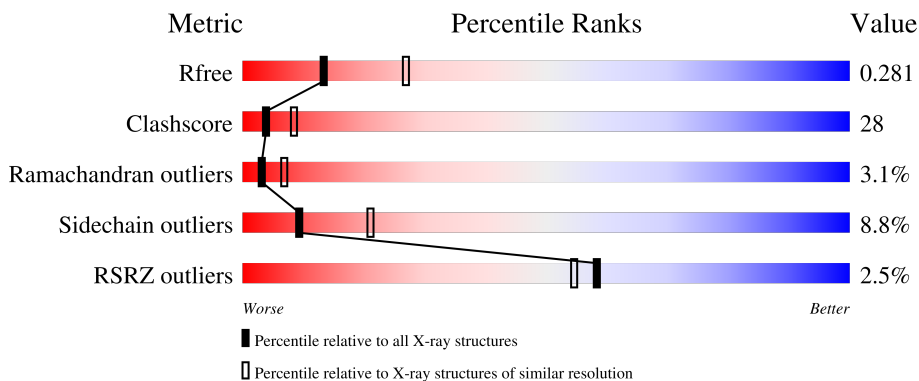
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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 $\leq 5\%$. 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	775	 3% 49% 42% 7%
2	B	248	 % 58% 35% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8254 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 DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	773	6204	4016	1029	1145	4	10	0	0	0

- Molecule 2 is a protein called DNA polymerase sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	B	247	1924	1234	306	376	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	LEU	MET	engineered mutation	UNP O73947
B	143	ALA	ASP	engineered mutation	UNP O73947
B	147	ALA	ASP	engineered mutation	UNP O73947

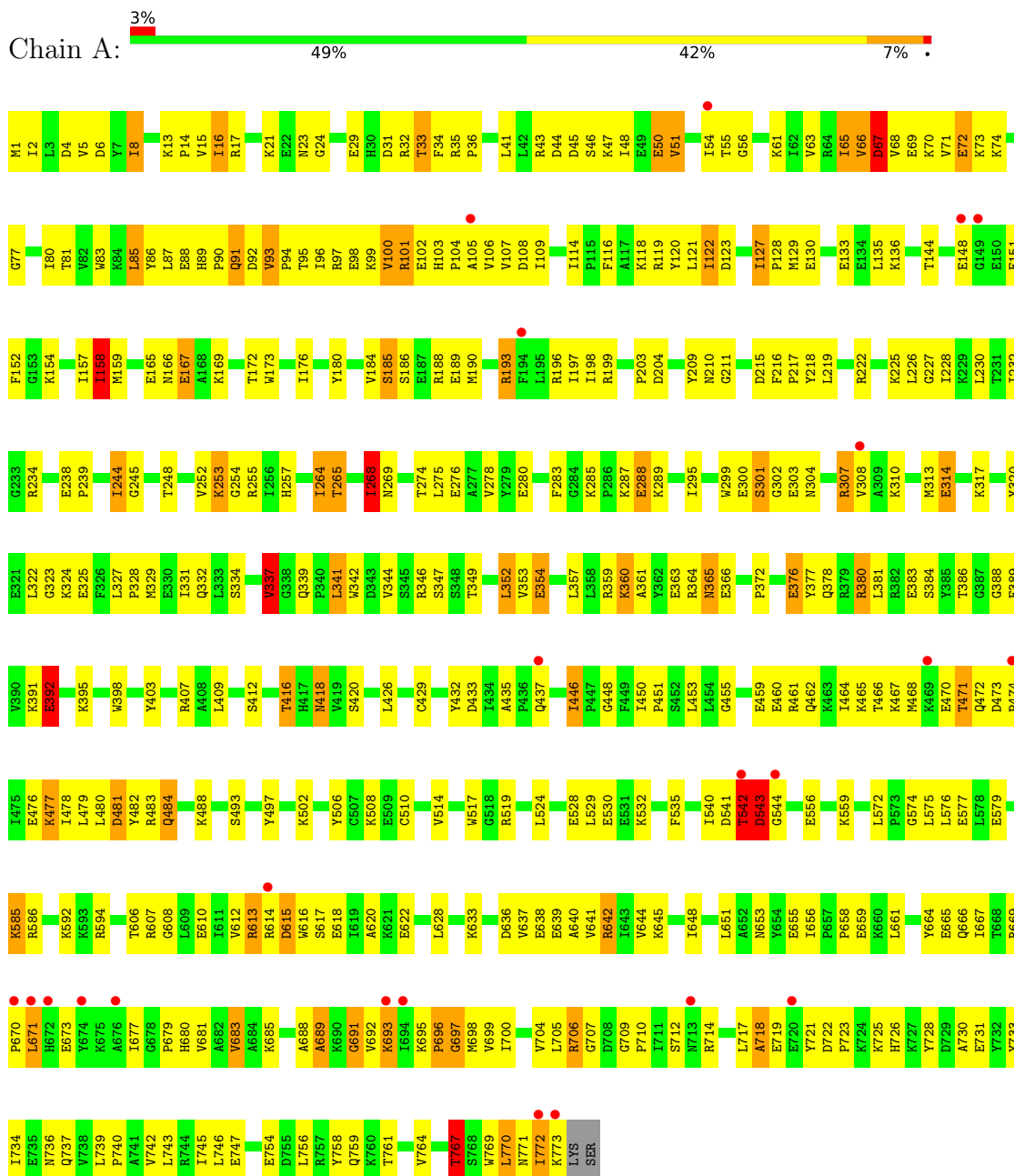
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	24	Total 24	O 24	0	0

3 Residue-property plots i

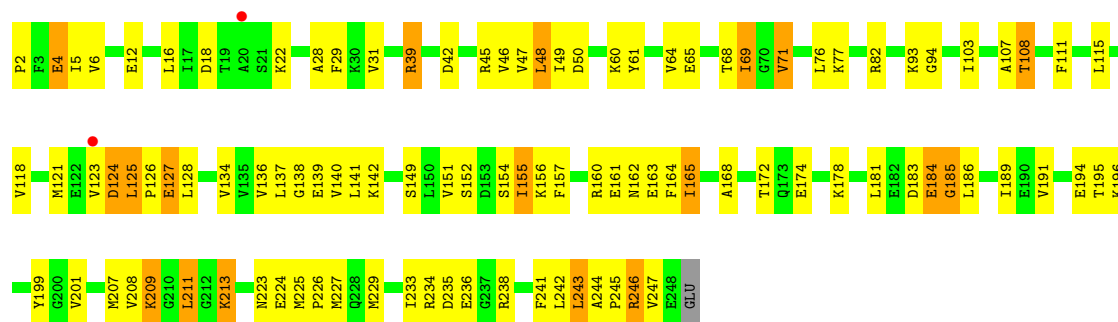
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA polymerase



- Molecule 2: DNA polymerase sliding clamp

Chain B:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.35Å 90.45Å 186.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.67 46.55 – 2.67	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.55-2.67) 99.0 (46.55-2.67)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.241 , 0.284 0.237 , 0.281	Depositor DCC
R_{free} test set	1867 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8254	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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	2/6338 (0.0%)	1.00	29/8566 (0.3%)
2	B	0.51	0/1942	0.97	6/2606 (0.2%)
All	All	0.48	2/8280 (0.0%)	1.00	35/11172 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	540	ILE	CA-C	-5.42	1.46	1.52
1	A	93	VAL	CA-CB	5.08	1.57	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ARG	N-CA-C	-10.38	97.14	110.53
1	A	127	ILE	CA-C-N	8.46	128.50	119.78
1	A	127	ILE	C-N-CA	8.46	128.50	119.78
1	A	543	ASP	CA-CB-CG	8.10	120.70	112.60
1	A	481	ASP	N-CA-C	-8.08	102.44	111.82
2	B	125	LEU	CA-C-N	7.04	126.96	119.85
2	B	125	LEU	C-N-CA	7.04	126.96	119.85
1	A	543	ASP	CB-CA-C	-7.04	95.52	109.67
2	B	185	GLY	N-CA-C	-6.81	97.03	113.18
1	A	433	ASP	N-CA-C	-6.76	98.38	109.40
1	A	185	SER	N-CA-C	6.49	118.02	111.07
1	A	158	ILE	N-CA-C	6.44	117.19	110.62
1	A	337	VAL	N-CA-C	-6.32	96.19	109.34
1	A	636	ASP	N-CA-C	6.17	118.82	108.02
1	A	114	ILE	N-CA-C	6.16	113.65	107.55
1	A	683	VAL	N-CA-C	-6.12	104.75	113.07
1	A	360	LYS	N-CA-C	-5.98	105.48	112.89
1	A	572	LEU	CA-C-N	5.95	126.45	120.14
1	A	572	LEU	C-N-CA	5.95	126.45	120.14
1	A	435	ALA	CA-C-N	5.86	127.16	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ALA	C-N-CA	5.86	127.16	119.84
1	A	426	LEU	N-CA-C	-5.85	103.22	110.41
1	A	35	ARG	CA-C-N	5.68	125.64	119.78
1	A	35	ARG	C-N-CA	5.68	125.64	119.78
2	B	246	ARG	N-CA-C	-5.50	98.25	107.99
1	A	388	GLY	N-CA-C	5.39	118.58	111.03
1	A	689	ALA	N-CA-C	-5.36	105.33	111.07
1	A	392	GLU	N-CA-C	-5.35	102.11	109.71
1	A	409	LEU	N-CA-C	5.28	117.46	111.02
2	B	243	LEU	N-CA-C	5.27	117.11	108.52
1	A	253	LYS	N-CA-C	5.20	121.87	110.80
1	A	677	ILE	N-CA-C	5.15	114.61	106.32
2	B	174	GLU	N-CA-C	5.11	116.06	108.86
1	A	767	THR	N-CA-C	5.03	121.52	110.80
1	A	386	THR	N-CA-C	5.03	117.17	110.53

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	6204	0	6122	369	0
2	B	1924	0	1967	100	0
3	A	102	0	0	6	0
3	B	24	0	0	2	0
All	All	8254	0	8089	461	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 28.

All (461) 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:541:ASP:OD1	1:A:542:THR:CG2	1.83	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ASP:OD1	1:A:542:THR:HG22	1.47	1.13
1:A:541:ASP:OD1	1:A:542:THR:HG23	1.53	1.05
1:A:188:ARG:HG3	1:A:228:ILE:HD11	1.41	1.01
1:A:2:ILE:HG23	1:A:128:PRO:HA	1.45	0.98
1:A:461:ARG:HH21	1:A:484:GLN:HE22	0.96	0.93
1:A:722:ASP:H	1:A:726:HIS:CD2	1.87	0.93
1:A:612:VAL:HG23	1:A:613:ARG:H	1.34	0.91
1:A:617:SER:H	1:A:737:GLN:NE2	1.69	0.91
1:A:418:ASN:ND2	1:A:448:GLY:H	1.70	0.89
2:B:213:LYS:HE3	2:B:213:LYS:N	1.89	0.88
1:A:418:ASN:HD21	1:A:448:GLY:N	1.72	0.88
1:A:461:ARG:NH2	1:A:484:GLN:HE22	1.71	0.87
1:A:541:ASP:OD1	1:A:542:THR:N	2.08	0.87
1:A:418:ASN:HD21	1:A:448:GLY:H	0.87	0.86
1:A:5:VAL:HG21	1:A:121:LEU:HD21	1.58	0.85
1:A:8:ILE:HD13	1:A:8:ILE:H	1.42	0.84
1:A:707:GLY:HA3	1:A:714:ARG:HD2	1.59	0.83
1:A:1:MSE:HE1	1:A:135:LEU:HD11	1.60	0.82
1:A:722:ASP:H	1:A:726:HIS:HD2	1.25	0.82
2:B:69:ILE:HD13	2:B:69:ILE:H	1.43	0.82
1:A:644:VAL:HG21	1:A:742:VAL:HG11	1.61	0.82
1:A:617:SER:H	1:A:737:GLN:HE21	1.25	0.81
2:B:207:MSE:HE1	2:B:227:MSE:HE1	1.61	0.81
1:A:461:ARG:HE	1:A:484:GLN:NE2	1.79	0.80
1:A:198:ILE:HD11	1:A:232:ILE:HA	1.63	0.80
1:A:692:VAL:HG12	1:A:693:LYS:H	1.46	0.80
1:A:461:ARG:HE	1:A:484:GLN:HE21	1.30	0.79
1:A:264:ILE:HD13	1:A:278:VAL:HG11	1.65	0.78
1:A:222:ARG:NH2	1:A:225:LYS:HD3	1.98	0.78
2:B:18:ASP:HA	2:B:77:LYS:HD3	1.65	0.77
1:A:412:SER:O	1:A:416:THR:HG23	1.84	0.77
1:A:90:PRO:O	1:A:93:VAL:HG12	1.84	0.76
1:A:301:SER:O	1:A:303:GLU:N	2.18	0.76
1:A:51:VAL:O	1:A:54:ILE:HD13	1.84	0.76
1:A:446:ILE:HD13	1:A:446:ILE:H	1.49	0.76
2:B:155:ILE:HD13	2:B:156:LYS:N	2.00	0.76
1:A:323:GLY:O	1:A:327:LEU:HB2	1.88	0.73
1:A:157:ILE:O	1:A:190:MSE:HE1	1.90	0.72
1:A:101:ARG:HA	1:A:106:VAL:HG21	1.71	0.71
1:A:93:VAL:CG1	1:A:94:PRO:HD3	2.20	0.71
1:A:91:GLN:O	1:A:94:PRO:HD2	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LEU:H	1:A:671:LEU:HD23	1.55	0.71
1:A:295:ILE:HG12	1:A:308:VAL:HG13	1.73	0.70
1:A:628:LEU:HD13	1:A:745:ILE:HD13	1.72	0.70
1:A:193:ARG:HD2	1:A:197:ILE:HD11	1.75	0.69
1:A:472:GLN:O	1:A:474:PRO:HD3	1.93	0.69
1:A:93:VAL:O	1:A:97:ARG:HG3	1.93	0.69
1:A:671:LEU:H	1:A:671:LEU:CD2	2.06	0.69
2:B:207:MSE:HE1	2:B:227:MSE:CE	2.23	0.68
1:A:151:GLU:HB3	1:A:154:LYS:HB2	1.76	0.68
1:A:288:GLU:CD	1:A:288:GLU:H	2.02	0.68
1:A:651:LEU:CD2	1:A:656:ILE:HD12	2.24	0.67
1:A:344:VAL:HG13	1:A:352:LEU:HD11	1.76	0.67
1:A:196:ARG:CD	1:A:199:ARG:HH21	2.07	0.67
1:A:658:PRO:HB3	1:A:721:TYR:CE2	2.30	0.67
1:A:541:ASP:CG	1:A:542:THR:HG23	2.19	0.66
2:B:5:ILE:HD12	2:B:61:TYR:CD1	2.31	0.66
1:A:620:ALA:HB2	1:A:737:GLN:HG3	1.77	0.66
1:A:165:GLU:HA	1:A:320:TYR:OH	1.96	0.66
1:A:467:LYS:NZ	1:A:471:THR:HG21	2.10	0.66
1:A:680:HIS:CE1	1:A:681:VAL:HG23	2.31	0.66
1:A:689:ALA:C	1:A:691:GLY:H	2.03	0.66
2:B:196:LYS:O	2:B:223:ASN:HA	1.96	0.66
1:A:392:GLU:HG2	1:A:592:LYS:NZ	2.10	0.66
1:A:1:MSE:HE3	1:A:129:MSE:SE	2.45	0.66
1:A:193:ARG:HD2	1:A:197:ILE:CD1	2.25	0.66
1:A:93:VAL:HG12	1:A:94:PRO:HD3	1.78	0.65
1:A:234:ARG:HB2	1:A:254:GLY:HA3	1.77	0.65
1:A:16:ILE:HD13	1:A:120:TYR:CG	2.31	0.65
1:A:664:TYR:O	1:A:665:GLU:HG3	1.96	0.65
2:B:196:LYS:H	2:B:223:ASN:ND2	1.95	0.65
1:A:74:LYS:HA	1:A:80:ILE:HG22	1.77	0.65
1:A:651:LEU:HD23	1:A:656:ILE:HD12	1.79	0.64
2:B:234:ARG:HG3	2:B:234:ARG:HH11	1.62	0.64
1:A:706:ARG:HG2	2:B:172:THR:HG23	1.80	0.63
1:A:706:ARG:HH22	1:A:730:ALA:HB3	1.63	0.63
2:B:5:ILE:HD12	2:B:61:TYR:CE1	2.34	0.63
1:A:244:ILE:HD13	1:A:245:GLY:N	2.14	0.63
1:A:666:GLN:HA	1:A:699:VAL:HA	1.79	0.63
1:A:1:MSE:CE	1:A:135:LEU:HD21	2.29	0.63
2:B:69:ILE:HB	2:B:115:LEU:HD22	1.81	0.63
1:A:198:ILE:CD1	1:A:232:ILE:HA	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD13	1:A:120:TYR:CD1	2.35	0.62
1:A:642:ARG:HG2	1:A:642:ARG:HH11	1.65	0.62
1:A:118:LYS:HD2	1:A:339:GLN:OE1	2.00	0.62
1:A:15:VAL:HG13	1:A:32:ARG:HG2	1.82	0.62
2:B:138:GLY:O	2:B:142:LYS:HG3	2.00	0.61
2:B:229:MSE:HE2	2:B:241:PHE:CD1	2.34	0.61
1:A:372:PRO:HB2	1:A:376:GLU:HB3	1.81	0.61
1:A:719:GLU:C	1:A:721:TYR:H	2.07	0.61
2:B:163:GLU:HG2	2:B:165:ILE:HD11	1.82	0.61
1:A:717:LEU:C	1:A:719:GLU:H	2.09	0.61
1:A:692:VAL:HG12	1:A:693:LYS:N	2.13	0.61
2:B:28:ALA:HB2	2:B:118:VAL:CG2	2.32	0.60
1:A:585:LYS:HE3	1:A:585:LYS:HA	1.82	0.60
1:A:606:THR:HG21	1:A:610:GLU:HG3	1.82	0.60
1:A:616:TRP:HA	1:A:737:GLN:HE22	1.67	0.60
2:B:22:LYS:HE3	2:B:209:LYS:HG2	1.82	0.60
1:A:127:ILE:HG12	1:A:130:GLU:OE2	2.01	0.60
1:A:407:ARG:HD2	1:A:579:GLU:OE1	2.01	0.60
1:A:303:GLU:O	1:A:304:ASN:HB2	2.01	0.60
1:A:136:LYS:HB2	1:A:203:PRO:HA	1.84	0.60
1:A:653:ASN:O	1:A:655:GLU:HG3	2.02	0.59
1:A:72:GLU:HG3	1:A:81:THR:HG22	1.84	0.59
1:A:594:ARG:HG2	1:A:608:GLY:O	2.01	0.59
2:B:28:ALA:HB2	2:B:118:VAL:HG21	1.83	0.59
2:B:238:ARG:HD2	3:B:1065:HOH:O	2.01	0.59
1:A:717:LEU:HD12	1:A:718:ALA:H	1.67	0.59
1:A:407:ARG:HH22	1:A:465:LYS:NZ	1.99	0.59
1:A:541:ASP:OD1	1:A:541:ASP:C	2.43	0.59
1:A:274:THR:O	1:A:278:VAL:HG23	2.02	0.59
1:A:66:VAL:O	1:A:67:ASP:HB2	2.02	0.59
1:A:158:ILE:CG2	1:A:159:MSE:HG3	2.32	0.59
2:B:163:GLU:H	2:B:189:ILE:HD13	1.68	0.58
1:A:301:SER:C	1:A:303:GLU:H	2.11	0.58
1:A:377:TYR:O	1:A:381:LEU:HG	2.04	0.58
1:A:679:PRO:O	1:A:683:VAL:HG23	2.03	0.58
1:A:159:MSE:HE1	1:A:308:VAL:HG12	1.85	0.58
1:A:119:ARG:HD2	1:A:123:ASP:OD2	2.05	0.57
1:A:767:THR:HA	1:A:770:LEU:HD22	1.86	0.57
1:A:706:ARG:NH2	1:A:730:ALA:H	2.03	0.57
1:A:377:TYR:CE1	1:A:502:LYS:HG2	2.40	0.56
2:B:155:ILE:HD12	2:B:157:PHE:CE1	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:LEU:O	1:A:747:GLU:HB2	2.05	0.56
2:B:12:GLU:HG2	2:B:233:ILE:HD11	1.87	0.56
1:A:129:MSE:HE2	1:A:341:LEU:HD12	1.86	0.56
1:A:148:GLU:OE2	1:A:148:GLU:HA	2.06	0.56
1:A:392:GLU:HG2	1:A:592:LYS:HZ1	1.68	0.56
2:B:164:PHE:C	2:B:165:ILE:HD13	2.30	0.56
2:B:234:ARG:HG3	2:B:234:ARG:NH1	2.21	0.56
1:A:48:ILE:HA	1:A:51:VAL:HG12	1.86	0.56
1:A:332:GLN:OE1	1:A:483:ARG:HG2	2.06	0.56
2:B:183:ASP:C	2:B:185:GLY:H	2.14	0.56
1:A:222:ARG:HH21	1:A:225:LYS:HD3	1.70	0.55
1:A:709:GLY:O	1:A:714:ARG:HD3	2.06	0.55
1:A:54:ILE:HD12	1:A:54:ILE:H	1.72	0.55
1:A:77:GLY:N	1:A:366:GLU:OE1	2.39	0.55
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.71	0.55
1:A:733:TYR:O	1:A:737:GLN:HB3	2.06	0.55
2:B:229:MSE:HE2	2:B:241:PHE:HD1	1.71	0.55
2:B:69:ILE:HD13	2:B:69:ILE:N	2.17	0.55
1:A:476:GLU:C	1:A:478:ILE:H	2.12	0.55
1:A:43:ARG:HB3	1:A:43:ARG:NH1	2.21	0.55
2:B:134:VAL:HG12	2:B:136:VAL:HG13	1.87	0.55
1:A:324:LYS:O	1:A:328:PRO:HD3	2.06	0.54
2:B:195:THR:HA	2:B:223:ASN:HD21	1.72	0.54
1:A:13:LYS:NZ	1:A:88:GLU:OE1	2.39	0.54
1:A:48:ILE:HA	1:A:51:VAL:CG1	2.37	0.54
1:A:99:LYS:O	1:A:101:ARG:N	2.40	0.54
1:A:541:ASP:O	1:A:542:THR:C	2.49	0.54
1:A:96:ILE:HD12	1:A:96:ILE:C	2.33	0.54
1:A:99:LYS:O	1:A:102:GLU:N	2.41	0.54
1:A:166:ASN:HA	3:A:1073:HOH:O	2.08	0.54
1:A:307:ARG:HH11	1:A:307:ARG:HB3	1.73	0.54
1:A:86:TYR:O	1:A:87:LEU:HD23	2.08	0.54
1:A:467:LYS:HG2	1:A:467:LYS:O	2.07	0.54
1:A:429:CYS:HB2	1:A:432:TYR:CZ	2.43	0.54
1:A:1:MSE:HE1	1:A:135:LEU:HD21	1.90	0.54
1:A:455:GLY:O	1:A:459:GLU:HG3	2.08	0.54
1:A:467:LYS:HZ3	1:A:471:THR:HG21	1.72	0.54
1:A:21:LYS:O	1:A:133:GLU:HG3	2.07	0.54
2:B:4:GLU:HG2	2:B:60:LYS:HE2	1.90	0.54
1:A:257:HIS:O	1:A:346:ARG:NH2	2.37	0.53
2:B:39:ARG:HD3	2:B:50:ASP:OD1	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:TYR:OH	1:A:324:LYS:HD3	2.08	0.53
2:B:6:VAL:HB	2:B:60:LYS:HB3	1.90	0.53
1:A:14:PRO:HG2	1:A:90:PRO:HD3	1.90	0.53
1:A:188:ARG:CG	1:A:228:ILE:HD11	2.28	0.53
1:A:461:ARG:NE	1:A:484:GLN:NE2	2.54	0.53
1:A:389:PHE:O	1:A:542:THR:N	2.42	0.53
1:A:754:GLU:H	1:A:754:GLU:CD	2.17	0.53
1:A:93:VAL:HG13	1:A:94:PRO:HD3	1.91	0.52
1:A:659:GLU:C	1:A:661:LEU:H	2.15	0.52
2:B:142:LYS:HD2	2:B:211:LEU:O	2.10	0.52
2:B:213:LYS:HE3	2:B:213:LYS:H	1.69	0.52
1:A:648:ILE:HD12	1:A:734:ILE:HG23	1.92	0.52
1:A:671:LEU:HD23	1:A:671:LEU:N	2.24	0.52
1:A:1:MSE:HE1	1:A:135:LEU:CD1	2.35	0.52
1:A:349:THR:O	1:A:353:VAL:HG23	2.10	0.52
2:B:69:ILE:O	2:B:69:ILE:HG12	2.10	0.52
1:A:73:LYS:HD2	1:A:365:ASN:ND2	2.24	0.52
1:A:119:ARG:HD2	1:A:123:ASP:CG	2.34	0.52
1:A:196:ARG:HD3	1:A:199:ARG:HH21	1.73	0.52
2:B:29:PHE:O	2:B:68:THR:HA	2.10	0.52
1:A:44:ASP:C	1:A:46:SER:H	2.17	0.52
2:B:199:TYR:CZ	2:B:227:MSE:HB2	2.45	0.52
1:A:378:GLN:HG3	3:A:1035:HOH:O	2.10	0.52
1:A:761:THR:HB	2:B:246:ARG:HB3	1.92	0.52
1:A:14:PRO:CG	1:A:90:PRO:HD3	2.40	0.51
2:B:163:GLU:H	2:B:189:ILE:CD1	2.22	0.51
1:A:460:GLU:O	1:A:464:ILE:HG12	2.10	0.51
1:A:479:LEU:O	1:A:479:LEU:HD23	2.10	0.51
1:A:707:GLY:CA	1:A:714:ARG:HD2	2.34	0.51
1:A:416:THR:HB	1:A:574:GLY:HA3	1.93	0.51
2:B:233:ILE:HG23	2:B:233:ILE:O	2.11	0.51
1:A:320:TYR:CZ	1:A:324:LYS:HD3	2.46	0.51
1:A:628:LEU:HD13	1:A:745:ILE:CD1	2.38	0.51
1:A:446:ILE:HD13	1:A:446:ILE:N	2.22	0.51
1:A:476:GLU:C	1:A:478:ILE:N	2.67	0.51
1:A:612:VAL:HG23	1:A:613:ARG:N	2.15	0.51
1:A:157:ILE:HG13	1:A:222:ARG:HG3	1.92	0.51
1:A:395:LYS:N	1:A:395:LYS:HD2	2.26	0.51
1:A:464:ILE:HG21	1:A:484:GLN:HB3	1.92	0.51
1:A:23:ASN:H	1:A:133:GLU:CD	2.18	0.51
1:A:96:ILE:O	1:A:100:VAL:HG23	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:O	1:A:331:ILE:HG13	2.11	0.51
1:A:612:VAL:CG2	1:A:613:ARG:H	2.14	0.51
1:A:287:LYS:HE3	3:A:1012:HOH:O	2.09	0.51
1:A:594:ARG:HA	1:A:607:ARG:O	2.11	0.51
1:A:728:TYR:CD1	1:A:728:TYR:C	2.89	0.51
1:A:288:GLU:OE1	1:A:288:GLU:N	2.45	0.50
1:A:416:THR:CG2	1:A:575:LEU:H	2.24	0.50
1:A:771:ASN:C	1:A:773:LYS:H	2.18	0.50
2:B:93:LYS:HD3	2:B:94:GLY:N	2.25	0.50
2:B:107:ALA:O	2:B:108:THR:C	2.55	0.50
2:B:140:VAL:HG23	2:B:141:LEU:N	2.26	0.50
1:A:2:ILE:HD11	1:A:4:ASP:O	2.11	0.50
1:A:36:PRO:HG3	1:A:116:PHE:CE1	2.47	0.50
1:A:85:LEU:N	1:A:85:LEU:HD23	2.27	0.50
1:A:158:ILE:HG23	1:A:159:MSE:HG3	1.92	0.50
1:A:420:SER:HB2	1:A:451:PRO:HD3	1.94	0.50
1:A:66:VAL:O	1:A:67:ASP:CB	2.59	0.50
2:B:155:ILE:HD12	2:B:157:PHE:HE1	1.76	0.50
1:A:211:GLY:HA2	1:A:215:ASP:HB2	1.93	0.50
1:A:530:GLU:HG2	1:A:535:PHE:O	2.12	0.50
1:A:89:HIS:HB3	1:A:92:ASP:OD1	2.12	0.50
2:B:68:THR:HG23	2:B:68:THR:O	2.12	0.50
1:A:6:ASP:OD2	1:A:6:ASP:C	2.54	0.49
1:A:342:TRP:CD1	1:A:346:ARG:NH2	2.80	0.49
1:A:704:VAL:C	1:A:705:LEU:HD12	2.37	0.49
1:A:689:ALA:C	1:A:691:GLY:N	2.67	0.49
1:A:384:SER:O	1:A:508:LYS:HE3	2.13	0.49
2:B:196:LYS:H	2:B:223:ASN:HD22	1.60	0.49
1:A:73:LYS:HD2	1:A:365:ASN:HD21	1.78	0.49
1:A:310:LYS:O	1:A:314:GLU:HB2	2.13	0.49
2:B:47:VAL:HG22	2:B:243:LEU:CD1	2.43	0.49
1:A:69:GLU:O	1:A:69:GLU:HG3	2.11	0.49
1:A:347:SER:HB2	1:A:352:LEU:HD13	1.93	0.49
1:A:420:SER:HB2	1:A:451:PRO:CD	2.43	0.49
1:A:722:ASP:N	1:A:726:HIS:HD2	2.02	0.49
2:B:183:ASP:O	2:B:185:GLY:N	2.45	0.49
1:A:8:ILE:H	1:A:8:ILE:CD1	2.21	0.49
1:A:54:ILE:HD12	1:A:54:ILE:N	2.27	0.49
1:A:276:GLU:HG2	1:A:289:LYS:HB2	1.93	0.49
1:A:44:ASP:O	1:A:46:SER:N	2.41	0.48
1:A:158:ILE:HG22	1:A:159:MSE:HG3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:PHE:N	2:B:111:PHE:CD1	2.81	0.48
2:B:47:VAL:HG22	2:B:243:LEU:HD13	1.95	0.48
1:A:173:TRP:CD1	1:A:173:TRP:O	2.66	0.48
1:A:376:GLU:OE1	1:A:380:ARG:HD3	2.12	0.48
2:B:82:ARG:HH11	2:B:111:PHE:HE2	1.61	0.48
2:B:134:VAL:HG13	2:B:186:LEU:CD2	2.42	0.48
1:A:152:PHE:CE1	1:A:218:TYR:HD1	2.31	0.48
1:A:383:GLU:HG2	1:A:508:LYS:NZ	2.28	0.48
1:A:391:LYS:HG2	1:A:392:GLU:O	2.13	0.48
1:A:769:TRP:CE2	2:B:226:PRO:HD3	2.48	0.48
1:A:308:VAL:HG12	1:A:308:VAL:O	2.13	0.48
1:A:717:LEU:C	1:A:719:GLU:N	2.71	0.48
1:A:666:GLN:HB2	1:A:699:VAL:HG12	1.95	0.48
2:B:183:ASP:C	2:B:185:GLY:N	2.71	0.48
1:A:232:ILE:HG22	1:A:252:VAL:HG11	1.96	0.48
1:A:398:TRP:O	1:A:586:ARG:HG3	2.14	0.48
1:A:542:THR:OG1	1:A:543:ASP:N	2.47	0.48
1:A:719:GLU:C	1:A:721:TYR:N	2.72	0.48
2:B:65:GLU:OE2	2:B:65:GLU:HA	2.12	0.48
1:A:658:PRO:HG2	1:A:659:GLU:OE2	2.13	0.48
1:A:639:GLU:OE2	1:A:642:ARG:NH1	2.47	0.47
1:A:695:LYS:O	1:A:697:GLY:N	2.47	0.47
2:B:163:GLU:HG3	2:B:178:LYS:HE3	1.95	0.47
1:A:285:LYS:HG3	3:A:1027:HOH:O	2.12	0.47
1:A:380:ARG:HD2	1:A:506:TYR:CE2	2.49	0.47
1:A:772:ILE:HD12	2:B:124:ASP:OD1	2.14	0.47
2:B:224:GLU:OE1	2:B:247:VAL:HG23	2.14	0.47
1:A:717:LEU:O	1:A:719:GLU:N	2.47	0.47
2:B:137:LEU:HD12	2:B:185:GLY:HA2	1.95	0.47
1:A:166:ASN:O	1:A:167:GLU:HB2	2.14	0.47
2:B:155:ILE:HD13	2:B:155:ILE:C	2.39	0.47
2:B:234:ARG:O	2:B:235:ASP:HB2	2.15	0.47
1:A:616:TRP:HA	1:A:737:GLN:NE2	2.29	0.47
2:B:154:SER:HB2	2:B:246:ARG:HD3	1.96	0.47
1:A:93:VAL:HG13	1:A:94:PRO:CD	2.45	0.47
1:A:378:GLN:NE2	1:A:381:LEU:HD12	2.30	0.47
1:A:437:GLN:OE1	1:A:519:ARG:NH2	2.41	0.47
1:A:476:GLU:O	1:A:480:LEU:HG	2.14	0.47
1:A:477:LYS:HA	1:A:480:LEU:HD11	1.95	0.47
2:B:139:GLU:HG2	2:B:140:VAL:N	2.30	0.47
1:A:47:LYS:HA	1:A:50:GLU:OE2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LEU:HD12	2:B:126:PRO:HG2	1.97	0.47
1:A:127:ILE:HA	1:A:128:PRO:HD3	1.72	0.47
1:A:761:THR:OG1	2:B:246:ARG:NH1	2.47	0.47
2:B:195:THR:HA	2:B:223:ASN:ND2	2.30	0.46
1:A:412:SER:O	1:A:416:THR:CG2	2.61	0.46
1:A:383:GLU:HG2	1:A:508:LYS:HZ1	1.81	0.46
2:B:103:ILE:O	2:B:108:THR:HA	2.15	0.46
1:A:103:HIS:O	1:A:105:ALA:N	2.48	0.46
1:A:360:LYS:HG2	1:A:453:LEU:HD22	1.96	0.46
1:A:158:ILE:HG13	1:A:299:TRP:CD2	2.50	0.46
1:A:606:THR:HG21	1:A:610:GLU:CG	2.45	0.46
1:A:21:LYS:HE2	1:A:24:GLY:HA2	1.98	0.46
1:A:466:THR:C	1:A:468:MSE:H	2.22	0.46
1:A:232:ILE:HD12	1:A:239:PRO:CG	2.46	0.46
1:A:90:PRO:HG3	1:A:116:PHE:CD1	2.51	0.46
1:A:479:LEU:O	1:A:482:TYR:HB2	2.15	0.46
2:B:69:ILE:H	2:B:69:ILE:CD1	2.22	0.46
2:B:127:GLU:HA	2:B:127:GLU:OE1	2.16	0.46
1:A:248:THR:O	1:A:248:THR:HG23	2.16	0.45
1:A:32:ARG:NH1	3:A:1056:HOH:O	2.48	0.45
1:A:103:HIS:C	1:A:105:ALA:H	2.24	0.45
1:A:479:LEU:HD23	1:A:479:LEU:C	2.40	0.45
1:A:710:PRO:O	1:A:714:ARG:HG3	2.17	0.45
1:A:65:ILE:C	1:A:67:ASP:H	2.25	0.45
1:A:71:VAL:HG12	1:A:72:GLU:N	2.31	0.45
1:A:94:PRO:HA	1:A:97:ARG:NE	2.32	0.45
1:A:65:ILE:O	1:A:67:ASP:N	2.50	0.45
1:A:706:ARG:NH2	1:A:730:ALA:HB3	2.28	0.45
1:A:448:GLY:C	1:A:451:PRO:HD2	2.41	0.45
2:B:242:LEU:HD12	2:B:242:LEU:HA	1.75	0.45
1:A:618:GLU:O	1:A:622:GLU:HB2	2.16	0.45
1:A:100:VAL:O	1:A:106:VAL:HG21	2.17	0.45
1:A:614:ARG:C	1:A:616:TRP:H	2.25	0.45
1:A:651:LEU:HG	1:A:656:ILE:HD12	1.98	0.45
1:A:354:GLU:OE2	1:A:497:TYR:OH	2.35	0.45
1:A:376:GLU:O	1:A:380:ARG:HB2	2.17	0.45
1:A:359:ARG:O	1:A:363:GLU:HG3	2.16	0.45
1:A:461:ARG:NH2	1:A:488:LYS:HD2	2.32	0.45
1:A:641:VAL:O	1:A:645:LYS:HG3	2.17	0.45
2:B:69:ILE:N	2:B:69:ILE:CD1	2.80	0.45
1:A:473:ASP:O	1:A:476:GLU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:PHE:HB2	2:B:69:ILE:HD11	1.97	0.44
2:B:125:LEU:HA	2:B:126:PRO:HD3	1.75	0.44
1:A:31:ASP:OD2	1:A:33:THR:HG23	2.16	0.44
1:A:295:ILE:HG12	1:A:308:VAL:CG1	2.44	0.44
1:A:717:LEU:HD12	1:A:718:ALA:N	2.31	0.44
1:A:723:PRO:C	1:A:725:LYS:N	2.73	0.44
2:B:121:MSE:HG2	2:B:123:VAL:HG23	2.00	0.44
1:A:34:PHE:CZ	1:A:119:ARG:HG3	2.52	0.44
1:A:158:ILE:CG2	1:A:159:MSE:HE3	2.47	0.44
1:A:429:CYS:HB2	1:A:432:TYR:CE1	2.53	0.44
1:A:670:PRO:HD2	1:A:673:GLU:OE2	2.17	0.44
2:B:71:VAL:HG21	2:B:76:LEU:HD22	1.98	0.44
1:A:43:ARG:NH1	1:A:43:ARG:CB	2.80	0.44
1:A:185:SER:HB3	1:A:189:GLU:HG3	1.98	0.44
1:A:659:GLU:OE2	1:A:659:GLU:N	2.45	0.44
1:A:56:GLY:O	1:A:63:VAL:N	2.51	0.44
1:A:70:LYS:HB2	1:A:83:TRP:CH2	2.51	0.44
1:A:196:ARG:HD3	1:A:199:ARG:NH2	2.32	0.44
1:A:416:THR:HG21	1:A:575:LEU:H	1.82	0.44
1:A:669:ARG:HA	1:A:696:PRO:HB3	1.99	0.44
1:A:692:VAL:CG1	1:A:693:LYS:H	2.25	0.44
1:A:736:ASN:HB3	3:A:1028:HOH:O	2.18	0.44
1:A:108:ASP:OD2	1:A:109:ILE:N	2.50	0.44
1:A:334:SER:HA	1:A:344:VAL:HG21	1.99	0.44
1:A:196:ARG:NE	1:A:199:ARG:HH21	2.16	0.44
1:A:651:LEU:CG	1:A:656:ILE:HD12	2.48	0.44
2:B:207:MSE:HE3	2:B:241:PHE:CB	2.48	0.44
1:A:67:ASP:O	1:A:68:VAL:CG1	2.66	0.44
1:A:67:ASP:O	1:A:68:VAL:HG13	2.18	0.44
1:A:334:SER:O	1:A:337:VAL:O	2.35	0.44
1:A:403:TYR:CE1	1:A:544:GLY:HA3	2.53	0.44
2:B:151:VAL:HG23	2:B:152:SER:N	2.33	0.44
1:A:56:GLY:HA3	1:A:95:THR:HG22	2.00	0.44
1:A:48:ILE:O	1:A:51:VAL:HG12	2.18	0.43
1:A:169:LYS:HD3	1:A:180:TYR:O	2.17	0.43
1:A:268:ILE:HD12	1:A:269:ASN:N	2.33	0.43
1:A:317:LYS:HD2	1:A:317:LYS:HA	1.72	0.43
2:B:225:MSE:HE3	2:B:225:MSE:HB2	1.88	0.43
1:A:667:ILE:HD11	1:A:700:ILE:HD12	2.00	0.43
2:B:161:GLU:N	2:B:191:VAL:HG21	2.33	0.43
1:A:392:GLU:HG2	1:A:592:LYS:HZ2	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:C	1:A:616:TRP:N	2.75	0.43
1:A:5:VAL:CG2	1:A:121:LEU:HD21	2.40	0.43
1:A:89:HIS:CG	1:A:90:PRO:HD2	2.53	0.43
1:A:196:ARG:NH1	1:A:196:ARG:HG2	2.33	0.43
1:A:613:ARG:C	1:A:615:ASP:N	2.75	0.43
2:B:152:SER:HB3	2:B:168:ALA:HB1	2.00	0.43
1:A:51:VAL:HG23	1:A:103:HIS:ND1	2.33	0.43
1:A:322:LEU:O	1:A:325:GLU:HB3	2.19	0.43
1:A:466:THR:C	1:A:468:MSE:N	2.76	0.43
1:A:103:HIS:C	1:A:105:ALA:N	2.76	0.43
1:A:659:GLU:C	1:A:661:LEU:N	2.77	0.43
1:A:772:ILE:O	1:A:772:ILE:HG22	2.18	0.43
2:B:16:LEU:HD13	2:B:233:ILE:HD13	2.00	0.43
2:B:29:PHE:HB2	2:B:69:ILE:CD1	2.49	0.43
1:A:450:ILE:HB	1:A:451:PRO:HD3	2.00	0.43
1:A:637:VAL:O	1:A:640:ALA:HB3	2.19	0.43
1:A:739:LEU:HB2	1:A:740:PRO:HD3	2.00	0.43
2:B:227:MSE:HE2	2:B:243:LEU:HB3	2.01	0.43
1:A:43:ARG:CB	1:A:43:ARG:HH11	2.32	0.43
1:A:327:LEU:HD12	1:A:327:LEU:HA	1.90	0.43
2:B:160:ARG:CG	2:B:194:GLU:HG3	2.49	0.43
1:A:127:ILE:O	1:A:130:GLU:HB2	2.18	0.42
1:A:472:GLN:C	1:A:474:PRO:HD3	2.44	0.42
1:A:510:CYS:O	1:A:514:VAL:HG23	2.19	0.42
1:A:41:LEU:HD22	1:A:107:VAL:CG2	2.49	0.42
2:B:162:ASN:O	2:B:163:GLU:HB2	2.18	0.42
1:A:2:ILE:CG2	1:A:128:PRO:HA	2.33	0.42
1:A:234:ARG:HG3	1:A:255:ARG:CZ	2.50	0.42
1:A:8:ILE:HD13	1:A:8:ILE:N	2.22	0.42
1:A:127:ILE:O	1:A:127:ILE:HG13	2.19	0.42
1:A:468:MSE:C	1:A:470:GLU:H	2.28	0.42
1:A:481:ASP:O	1:A:484:GLN:HG3	2.19	0.42
1:A:5:VAL:HG21	1:A:121:LEU:CD2	2.41	0.42
1:A:172:THR:HG21	1:A:176:ILE:HD12	2.01	0.42
1:A:216:PHE:HB2	1:A:217:PRO:HD3	2.01	0.42
1:A:476:GLU:O	1:A:478:ILE:N	2.52	0.42
1:A:21:LYS:NZ	1:A:204:ASP:OD2	2.52	0.42
1:A:89:HIS:ND1	1:A:90:PRO:HD2	2.34	0.42
1:A:644:VAL:HG11	1:A:756:LEU:HD13	2.02	0.42
1:A:742:VAL:HG12	1:A:746:LEU:HD12	2.02	0.42
2:B:238:ARG:HD3	3:B:1079:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:HA	1:A:29:GLU:O	2.20	0.42
1:A:159:MSE:HG2	1:A:172:THR:HB	2.01	0.42
1:A:283:PHE:C	1:A:285:LYS:H	2.27	0.42
1:A:680:HIS:HB2	1:A:700:ILE:HB	2.00	0.42
2:B:186:LEU:HD13	2:B:186:LEU:C	2.45	0.42
1:A:357:LEU:O	1:A:361:ALA:N	2.52	0.42
1:A:188:ARG:NH2	1:A:227:GLY:O	2.53	0.42
1:A:706:ARG:O	1:A:706:ARG:HG3	2.19	0.42
1:A:54:ILE:H	1:A:54:ILE:CD1	2.33	0.41
1:A:196:ARG:HG2	1:A:196:ARG:HH11	1.84	0.41
1:A:209:TYR:O	1:A:210:ASN:HB3	2.19	0.41
2:B:82:ARG:NH1	2:B:111:PHE:HE2	2.18	0.41
1:A:54:ILE:HG22	1:A:55:THR:N	2.35	0.41
1:A:98:GLU:O	1:A:102:GLU:HG2	2.20	0.41
1:A:1:MSE:HE2	1:A:135:LEU:HD21	2.03	0.41
1:A:67:ASP:C	1:A:68:VAL:HG13	2.46	0.41
1:A:288:GLU:CD	1:A:288:GLU:N	2.75	0.41
2:B:160:ARG:HG2	2:B:194:GLU:HG3	2.02	0.41
1:A:389:PHE:CD2	1:A:389:PHE:C	2.99	0.41
1:A:529:LEU:O	1:A:535:PHE:HB2	2.20	0.41
1:A:244:ILE:HD13	1:A:244:ILE:C	2.45	0.41
1:A:528:GLU:HG2	1:A:532:LYS:HD2	2.03	0.41
1:A:613:ARG:HG3	1:A:615:ASP:HB2	2.03	0.41
2:B:48:LEU:HD23	2:B:49:ILE:N	2.35	0.41
1:A:93:VAL:CG1	1:A:94:PRO:CD	2.96	0.41
1:A:230:LEU:O	1:A:238:GLU:HA	2.20	0.41
1:A:644:VAL:CG2	1:A:742:VAL:HG11	2.42	0.41
1:A:767:THR:HB	2:B:45:ARG:NH2	2.35	0.41
1:A:770:LEU:HD12	2:B:126:PRO:CG	2.50	0.41
2:B:211:LEU:HD12	2:B:211:LEU:HA	1.95	0.41
2:B:226:PRO:HA	2:B:245:PRO:HD3	2.02	0.41
1:A:685:LYS:HA	1:A:688:ALA:CB	2.50	0.41
1:A:698:MSE:HE3	1:A:698:MSE:HB2	1.89	0.41
1:A:758:TYR:CG	1:A:759:GLN:N	2.88	0.41
1:A:48:ILE:HG12	1:A:83:TRP:CZ3	2.56	0.41
1:A:186:SER:H	1:A:189:GLU:HB2	1.86	0.41
1:A:541:ASP:O	1:A:543:ASP:N	2.53	0.41
1:A:51:VAL:O	1:A:54:ILE:CD1	2.64	0.41
1:A:122:ILE:HG23	1:A:359:ARG:HA	2.03	0.41
1:A:158:ILE:HG21	1:A:159:MSE:HE3	2.02	0.41
2:B:46:VAL:HG13	2:B:244:ALA:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:CE1	1:A:90:PRO:HD2	2.56	0.40
2:B:149:SER:CB	2:B:201:VAL:HG11	2.51	0.40
2:B:208:VAL:HA	2:B:211:LEU:HD22	2.02	0.40
1:A:255:ARG:HH11	1:A:255:ARG:HG2	1.87	0.40
1:A:671:LEU:HD12	1:A:685:LYS:CA	2.51	0.40
2:B:2:PRO:HB3	2:B:94:GLY:HA2	2.04	0.40
1:A:349:THR:HB	1:A:493:SER:OG	2.22	0.40
1:A:461:ARG:NH2	1:A:484:GLN:NE2	2.54	0.40
2:B:207:MSE:HE3	2:B:241:PHE:HB3	2.03	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	771/775 (100%)	667 (86%)	75 (10%)	29 (4%)	2 5
2	B	245/248 (99%)	227 (93%)	15 (6%)	3 (1%)	10 24
All	All	1016/1023 (99%)	894 (88%)	90 (9%)	32 (3%)	3 7

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	100	VAL
1	A	302	GLY
1	A	542	THR
1	A	693	LYS
1	A	45	ASP
1	A	61	LYS
1	A	167	GLU
1	A	613	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	691	GLY
1	A	696	PRO
1	A	718	ALA
1	A	767	THR
2	B	184	GLU
1	A	67	ASP
1	A	300	GLU
2	B	108	THR
1	A	253	LYS
1	A	265	THR
1	A	471	THR
1	A	615	ASP
2	B	64	VAL
1	A	104	PRO
1	A	477	LYS
1	A	697	GLY
1	A	706	ARG
1	A	712	SER
1	A	65	ILE
1	A	268	ILE
1	A	772	ILE
1	A	122	ILE
1	A	264	ILE

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	639/671 (95%)	582 (91%)	57 (9%)	9 21
2	B	211/208 (101%)	193 (92%)	18 (8%)	10 23
All	All	850/879 (97%)	775 (91%)	75 (9%)	9 21

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	16	ILE
1	A	33	THR
1	A	50	GLU
1	A	51	VAL
1	A	67	ASP
1	A	72	GLU
1	A	85	LEU
1	A	91	GLN
1	A	101	ARG
1	A	144	THR
1	A	158	ILE
1	A	184	VAL
1	A	193	ARG
1	A	219	LEU
1	A	226	LEU
1	A	244	ILE
1	A	265	THR
1	A	268	ILE
1	A	275	LEU
1	A	280	GLU
1	A	288	GLU
1	A	301	SER
1	A	307	ARG
1	A	313	MSE
1	A	314	GLU
1	A	329	MSE
1	A	337	VAL
1	A	341	LEU
1	A	352	LEU
1	A	354	GLU
1	A	365	ASN
1	A	376	GLU
1	A	380	ARG
1	A	392	GLU
1	A	416	THR
1	A	418	ASN
1	A	446	ILE
1	A	462	GLN
1	A	484	GLN
1	A	517	TRP
1	A	524	LEU
1	A	542	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	543	ASP
1	A	556	GLU
1	A	559	LYS
1	A	576	LEU
1	A	577	GLU
1	A	585	LYS
1	A	633	LYS
1	A	638	GLU
1	A	642	ARG
1	A	671	LEU
1	A	731	GLU
1	A	764	VAL
1	A	767	THR
1	A	770	LEU
2	B	4	GLU
2	B	31	VAL
2	B	39	ARG
2	B	42	ASP
2	B	48	LEU
2	B	69	ILE
2	B	71	VAL
2	B	124	ASP
2	B	127	GLU
2	B	128	LEU
2	B	155	ILE
2	B	165	ILE
2	B	181	LEU
2	B	184	GLU
2	B	209	LYS
2	B	211	LEU
2	B	213	LYS
2	B	236	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	91	GLN
1	A	147	HIS
1	A	365	ASN
1	A	378	GLN
1	A	400	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	418	ASN
1	A	431	ASN
1	A	440	HIS
1	A	462	GLN
1	A	484	GLN
1	A	492	ASN
1	A	649	GLN
1	A	666	GLN
1	A	726	HIS
1	A	736	ASN
1	A	737	GLN
1	A	759	GLN
2	B	173	GLN
2	B	192	GLN
2	B	223	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 oligosaccharides 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, 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	763/775 (98%)	0.25	23 (3%) 52 48	29, 63, 101, 109	0
2	B	239/248 (96%)	0.06	2 (0%) 82 81	38, 60, 83, 97	0
All	All	1002/1023 (97%)	0.20	25 (2%) 58 54	29, 62, 99, 109	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	773	LYS	4.2
1	A	772	ILE	3.4
1	A	149	GLY	3.1
1	A	542	THR	3.1
2	B	20	ALA	3.0
1	A	720	GLU	3.0
1	A	671	LEU	2.9
1	A	676	ALA	2.7
1	A	614	ARG	2.7
1	A	308	VAL	2.6
1	A	194	PHE	2.5
1	A	54	ILE	2.3
1	A	674	TYR	2.3
1	A	670	PRO	2.3
1	A	713	ASN	2.2
1	A	544	GLY	2.2
1	A	105	ALA	2.2
1	A	148	GLU	2.2
1	A	474	PRO	2.2
1	A	469	LYS	2.2
1	A	693	LYS	2.1
2	B	123	VAL	2.1
1	A	694	ILE	2.1
1	A	437	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	672	HIS	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 oligosaccharides 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.