



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:51 AM UTC

PDB ID : 1Z2Z / pdb_00001z2z
Title : Crystal Structure of the Putative tRNA pseudouridine synthase D (TruD) from Methanosarcina mazei, Northeast Structural Genomics Target MaR1
Authors : Forouhar, F.; Yong, W.; Ciano, M.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-03-10
Resolution : 2.60 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

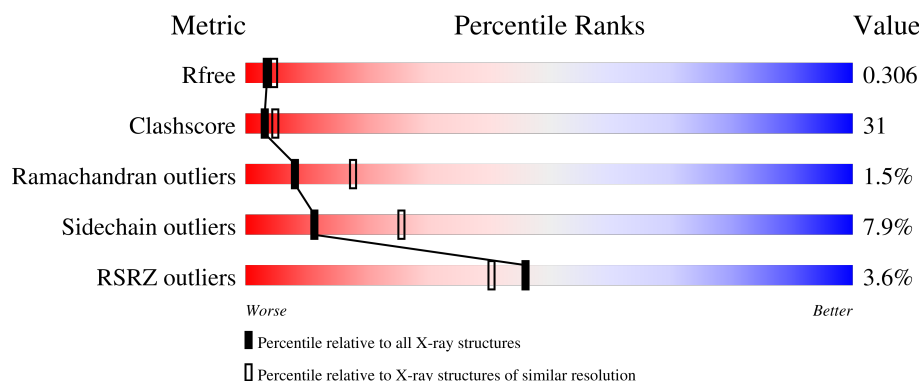
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

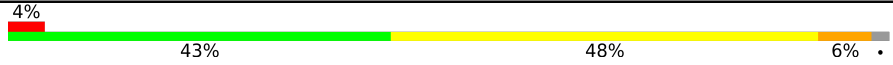
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	446	
1	B	446	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7176 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 Probable tRNA pseudouridine synthase D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	Se	0	0	0
			3478	2204	599	664	2	9			
1	B	437	Total	C	N	O	S	Se	0	0	0
			3478	2204	599	664	2	9			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8Q0M2
A	243	MSE	MET	modified residue	UNP Q8Q0M2
A	244	MSE	MET	modified residue	UNP Q8Q0M2
A	268	MSE	MET	modified residue	UNP Q8Q0M2
A	326	MSE	MET	modified residue	UNP Q8Q0M2
A	379	MSE	MET	modified residue	UNP Q8Q0M2
A	415	MSE	MET	modified residue	UNP Q8Q0M2
A	430	MSE	MET	modified residue	UNP Q8Q0M2
A	437	MSE	MET	modified residue	UNP Q8Q0M2
A	439	LEU	-	cloning artifact	UNP Q8Q0M2
A	440	GLU	-	cloning artifact	UNP Q8Q0M2
A	441	HIS	-	expression tag	UNP Q8Q0M2
A	442	HIS	-	expression tag	UNP Q8Q0M2
A	443	HIS	-	expression tag	UNP Q8Q0M2
A	444	HIS	-	expression tag	UNP Q8Q0M2
A	445	HIS	-	expression tag	UNP Q8Q0M2
A	446	HIS	-	expression tag	UNP Q8Q0M2
B	1	MSE	MET	modified residue	UNP Q8Q0M2
B	243	MSE	MET	modified residue	UNP Q8Q0M2
B	244	MSE	MET	modified residue	UNP Q8Q0M2
B	268	MSE	MET	modified residue	UNP Q8Q0M2
B	326	MSE	MET	modified residue	UNP Q8Q0M2
B	379	MSE	MET	modified residue	UNP Q8Q0M2
B	415	MSE	MET	modified residue	UNP Q8Q0M2
B	430	MSE	MET	modified residue	UNP Q8Q0M2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	437	MSE	MET	modified residue	UNP Q8Q0M2
B	439	LEU	-	cloning artifact	UNP Q8Q0M2
B	440	GLU	-	cloning artifact	UNP Q8Q0M2
B	441	HIS	-	expression tag	UNP Q8Q0M2
B	442	HIS	-	expression tag	UNP Q8Q0M2
B	443	HIS	-	expression tag	UNP Q8Q0M2
B	444	HIS	-	expression tag	UNP Q8Q0M2
B	445	HIS	-	expression tag	UNP Q8Q0M2
B	446	HIS	-	expression tag	UNP Q8Q0M2

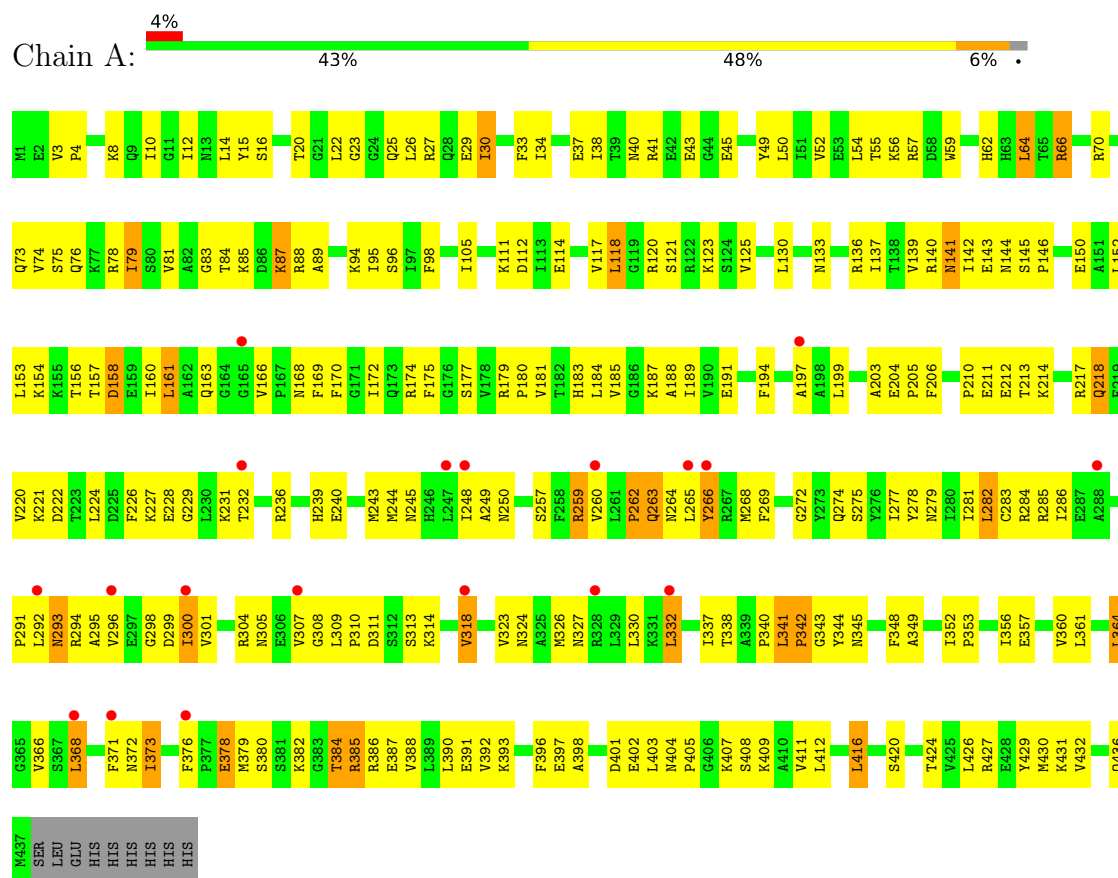
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	106	Total O 106 106	0	0
2	B	114	Total O 114 114	0	0

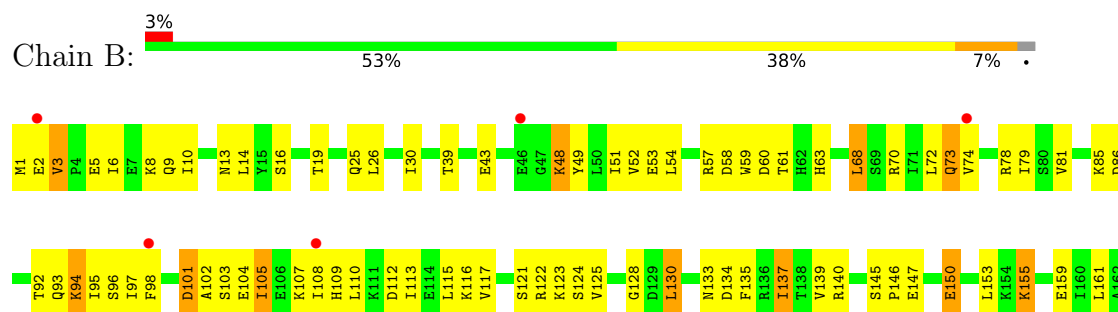
3 Residue-property plots

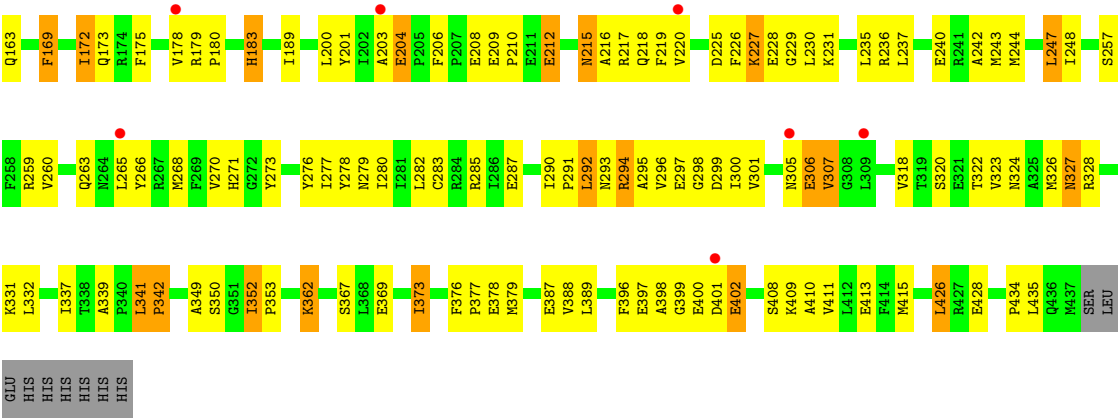
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Probable tRNA pseudouridine synthase D





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.56Å 132.53Å 66.78Å 90.00° 116.98° 90.00°	Depositor
Resolution (Å)	29.03 – 2.60 29.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.03-2.60) 96.6 (29.03-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.89 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.296 0.246 , 0.306	Depositor DCC
R_{free} test set	5735 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7176	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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	0.50	0/3531	0.90	4/4748 (0.1%)
1	B	0.54	0/3531	0.93	9/4748 (0.2%)
All	All	0.52	0/7062	0.91	13/9496 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	LEU	CA-C-N	8.58	130.56	119.84
1	B	341	LEU	C-N-CA	8.58	130.56	119.84
1	B	307	VAL	N-CA-C	-7.63	105.88	113.20
1	B	206	PHE	CA-C-N	6.66	126.17	119.24
1	B	206	PHE	C-N-CA	6.66	126.17	119.24
1	A	118	LEU	N-CA-C	-6.35	105.55	113.55
1	B	373	ILE	N-CA-C	5.79	116.74	108.93
1	B	3	VAL	N-CA-C	5.59	113.44	108.63
1	B	341	LEU	N-CA-C	-5.57	98.84	108.97
1	A	84	THR	N-CA-C	5.49	117.18	108.67
1	A	341	LEU	CA-C-N	5.46	126.67	119.84
1	A	341	LEU	C-N-CA	5.46	126.67	119.84
1	B	352	ILE	CB-CA-C	-5.14	108.82	113.70

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	3478	0	3522	237	0
1	B	3478	0	3522	208	0
2	A	106	0	0	4	0
2	B	114	0	0	11	0
All	All	7176	0	7044	437	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 31.

All (437) 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:401:ASP:HB3	1:B:409:LYS:HB3	1.44	0.97
1:B:6:ILE:HD12	1:B:6:ILE:H	1.31	0.95
1:A:170:PHE:H	1:A:279:ASN:HD21	1.14	0.92
1:A:309:LEU:HD12	1:A:310:PRO:HD2	1.51	0.90
1:B:291:PRO:HG2	1:B:294:ARG:HB2	1.54	0.88
1:A:373:ILE:HD12	1:A:373:ILE:H	1.39	0.87
1:A:373:ILE:HG22	1:A:376:PHE:H	1.37	0.87
1:B:373:ILE:HG22	1:B:376:PHE:H	1.38	0.87
1:A:401:ASP:HB3	1:A:409:LYS:HB3	1.58	0.85
1:B:226:PHE:HA	1:B:244:MSE:HE2	1.58	0.85
1:B:5:GLU:HG3	1:B:9:GLN:HE21	1.42	0.84
1:B:277:ILE:HG21	1:B:342:PRO:HG3	1.60	0.84
1:A:293:ASN:H	1:A:293:ASN:HD22	1.27	0.83
1:B:243:MSE:HG2	1:B:257:SER:O	1.80	0.81
1:B:295:ALA:H	1:B:327:ASN:HD21	1.31	0.79
1:B:247:LEU:HD13	1:B:257:SER:HB3	1.64	0.78
1:A:16:SER:HB2	1:A:163:GLN:HE22	1.48	0.78
1:A:364:LEU:HB3	1:A:366:VAL:HG23	1.65	0.78
1:B:282:LEU:HD11	1:B:388:VAL:HG23	1.62	0.78
1:B:74:VAL:HB	1:B:78:ARG:HD2	1.66	0.78
1:A:285:ARG:HA	1:A:356:ILE:HD13	1.65	0.77
1:A:96:SER:HB3	1:A:125:VAL:HG23	1.67	0.77
1:A:205:PRO:HG3	1:A:218:GLN:HG2	1.65	0.76
1:A:402:GLU:CD	1:A:402:GLU:H	1.94	0.76
1:B:49:TYR:CD1	1:B:98:PHE:HB3	2.21	0.76
1:B:294:ARG:NH2	1:B:331:LYS:HD3	1.99	0.76
1:A:141:ASN:HD22	1:A:407:LYS:HG3	1.50	0.75
1:A:245:ASN:O	1:A:248:ILE:HG12	1.86	0.75
1:A:199:LEU:HD21	1:A:224:LEU:HD21	1.70	0.74
1:B:265:LEU:HD13	1:B:268:MSE:SE	2.38	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LYS:HE3	1:B:227:LYS:HA	1.71	0.73
1:B:153:LEU:HD13	1:B:396:PHE:HB2	1.69	0.73
1:B:402:GLU:CD	1:B:402:GLU:H	1.96	0.72
1:B:81:VAL:HG12	1:B:95:ILE:HG22	1.70	0.72
1:A:50:LEU:HD23	1:A:120:ARG:HH21	1.55	0.71
1:A:50:LEU:HD23	1:A:120:ARG:NH2	2.04	0.71
1:A:161:LEU:HD11	1:A:393:LYS:HG3	1.72	0.71
1:A:37:GLU:HA	1:A:133:ASN:HD22	1.55	0.71
1:A:142:ILE:HG22	1:A:408:SER:O	1.91	0.71
1:A:66:ARG:NH1	1:A:70:ARG:HH12	1.89	0.71
1:A:105:ILE:HD11	1:A:117:VAL:HG22	1.71	0.71
1:B:215:ASN:H	1:B:215:ASN:HD22	1.39	0.71
1:B:6:ILE:H	1:B:6:ILE:CD1	2.04	0.70
1:A:37:GLU:HG3	1:A:130:LEU:HD12	1.74	0.69
1:B:294:ARG:CZ	1:B:331:LYS:HD3	2.22	0.69
1:A:373:ILE:HD12	1:A:373:ILE:N	2.08	0.69
1:A:373:ILE:H	1:A:373:ILE:CD1	2.05	0.69
1:A:372:ASN:HA	1:A:380:SER:HB2	1.75	0.69
1:B:265:LEU:HD12	1:B:268:MSE:HB3	1.75	0.69
1:B:282:LEU:CD1	1:B:388:VAL:HG23	2.22	0.68
1:A:262:PRO:O	1:A:266:TYR:HB2	1.93	0.68
1:B:203:ALA:O	1:B:217:ARG:HD3	1.93	0.68
1:A:141:ASN:ND2	1:A:407:LYS:HG3	2.08	0.68
1:A:293:ASN:HD22	1:A:293:ASN:N	1.90	0.68
1:B:305:ASN:C	1:B:307:VAL:H	2.02	0.67
1:A:121:SER:OG	1:A:123:LYS:HG2	1.94	0.67
1:B:270:VAL:HG23	2:B:508:HOH:O	1.95	0.67
1:B:94:LYS:HD3	2:B:456:HOH:O	1.93	0.67
1:A:54:LEU:HD11	1:A:64:LEU:HD11	1.76	0.67
1:A:226:PHE:HA	1:A:244:MSE:HE2	1.77	0.66
1:A:348:PHE:HZ	1:A:368:LEU:HD21	1.61	0.66
1:A:49:TYR:HB2	1:A:121:SER:O	1.95	0.66
1:A:318:VAL:HB	1:A:326:MSE:HG3	1.78	0.65
1:A:397:GLU:HB3	1:A:411:VAL:HB	1.78	0.65
1:A:298:GLY:O	1:A:349:ALA:HB1	1.98	0.64
1:B:85:LYS:NZ	1:B:133:ASN:HD21	1.96	0.64
1:A:8:LYS:HA	1:A:12:ILE:O	1.97	0.64
1:A:22:LEU:CD2	1:A:142:ILE:HD12	2.27	0.64
1:A:338:THR:OG1	1:A:385:ARG:HG2	1.97	0.64
1:A:66:ARG:HH11	1:A:70:ARG:HH12	1.45	0.64
1:A:293:ASN:H	1:A:293:ASN:ND2	1.93	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ILE:HD13	1:B:426:LEU:HD21	1.80	0.64
1:B:294:ARG:HH22	1:B:331:LYS:CE	2.11	0.64
1:A:301:VAL:HG12	1:A:337:ILE:HD13	1.80	0.64
1:B:210:PRO:HB2	1:B:212:GLU:HG3	1.79	0.64
1:B:257:SER:O	1:B:260:VAL:HG12	1.98	0.63
1:B:183:HIS:CD2	1:B:183:HIS:H	2.16	0.63
1:A:292:LEU:HD22	1:A:388:VAL:HG11	1.80	0.63
1:B:294:ARG:NH1	1:B:331:LYS:HD3	2.14	0.63
1:A:179:ARG:HG3	1:A:206:PHE:CG	2.35	0.62
1:A:345:ASN:CB	1:A:382:LYS:HB2	2.30	0.62
1:B:397:GLU:HB3	1:B:411:VAL:HB	1.80	0.62
1:A:344:TYR:CZ	1:A:382:LYS:HB3	2.34	0.62
1:B:52:VAL:HG22	1:B:117:VAL:HA	1.81	0.62
1:A:141:ASN:HD21	1:A:407:LYS:NZ	1.97	0.62
1:A:345:ASN:HB3	1:A:382:LYS:HB2	1.82	0.62
1:B:96:SER:HB3	1:B:125:VAL:HG23	1.81	0.61
1:A:141:ASN:HD21	1:A:407:LYS:HZ3	1.47	0.61
1:B:48:LYS:NZ	1:B:122:ARG:HG3	2.15	0.61
1:A:163:GLN:O	1:A:163:GLN:HG2	1.99	0.61
1:B:134:ASP:OD1	1:B:415:MSE:HE2	2.00	0.61
1:B:155:LYS:O	1:B:159:GLU:HG3	2.01	0.61
1:A:66:ARG:HH11	1:A:70:ARG:NH1	1.99	0.61
1:A:166:VAL:HG13	1:A:392:VAL:HG21	1.83	0.60
1:B:6:ILE:HD12	1:B:6:ILE:N	2.10	0.60
1:A:305:ASN:O	1:A:307:VAL:HG23	2.01	0.60
1:A:38:ILE:HG12	1:B:70:ARG:HH21	1.67	0.60
1:B:163:GLN:HB2	2:B:450:HOH:O	2.01	0.60
1:B:26:LEU:HD22	1:B:137:ILE:HD12	1.84	0.60
1:A:56:LYS:HG3	2:A:448:HOH:O	2.02	0.59
1:B:169:PHE:HB2	1:B:279:ASN:ND2	2.16	0.59
1:A:299:ASP:H	1:A:318:VAL:HG13	1.67	0.59
1:B:3:VAL:HG13	1:B:8:LYS:HE3	1.83	0.59
1:B:72:LEU:O	1:B:73:GLN:HB2	1.99	0.59
1:B:172:ILE:HD13	1:B:173:GLN:H	1.68	0.59
1:B:242:ALA:HB1	1:B:260:VAL:HG21	1.84	0.59
1:B:399:GLY:O	1:B:408:SER:HB2	2.03	0.59
1:A:85:LYS:HZ2	1:A:133:ASN:HD21	1.50	0.59
1:B:215:ASN:HD22	1:B:215:ASN:N	1.98	0.59
1:A:137:ILE:HD13	1:A:426:LEU:HD11	1.85	0.58
1:B:369:GLU:CD	1:B:369:GLU:H	2.10	0.58
1:A:412:LEU:HD21	1:A:429:TYR:CE2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:TYR:O	1:B:280:ILE:HG12	2.03	0.58
1:B:297:GLU:OE1	1:B:320:SER:HB3	2.03	0.58
1:B:172:ILE:HD12	1:B:434:PRO:HB2	1.85	0.58
1:B:26:LEU:HD21	1:B:139:VAL:HG22	1.86	0.58
1:B:30:ILE:HG21	1:B:57:ARG:HG3	1.86	0.58
1:A:66:ARG:HD3	1:A:70:ARG:CZ	2.33	0.58
1:B:48:LYS:HZ1	1:B:122:ARG:HG3	1.69	0.58
1:A:304:ARG:NH1	1:B:107:LYS:HG3	2.19	0.58
1:B:294:ARG:HH22	1:B:331:LYS:HD3	1.66	0.57
1:B:3:VAL:HG13	1:B:8:LYS:CE	2.35	0.57
1:A:188:ALA:HB3	1:A:197:ALA:HB2	1.86	0.57
1:A:22:LEU:HD23	1:A:142:ILE:HD12	1.86	0.57
1:A:34:ILE:HB	1:A:136:ARG:HB3	1.87	0.57
1:A:277:ILE:HG21	1:A:342:PRO:HG3	1.85	0.57
1:B:225:ASP:OD1	1:B:228:GLU:HB2	2.05	0.57
1:A:56:LYS:HE2	1:A:59:TRP:O	2.04	0.57
1:A:78:ARG:HB3	1:A:98:PHE:HB3	1.86	0.57
1:A:327:ASN:HA	1:A:330:LEU:HD12	1.87	0.57
1:A:391:GLU:O	1:A:392:VAL:HG13	2.05	0.56
1:A:57:ARG:HB3	1:A:112:ASP:HB3	1.87	0.56
1:B:74:VAL:HG12	1:B:78:ARG:HH21	1.70	0.56
1:B:200:LEU:O	1:B:204:GLU:HB3	2.05	0.56
1:B:226:PHE:CZ	1:B:247:LEU:HD23	2.40	0.56
1:B:296:VAL:O	1:B:299:ASP:HB2	2.05	0.56
1:B:283:CYS:O	1:B:287:GLU:HG3	2.05	0.56
1:A:304:ARG:CZ	1:B:107:LYS:HG3	2.35	0.56
1:A:373:ILE:HD13	1:A:380:SER:HA	1.87	0.56
1:A:430:MSE:O	1:A:432:VAL:HG13	2.06	0.56
1:B:294:ARG:HH22	1:B:331:LYS:CD	2.19	0.56
1:B:305:ASN:ND2	1:B:306:GLU:H	2.04	0.56
1:A:360:VAL:O	1:A:364:LEU:HB2	2.06	0.55
1:A:180:PRO:HD2	1:A:206:PHE:CD1	2.42	0.55
1:B:278:TYR:CE2	1:B:339:ALA:HB3	2.40	0.55
1:B:215:ASN:ND2	1:B:216:ALA:H	2.05	0.55
1:B:294:ARG:HG2	1:B:294:ARG:HH11	1.70	0.55
1:A:75:SER:O	1:A:78:ARG:HG2	2.07	0.55
1:A:153:LEU:HD12	1:A:398:ALA:HB2	1.89	0.55
1:A:282:LEU:O	1:A:286:ILE:HG13	2.06	0.55
1:B:105:ILE:HA	1:B:108:ILE:HG22	1.89	0.55
1:B:179:ARG:HG3	1:B:204:GLU:OE1	2.07	0.55
1:B:294:ARG:NH1	1:B:294:ARG:HG2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ASP:OD2	1:A:404:ASN:HB2	2.07	0.54
1:A:145:SER:HB2	1:A:146:PRO:HD2	1.87	0.54
1:A:344:TYR:CE1	1:A:382:LYS:HB3	2.42	0.54
1:B:140:ARG:NH2	1:B:401:ASP:HB2	2.23	0.54
1:A:140:ARG:HH21	1:A:401:ASP:HB2	1.73	0.54
1:A:384:THR:OG1	1:A:385:ARG:N	2.40	0.54
1:A:154:LYS:HZ2	1:A:158:ASP:HB2	1.73	0.54
1:A:416:LEU:HB3	1:A:420:SER:OG	2.08	0.54
1:B:68:LEU:HD12	1:B:79:ILE:CD1	2.38	0.54
1:A:14:LEU:O	1:A:427:ARG:NH2	2.34	0.53
1:A:85:LYS:NZ	1:A:133:ASN:HD21	2.06	0.53
1:A:94:LYS:HE2	1:A:118:LEU:HD13	1.90	0.53
1:A:291:PRO:HG2	1:A:294:ARG:HB2	1.89	0.53
1:B:285:ARG:HH22	1:B:299:ASP:CG	2.17	0.53
1:B:291:PRO:HG2	1:B:294:ARG:CB	2.33	0.53
1:A:20:THR:HG23	1:A:152:LEU:HD11	1.89	0.53
1:B:101:ASP:C	1:B:103:SER:H	2.15	0.53
1:B:102:ALA:HB1	1:B:117:VAL:HG11	1.90	0.53
1:B:244:MSE:O	1:B:248:ILE:HG13	2.08	0.53
1:B:277:ILE:CG2	1:B:342:PRO:HG3	2.36	0.53
1:B:179:ARG:O	1:B:179:ARG:HG2	2.09	0.53
1:A:168:ASN:OD1	1:A:390:LEU:HD12	2.09	0.53
1:B:53:GLU:OE2	1:B:116:LYS:HD3	2.09	0.53
1:B:350:SER:O	1:B:353:PRO:HG2	2.07	0.53
1:A:249:ALA:C	1:A:250:ASN:HD22	2.17	0.53
1:B:146:PRO:HG2	1:B:147:GLU:OE2	2.08	0.53
1:A:29:GLU:O	1:A:30:ILE:C	2.51	0.53
1:A:203:ALA:HB1	1:A:221:LYS:HB2	1.90	0.53
1:A:220:VAL:HG11	1:A:244:MSE:HE1	1.90	0.53
1:A:96:SER:HB3	1:A:125:VAL:CG2	2.39	0.53
1:A:154:LYS:NZ	1:A:158:ASP:HB2	2.24	0.53
1:B:305:ASN:O	1:B:307:VAL:N	2.41	0.53
1:A:15:TYR:CE1	1:A:431:LYS:HG2	2.45	0.52
1:A:343:GLY:HA3	1:A:382:LYS:C	2.34	0.52
1:A:265:LEU:HA	1:A:268:MSE:HB2	1.91	0.52
1:A:386:ARG:HD2	1:A:387:GLU:OE2	2.09	0.52
1:A:38:ILE:HG12	1:B:70:ARG:NH2	2.24	0.52
1:A:248:ILE:HG13	1:A:249:ALA:N	2.23	0.52
1:B:220:VAL:HG11	1:B:244:MSE:HE3	1.90	0.52
1:B:290:ILE:HD11	1:B:352:ILE:CG2	2.38	0.52
1:B:85:LYS:HZ2	1:B:133:ASN:HD21	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:HD13	1:A:340:PRO:HG2	1.92	0.52
1:A:372:ASN:HA	1:A:380:SER:CB	2.40	0.52
1:A:10:ILE:HD13	1:A:172:ILE:HD13	1.91	0.52
1:B:290:ILE:HD11	1:B:352:ILE:HG21	1.91	0.52
1:B:147:GLU:CD	1:B:147:GLU:N	2.68	0.51
1:A:59:TRP:O	1:A:87:LYS:HA	2.09	0.51
1:B:39:THR:CB	1:B:94:LYS:HZ2	2.22	0.51
1:B:105:ILE:HA	1:B:108:ILE:CG2	2.40	0.51
1:B:226:PHE:CE1	1:B:247:LEU:HD23	2.46	0.51
1:A:33:PHE:O	1:A:89:ALA:HB1	2.11	0.51
1:B:49:TYR:HB2	1:B:121:SER:O	2.11	0.51
1:B:265:LEU:CD1	1:B:268:MSE:HB3	2.40	0.51
1:A:296:VAL:HG21	1:A:353:PRO:HD3	1.92	0.51
1:A:179:ARG:HG3	1:A:206:PHE:CD1	2.45	0.51
1:A:229:GLY:HA2	1:A:232:THR:HG22	1.93	0.51
1:A:66:ARG:NH1	1:A:70:ARG:NH1	2.56	0.50
1:A:180:PRO:HG2	1:A:206:PHE:HE1	1.76	0.50
1:A:292:LEU:HD22	1:A:388:VAL:CG1	2.41	0.50
1:A:371:PHE:O	1:A:380:SER:HB2	2.12	0.50
1:B:74:VAL:HG12	1:B:78:ARG:NH2	2.26	0.50
1:A:204:GLU:H	1:A:221:LYS:HD2	1.75	0.50
1:B:183:HIS:H	1:B:183:HIS:HD2	1.57	0.50
1:A:41:ARG:HH12	1:A:123:LYS:HG3	1.77	0.50
1:A:352:ILE:N	1:A:353:PRO:HD2	2.27	0.50
1:A:368:LEU:N	1:A:368:LEU:HD22	2.27	0.50
1:B:402:GLU:CD	1:B:402:GLU:N	2.67	0.50
1:A:378:GLU:CD	1:A:378:GLU:H	2.19	0.49
1:A:26:LEU:HD21	1:A:139:VAL:HG22	1.92	0.49
1:B:39:THR:HB	1:B:94:LYS:HZ2	1.78	0.49
1:A:16:SER:HB2	1:A:163:GLN:NE2	2.21	0.49
1:A:30:ILE:HG21	1:A:57:ARG:HG3	1.94	0.49
1:A:79:ILE:CD1	1:A:95:ILE:HD12	2.41	0.49
1:A:344:TYR:H	1:A:382:LYS:HA	1.76	0.49
1:B:323:VAL:HG13	1:B:324:ASN:H	1.77	0.49
1:A:29:GLU:CG	1:A:403:LEU:HD21	2.42	0.49
1:A:282:LEU:O	1:A:282:LEU:HD23	2.12	0.49
1:A:14:LEU:HD12	1:A:15:TYR:N	2.28	0.49
1:A:357:GLU:O	1:A:361:LEU:HG	2.13	0.49
1:B:215:ASN:ND2	1:B:216:ALA:N	2.60	0.49
1:A:41:ARG:NH1	1:A:123:LYS:HG3	2.28	0.49
1:A:179:ARG:HH12	1:A:217:ARG:NH1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:O	1:B:8:LYS:HE3	2.13	0.49
1:B:215:ASN:HD22	1:B:216:ALA:H	1.60	0.49
1:A:368:LEU:H	1:A:368:LEU:CD2	2.26	0.49
1:B:78:ARG:HG2	1:B:98:PHE:CZ	2.48	0.49
1:A:74:VAL:HB	1:A:78:ARG:HG3	1.94	0.48
1:A:140:ARG:NH2	1:A:401:ASP:HB2	2.27	0.48
1:B:146:PRO:HG3	1:B:400:GLU:HG3	1.96	0.48
1:A:189:ILE:HG23	1:A:194:PHE:CZ	2.48	0.48
1:A:344:TYR:CD1	1:A:344:TYR:C	2.91	0.48
1:A:26:LEU:HD11	1:A:426:LEU:HD13	1.94	0.48
1:A:15:TYR:CD1	1:A:431:LYS:HG2	2.48	0.48
1:A:105:ILE:CD1	1:A:117:VAL:HG22	2.42	0.48
1:A:175:PHE:O	1:A:180:PRO:HA	2.13	0.48
1:B:260:VAL:O	1:B:260:VAL:HG22	2.13	0.48
1:A:187:LYS:HE3	2:A:503:HOH:O	2.13	0.48
1:B:16:SER:OG	1:B:428:GLU:OE1	2.28	0.48
1:B:93:GLN:HG2	2:B:455:HOH:O	2.14	0.48
1:B:219:PHE:CE1	1:B:228:GLU:HG2	2.49	0.48
1:A:156:THR:O	1:A:160:ILE:HG13	2.13	0.48
1:A:169:PHE:HD1	1:A:279:ASN:HD22	1.62	0.48
1:A:368:LEU:HD22	1:A:368:LEU:H	1.77	0.48
1:A:304:ARG:HH11	1:A:308:GLY:HA2	1.78	0.48
1:B:128:GLY:C	1:B:130:LEU:H	2.22	0.48
1:A:285:ARG:HG2	1:A:285:ARG:HH21	1.77	0.48
1:A:345:ASN:HB2	1:A:382:LYS:HB2	1.96	0.48
1:A:392:VAL:HG12	1:A:416:LEU:HD11	1.96	0.48
1:A:436:GLN:O	1:A:436:GLN:HG2	2.14	0.48
1:B:201:TYR:O	1:B:204:GLU:HG2	2.14	0.48
1:B:296:VAL:HG12	2:B:517:HOH:O	2.13	0.48
1:A:10:ILE:HD13	1:A:172:ILE:CD1	2.43	0.47
1:B:228:GLU:O	1:B:231:LYS:HB3	2.14	0.47
1:A:265:LEU:O	1:A:266:TYR:C	2.57	0.47
1:A:332:LEU:O	1:B:103:SER:HB2	2.14	0.47
1:B:240:GLU:O	1:B:244:MSE:HG3	2.15	0.47
1:A:257:SER:O	1:A:260:VAL:HG22	2.14	0.47
1:A:300:ILE:HG21	1:A:385:ARG:HD3	1.95	0.47
1:A:55:THR:HB	1:A:114:GLU:HB3	1.95	0.47
1:A:259:ARG:HG3	1:A:259:ARG:HH11	1.80	0.47
1:B:140:ARG:HH21	1:B:401:ASP:HB2	1.79	0.47
1:A:353:PRO:O	1:A:357:GLU:HG3	2.14	0.47
1:B:178:VAL:HG23	1:B:179:ARG:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:HB2	2:B:512:HOH:O	2.15	0.47
1:B:305:ASN:C	1:B:307:VAL:N	2.71	0.47
1:A:274:GLN:HB3	1:A:341:LEU:HD22	1.97	0.47
1:B:1:MSE:HG3	2:B:526:HOH:O	2.15	0.47
1:B:14:LEU:HD12	1:B:14:LEU:C	2.40	0.47
1:A:37:GLU:HG3	1:A:130:LEU:CD1	2.44	0.46
1:A:213:THR:HG21	1:A:236:ARG:NH2	2.31	0.46
1:B:285:ARG:CD	1:B:292:LEU:HD12	2.45	0.46
1:A:304:ARG:NH1	1:A:304:ARG:HB3	2.30	0.46
1:A:37:GLU:HA	1:A:133:ASN:ND2	2.27	0.46
1:A:83:GLY:O	1:A:85:LYS:HE2	2.15	0.46
1:B:273:TYR:O	1:B:276:TYR:HB3	2.16	0.46
1:A:265:LEU:HD13	1:A:268:MSE:SE	2.66	0.46
1:A:153:LEU:HD13	1:A:396:PHE:HB2	1.98	0.46
1:B:145:SER:HB2	1:B:146:PRO:HD2	1.98	0.46
1:B:215:ASN:H	1:B:215:ASN:ND2	2.10	0.46
1:B:298:GLY:O	1:B:349:ALA:HB1	2.16	0.46
1:A:14:LEU:HD21	1:A:283:CYS:HB3	1.97	0.46
1:A:323:VAL:HG13	1:A:324:ASN:N	2.31	0.46
1:A:142:ILE:C	1:A:144:ASN:H	2.24	0.45
1:A:295:ALA:HB2	1:A:337:ILE:HD11	1.97	0.45
1:A:405:PRO:HB3	2:A:522:HOH:O	2.16	0.45
1:B:78:ARG:HG2	1:B:98:PHE:CE2	2.52	0.45
1:B:79:ILE:HG12	1:B:97:ILE:HG23	1.98	0.45
1:A:45:GLU:OE1	1:A:45:GLU:HA	2.16	0.45
1:B:57:ARG:O	1:B:112:ASP:HB3	2.15	0.45
1:B:172:ILE:HD13	1:B:172:ILE:N	2.31	0.45
1:B:341:LEU:HA	1:B:342:PRO:HD2	1.84	0.45
1:A:364:LEU:HB3	1:A:366:VAL:CG2	2.43	0.45
1:B:203:ALA:O	1:B:217:ARG:HB3	2.16	0.45
1:A:390:LEU:HD13	1:A:424:THR:HG21	1.97	0.45
1:B:208:GLU:OE2	1:B:208:GLU:HA	2.17	0.45
1:A:27:ARG:NH1	1:A:33:PHE:CG	2.85	0.45
1:A:373:ILE:HD13	1:A:380:SER:CA	2.47	0.45
1:B:387:GLU:HG3	2:B:476:HOH:O	2.15	0.45
1:B:68:LEU:HD12	1:B:79:ILE:HD13	1.99	0.45
1:A:244:MSE:O	1:A:248:ILE:HG23	2.17	0.45
1:B:49:TYR:CE1	1:B:98:PHE:HB3	2.50	0.45
1:A:3:VAL:HG13	1:A:4:PRO:HD2	1.98	0.45
1:A:307:VAL:HG13	1:B:109:HIS:CD2	2.52	0.45
1:B:373:ILE:HD12	1:B:373:ILE:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG12	1:A:95:ILE:HG22	1.98	0.44
1:A:179:ARG:HG2	1:A:181:VAL:HG13	1.98	0.44
1:A:204:GLU:OE1	1:A:221:LYS:HE3	2.16	0.44
1:B:352:ILE:N	1:B:353:PRO:HD2	2.32	0.44
1:A:226:PHE:HD1	1:A:244:MSE:HE2	1.82	0.44
1:B:401:ASP:CB	1:B:409:LYS:HB3	2.32	0.44
1:A:169:PHE:HD1	1:A:279:ASN:ND2	2.15	0.44
1:A:41:ARG:HD3	1:A:43:GLU:OE2	2.17	0.44
1:A:142:ILE:CG2	1:A:408:SER:HB2	2.47	0.44
1:B:59:TRP:CD1	1:B:113:ILE:HD11	2.53	0.44
1:B:150:GLU:HG2	1:B:398:ALA:HB3	1.99	0.44
1:A:265:LEU:HB3	1:A:269:PHE:CZ	2.53	0.44
1:B:1:MSE:HG2	1:B:2:GLU:N	2.33	0.44
1:A:187:LYS:O	1:A:191:GLU:HG3	2.17	0.44
1:A:205:PRO:O	1:A:206:PHE:HD2	2.00	0.44
1:A:211:GLU:HA	1:A:214:LYS:HB3	1.99	0.44
1:A:239:HIS:O	1:A:243:MSE:HG3	2.18	0.44
1:B:30:ILE:HD13	1:B:58:ASP:HB2	1.99	0.44
1:A:87:LYS:HG3	1:A:88:ARG:N	2.33	0.43
1:A:154:LYS:HD3	1:A:154:LYS:C	2.43	0.43
1:A:181:VAL:HA	1:A:184:LEU:HD12	1.98	0.43
1:A:293:ASN:N	1:A:293:ASN:ND2	2.55	0.43
1:B:292:LEU:HB3	1:B:389:LEU:HG	2.00	0.43
1:B:301:VAL:HG12	1:B:337:ILE:HD13	2.00	0.43
1:A:240:GLU:O	1:A:244:MSE:HG3	2.19	0.43
1:A:263:GLN:HA	1:A:266:TYR:CB	2.48	0.43
1:A:307:VAL:HG13	1:B:109:HIS:HD2	1.83	0.43
1:A:307:VAL:HG12	1:A:307:VAL:O	2.18	0.43
1:B:85:LYS:HZ1	1:B:133:ASN:HD21	1.66	0.43
1:A:23:GLY:HA2	1:A:432:VAL:HG11	1.99	0.43
1:A:111:LYS:O	1:A:112:ASP:HB2	2.18	0.43
1:B:60:ASP:O	1:B:61:THR:C	2.60	0.43
1:B:172:ILE:HD13	1:B:173:GLN:N	2.31	0.43
1:B:183:HIS:CD2	1:B:183:HIS:N	2.84	0.43
1:B:322:THR:O	1:B:326:MSE:HG2	2.19	0.43
1:A:284:ARG:HB3	1:A:356:ILE:HG23	2.00	0.43
1:B:43:GLU:OE1	1:B:51:ILE:HG13	2.18	0.43
1:B:135:PHE:O	1:B:413:GLU:HA	2.18	0.43
1:A:390:LEU:O	1:A:392:VAL:HG22	2.19	0.43
1:B:68:LEU:HD12	1:B:79:ILE:HD11	2.01	0.43
1:B:294:ARG:HH12	1:B:331:LYS:HD3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PRO:HD2	1:A:206:PHE:CE1	2.54	0.43
1:B:74:VAL:CG1	1:B:78:ARG:HH21	2.32	0.43
1:B:128:GLY:O	1:B:130:LEU:N	2.45	0.43
1:A:189:ILE:HD13	1:A:379:MSE:SE	2.69	0.43
1:A:228:GLU:O	1:A:231:LYS:HB3	2.19	0.43
1:B:19:THR:HG21	1:B:155:LYS:HB3	2.00	0.43
1:B:259:ARG:HD2	1:B:376:PHE:CZ	2.54	0.43
1:A:341:LEU:HA	1:A:342:PRO:HD2	1.84	0.42
1:B:169:PHE:CB	1:B:279:ASN:ND2	2.80	0.42
1:A:278:TYR:CD1	1:A:278:TYR:C	2.97	0.42
1:B:175:PHE:O	1:B:180:PRO:HA	2.20	0.42
1:B:220:VAL:HG11	1:B:244:MSE:CE	2.50	0.42
1:A:3:VAL:HG22	1:A:15:TYR:CE2	2.54	0.42
1:A:25:GLN:HG2	1:A:140:ARG:O	2.20	0.42
1:B:209:GLU:HA	2:B:547:HOH:O	2.19	0.42
1:B:210:PRO:HB2	1:B:212:GLU:CG	2.48	0.42
1:A:22:LEU:HB2	1:A:429:TYR:O	2.19	0.42
1:B:1:MSE:HE2	2:B:559:HOH:O	2.19	0.42
1:A:390:LEU:O	1:A:391:GLU:C	2.63	0.42
1:B:294:ARG:HD3	1:B:327:ASN:ND2	2.35	0.42
1:A:174:ARG:HD3	2:A:506:HOH:O	2.19	0.42
1:B:161:LEU:HD13	1:B:161:LEU:HA	1.86	0.42
1:A:50:LEU:HD12	1:A:52:VAL:CG2	2.50	0.42
1:A:70:ARG:O	1:A:73:GLN:NE2	2.40	0.42
1:A:272:GLY:O	1:A:275:SER:N	2.53	0.42
1:B:179:ARG:HA	1:B:180:PRO:HD2	1.94	0.42
1:A:175:PHE:HB3	1:A:183:HIS:HD2	1.85	0.42
1:B:3:VAL:HG11	1:B:13:ASN:O	2.20	0.42
1:B:122:ARG:HG3	1:B:122:ARG:HH21	1.85	0.42
1:A:142:ILE:HG22	1:A:408:SER:C	2.45	0.41
1:B:189:ILE:HD13	1:B:379:MSE:SE	2.70	0.41
1:A:150:GLU:HB2	1:A:398:ALA:HB3	2.01	0.41
1:B:60:ASP:HB3	1:B:63:HIS:HB2	2.02	0.41
1:A:170:PHE:O	1:A:175:PHE:HE2	2.04	0.41
1:A:430:MSE:O	1:A:431:LYS:C	2.63	0.41
1:B:10:ILE:HD13	1:B:172:ILE:HG22	2.02	0.41
1:B:295:ALA:H	1:B:327:ASN:ND2	2.08	0.41
1:B:352:ILE:H	1:B:352:ILE:HG12	1.72	0.41
1:A:210:PRO:C	1:A:212:GLU:H	2.28	0.41
1:A:217:ARG:HH12	1:A:240:GLU:HG2	1.84	0.41
1:B:137:ILE:CD1	1:B:426:LEU:HD21	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HA	1:B:236:ARG:CZ	2.49	0.41
1:A:181:VAL:O	1:A:185:VAL:HG23	2.20	0.41
1:B:227:LYS:HE3	1:B:227:LYS:CA	2.46	0.41
1:A:26:LEU:HD23	1:A:139:VAL:HA	2.03	0.41
1:B:121:SER:OG	1:B:122:ARG:N	2.54	0.41
1:A:40:ASN:HB2	1:B:110:LEU:HD22	2.03	0.41
1:A:157:THR:O	1:A:160:ILE:HB	2.21	0.41
1:A:179:ARG:NH1	1:A:217:ARG:NH1	2.68	0.41
1:A:304:ARG:HA	1:A:309:LEU:O	2.21	0.41
1:B:163:GLN:O	1:B:293:ASN:HB3	2.21	0.41
1:B:235:LEU:C	1:B:237:LEU:H	2.29	0.41
1:B:259:ARG:NH1	1:B:378:GLU:OE1	2.54	0.41
1:B:377:PRO:C	1:B:379:MSE:H	2.29	0.41
1:A:210:PRO:C	1:A:212:GLU:N	2.79	0.41
1:A:376:PHE:O	1:A:379:MSE:HB3	2.21	0.41
1:B:178:VAL:HG23	1:B:179:ARG:H	1.86	0.41
1:B:203:ALA:O	1:B:217:ARG:CD	2.67	0.41
1:B:229:GLY:C	1:B:231:LYS:H	2.28	0.41
1:B:320:SER:O	1:B:323:VAL:HG12	2.21	0.41
1:A:373:ILE:HB	1:A:376:PHE:O	2.20	0.40
1:A:29:GLU:HG3	1:A:403:LEU:HD21	2.01	0.40
1:A:50:LEU:C	1:A:50:LEU:HD13	2.47	0.40
1:B:212:GLU:HG3	1:B:212:GLU:H	1.54	0.40
1:B:247:LEU:CD1	1:B:257:SER:HB3	2.45	0.40
1:B:362:LYS:HB2	1:B:362:LYS:NZ	2.36	0.40
1:A:87:LYS:O	1:A:89:ALA:N	2.53	0.40
1:A:311:ASP:C	1:A:313:SER:H	2.29	0.40
1:B:39:THR:HG22	1:B:94:LYS:NZ	2.36	0.40
1:B:54:LEU:O	1:B:92:THR:HA	2.22	0.40
1:B:323:VAL:HG13	1:B:324:ASN:N	2.35	0.40
1:B:49:TYR:CZ	1:B:124:SER:HB2	2.56	0.40
1:B:68:LEU:HD22	1:B:68:LEU:HA	1.94	0.40
1:B:81:VAL:HG22	2:B:485:HOH:O	2.22	0.40
1:B:139:VAL:HB	1:B:410:ALA:HB3	2.04	0.40
1:B:229:GLY:C	1:B:231:LYS:N	2.79	0.40
1:B:327:ASN:O	1:B:331:LYS:HG2	2.21	0.40
1:A:170:PHE:CG	1:A:275:SER:HB3	2.57	0.40
1:B:328:ARG:NH2	1:B:332:LEU:HD11	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	435/446 (98%)	380 (87%)	47 (11%)	8 (2%)	6	14
1	B	435/446 (98%)	397 (91%)	33 (8%)	5 (1%)	11	25
All	All	870/892 (98%)	777 (89%)	80 (9%)	13 (2%)	8	18

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	B	73	GLN
1	B	306	GLU
1	A	143	GLU
1	B	86	ASP
1	A	177	SER
1	A	342	PRO
1	B	342	PRO
1	A	266	TYR
1	A	300	ILE
1	B	300	ILE
1	A	30	ILE
1	A	262	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	382/382 (100%)	356 (93%)	26 (7%)	14	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	382/382 (100%)	348 (91%)	34 (9%)	9	20
All	All	764/764 (100%)	704 (92%)	60 (8%)	11	26

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	64	LEU
1	A	66	ARG
1	A	76	GLN
1	A	79	ILE
1	A	87	LYS
1	A	141	ASN
1	A	158	ASP
1	A	161	LEU
1	A	218	GLN
1	A	222	ASP
1	A	227	LYS
1	A	259	ARG
1	A	263	GLN
1	A	282	LEU
1	A	293	ASN
1	A	314	LYS
1	A	318	VAL
1	A	332	LEU
1	A	364	LEU
1	A	368	LEU
1	A	373	ILE
1	A	378	GLU
1	A	384	THR
1	A	385	ARG
1	A	416	LEU
1	B	25	GLN
1	B	48	LYS
1	B	68	LEU
1	B	94	LYS
1	B	101	ASP
1	B	104	GLU
1	B	105	ILE
1	B	115	LEU
1	B	123	LYS
1	B	130	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	137	ILE
1	B	150	GLU
1	B	155	LYS
1	B	169	PHE
1	B	172	ILE
1	B	183	HIS
1	B	204	GLU
1	B	212	GLU
1	B	215	ASN
1	B	218	GLN
1	B	227	LYS
1	B	230	LEU
1	B	247	LEU
1	B	263	GLN
1	B	266	TYR
1	B	292	LEU
1	B	294	ARG
1	B	318	VAL
1	B	327	ASN
1	B	362	LYS
1	B	367	SER
1	B	402	GLU
1	B	426	LEU
1	B	435	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	25	GLN
1	A	133	ASN
1	A	141	ASN
1	A	144	ASN
1	A	163	GLN
1	A	183	HIS
1	A	250	ASN
1	A	264	ASN
1	A	274	GLN
1	A	279	ASN
1	A	293	ASN
1	A	358	ASN
1	B	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	25	GLN
1	B	109	HIS
1	B	133	ASN
1	B	144	ASN
1	B	168	ASN
1	B	183	HIS
1	B	215	ASN
1	B	218	GLN
1	B	264	ASN
1	B	279	ASN
1	B	305	ASN
1	B	324	ASN
1	B	327	ASN
1	B	436	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 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	428/446 (95%)	0.53	19 (4%) 39 33	12, 49, 76, 83	0
1	B	428/446 (95%)	0.12	12 (2%) 55 49	14, 36, 66, 77	0
All	All	856/892 (95%)	0.33	31 (3%) 46 40	12, 41, 74, 83	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	LEU	4.2
1	B	265	LEU	3.6
1	A	266	TYR	3.3
1	B	178	VAL	3.3
1	B	305	ASN	3.3
1	A	318	VAL	3.2
1	B	2	GLU	3.2
1	A	332	LEU	2.7
1	B	46	GLU	2.7
1	B	401	ASP	2.6
1	A	247	LEU	2.6
1	A	307	VAL	2.5
1	A	288	ALA	2.5
1	A	197	ALA	2.5
1	B	74	VAL	2.4
1	A	376	PHE	2.4
1	A	292	LEU	2.3
1	A	232	THR	2.3
1	B	98	PHE	2.3
1	A	296	VAL	2.2
1	A	328	ARG	2.2
1	A	165	GLY	2.2
1	A	300	ILE	2.2
1	B	220	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	260	VAL	2.1
1	B	108	ILE	2.1
1	A	371	PHE	2.1
1	A	248	ILE	2.1
1	B	203	ALA	2.0
1	A	368	LEU	2.0
1	B	309	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 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.