



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:55 PM GMT

PDB ID : 1Z2Z
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

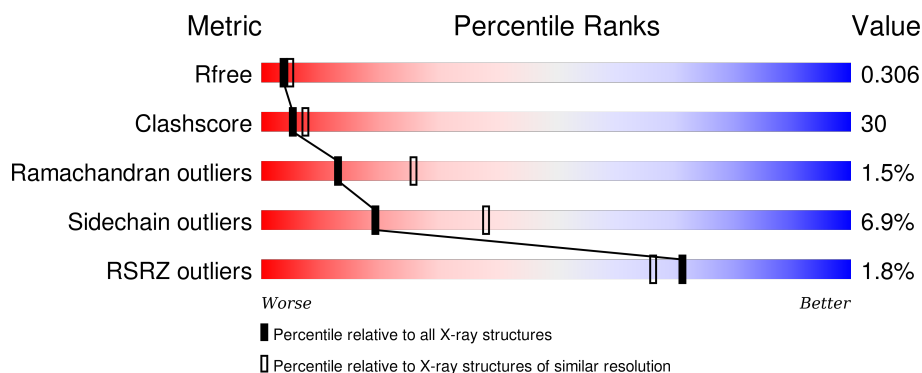
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

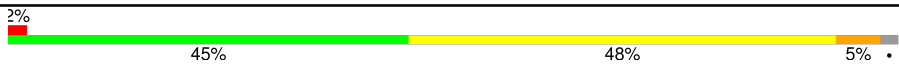
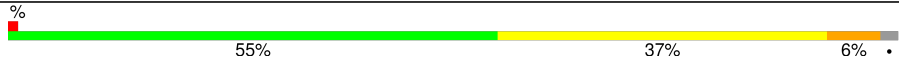
The reported resolution of this entry is 2.60 Å.

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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

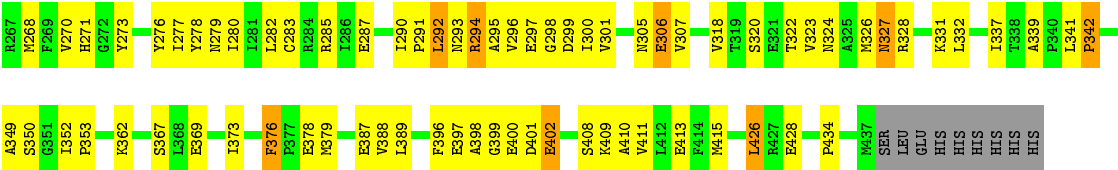
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Chain	Residue	Modelled	Actual	Comment	Reference
B	437	MSE	MET	MODIFIED RESIDUE	UNP Q8Q0M2
B	439	LEU	-	CLONING ARTIFACT	UNP Q8Q0M2
B	440	GLU	-	CLONING ARTIFACT	UNP Q8Q0M2
B	441	HIS	-	EXPRESSION TAG	UNP Q8Q0M2
B	442	HIS	-	EXPRESSION TAG	UNP Q8Q0M2
B	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 106	O 106	0	0
2	B	114	Total 114	O 114	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.56 Å 132.53 Å 66.78 Å 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) 98.5 (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 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.296 0.246 , 0.306	Depositor DCC
R_{free} test set	2895 reflections (9.86%)	DCC
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.6	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 58135 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/3531	0.59	0/4748
1	B	0.43	0/3531	0.63	0/4748
All	All	0.42	0/7062	0.61	0/9496

There are no bond length outliers.

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	3478	0	3522	228	0
1	B	3478	0	3522	203	0
2	A	106	0	0	4	0
2	B	114	0	0	11	0
All	All	7176	0	7044	423	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 30.

All (423) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:373:ILE:HD12	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:B:294:ARG:NH2	1:B:331:LYS:HD3	1.99	0.76
1:B:49:TYR:CD1	1:B:98:PHE:HB3	2.21	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
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: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:142:ILE:HG22	1:A:408:SER:O	1.91	0.71
1:A:37:GLU:HA	1:A:133:ASN:HD22	1.55	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:HD22	1:B:215:ASN:H	1.39	0.71
1:B:6:ILE:CD1	1:B:6:ILE:H	2.04	0.70
1:A:37:GLU:HG3	1:A:130:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLU:CD	1:A:402:GLU:H	1.94	0.69
1:B:294:ARG:CZ	1:B:331:LYS:HD3	2.22	0.69
1:A:373:ILE:H	1:A:373:ILE:CD1	2.05	0.69
1:A:373:ILE:N	1:A:373:ILE:HD12	2.08	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:B:203:ALA:O	1:B:217:ARG:HD3	1.93	0.68
1:A:262:PRO:O	1:A:266:TYR:HB2	1.93	0.68
1:A:293:ASN:N	1:A:293:ASN:HD22	1.90	0.68
1:A:141:ASN:ND2	1:A:407:LYS:HG3	2.08	0.68
1:B:402:GLU:CD	1:B:402:GLU:H	1.96	0.68
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:22:LEU:CD2	1:A:142:ILE:HD12	2.27	0.64
1:A:8:LYS:HA	1:A:12:ILE:O	1.97	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
1:B:294:ARG:HH22	1:B:331:LYS:CE	2.11	0.64
1:B:137:ILE:HD13	1:B:426:LEU:HD21	1.80	0.64
1:B:210:PRO:HB2	1:B:212:GLU:HG3	1.79	0.64
1:A:301:VAL:HG12	1:A:337:ILE:HD13	1.80	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:305:ASN:C	1:B:307:VAL:H	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:48:LYS:NZ	1:B:122:ARG:HG3	2.15	0.61
1:A:141:ASN:HD21	1:A:407:LYS:HZ3	1.47	0.61
1:A:163:GLN:HG2	1:A:163:GLN:O	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:B:6:ILE:N	1:B:6:ILE:HD12	2.10	0.60
1:A:166:VAL:HG13	1:A:392:VAL:HG21	1.83	0.60
1:A:305:ASN:O	1:A:307:VAL:HG23	2.01	0.60
1:B:163:GLN:HB2	2:B:450:HOH:O	2.01	0.60
1:A:38:ILE:HG12	1:B:70:ARG:HH21	1.67	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:B:242:ALA:HB1	1:B:260:VAL:HG21	1.84	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:399:GLY:O	1:B:408:SER:HB2	2.03	0.59
1:B:215:ASN:HD22	1:B:215:ASN:N	1.98	0.59
1:A:85:LYS:HZ2	1:A:133:ASN:HD21	1.50	0.59
1:A:137:ILE:HD13	1:A:426:LEU:HD11	1.85	0.58
1:A:412:LEU:HD21	1:A:429:TYR:CE2	2.37	0.58
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:B:48:LYS:HZ1	1:B:122:ARG:HG3	1.69	0.58
1:A:66:ARG:HD3	1:A:70:ARG:CZ	2.33	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:277:ILE:HG21	1:A:342:PRO:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HB	1:A:136:ARG:HB3	1.87	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:B:74:VAL:HG12	1:B:78:ARG:HH21	1.70	0.56
1:A:57:ARG:HB3	1:A:112:ASP:HB3	1.87	0.56
1:B:226:PHE:CZ	1:B:247:LEU:HD23	2.40	0.56
1:B:200:LEU:O	1:B:204:GLU:HB3	2.05	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:B:294:ARG:HH22	1:B:331:LYS:CD	2.19	0.56
1:A:373:ILE:HD13	1:A:380:SER:HA	1.87	0.56
1:B:305:ASN:ND2	1:B:306:GLU:H	2.04	0.56
1:A:430:MSE:O	1:A:432:VAL:HG13	2.06	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:B:179:ARG:HG3	1:B:204:GLU:OE1	2.07	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:294:ARG:HG2	1:B:294:ARG:NH1	2.22	0.54
1:A:401:ASP:OD2	1:A:404:ASN:HB2	2.07	0.54
1:B:140:ARG:NH2	1:B:401:ASP:HB2	2.23	0.54
1:A:344:TYR:CE1	1:A:382:LYS:HB3	2.42	0.54
1:A:145:SER:HB2	1:A:146:PRO:HD2	1.87	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:B:369:GLU:CD	1:B:369:GLU:H	2.10	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:B:291:PRO:HG2	1:B:294:ARG:CB	2.33	0.53
1:A:85:LYS:NZ	1:A:133:ASN:HD21	2.06	0.53
1:A:291:PRO:HG2	1:A:294:ARG:HB2	1.89	0.53
1:A:94:LYS:HE2	1:A:118:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:O	1:A:427:ARG:NH2	2.34	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:102:ALA:HB1	1:B:117:VAL:HG11	1.90	0.53
1:A:20:THR:HG23	1:A:152:LEU:HD11	1.89	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:B:146:PRO:HG2	1:B:147:GLU:OE2	2.08	0.53
1:A:220:VAL:HG11	1:A:244:MSE:HE1	1.90	0.53
1:A:203:ALA:HB1	1:A:221:LYS:HB2	1.90	0.53
1:A:96:SER:HB3	1:A:125:VAL:CG2	2.39	0.53
1:B:305:ASN:O	1:B:307:VAL:N	2.41	0.53
1:A:154:LYS:NZ	1:A:158:ASP:HB2	2.24	0.53
1:A:15:TYR:CE1	1:A:431:LYS:HG2	2.45	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: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:A:38:ILE:HG12	1:B:70:ARG:NH2	2.24	0.52
1:B:290:ILE:HD11	1:B:352:ILE:CG2	2.38	0.52
1:B:85:LYS:HZ3	1:B:133:ASN:HD21	1.57	0.52
1:A:372:ASN:HA	1:A:380:SER:CB	2.40	0.52
1:A:281:ILE:HD13	1:A:340:PRO:HG2	1.92	0.52
1:B:290:ILE:HD11	1:B:352:ILE:HG21	1.91	0.52
1:A:10:ILE:HD13	1:A:172:ILE:HD13	1.91	0.52
1:B:39:THR:CB	1:B:94:LYS:HZ2	2.22	0.51
1:A:59:TRP:O	1:A:87:LYS:HA	2.09	0.51
1:B:226:PHE:CE1	1:B:247:LEU:HD23	2.46	0.51
1:B:105:ILE:HA	1:B:108:ILE:CG2	2.40	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:180:PRO:HG2	1:A:206:PHE:HE1	1.76	0.50
1:A:66:ARG:NH1	1:A:70:ARG:NH1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD22	1:A:388:VAL:CG1	2.41	0.50
1:B:183:HIS:HD2	1:B:183:HIS:H	1.57	0.50
1:A:204:GLU:H	1:A:221:LYS:HD2	1.75	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:HD22	1:A:368:LEU:N	2.27	0.50
1:B:39:THR:HB	1:B:94:LYS:HZ2	1.78	0.49
1:A:26:LEU:HD21	1:A:139:VAL:HG22	1.92	0.49
1:A:16:SER:HB2	1:A:163:GLN:NE2	2.21	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: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:29:GLU:CG	1:A:403:LEU:HD21	2.42	0.49
1:A:282:LEU:HD23	1:A:282:LEU:O	2.12	0.49
1:B:215:ASN:ND2	1:B:216:ALA:N	2.60	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:A:179:ARG:HH12	1:A:217:ARG:NH1	2.11	0.49
1:A:41:ARG:NH1	1:A:123:LYS:HG3	2.28	0.49
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:B:78:ARG:HG2	1:B:98:PHE:CZ	2.48	0.49
1:A:368:LEU:CD2	1:A:368:LEU:H	2.26	0.49
1:B:285:ARG:HH22	1:B:299:ASP:CG	2.17	0.49
1:A:140:ARG:NH2	1:A:401:ASP:HB2	2.27	0.48
1:A:74:VAL:HB	1:A:78:ARG:HG3	1.94	0.48
1:B:146:PRO:HG3	1:B:400:GLU:HG3	1.96	0.48
1:B:101:ASP:C	1:B:103:SER:H	2.15	0.48
1:A:189:ILE:HG23	1:A:194:PHE:CZ	2.48	0.48
1:A:26:LEU:HD11	1:A:426:LEU:HD13	1.94	0.48
1:A:175:PHE:O	1:A:180:PRO:HA	2.13	0.48
1:A:249:ALA:C	1:A:250:ASN:HD22	2.17	0.48
1:B:260:VAL:HG22	1:B:260:VAL:O	2.13	0.48
1:A:105:ILE:CD1	1:A:117:VAL:HG22	2.42	0.48
1:A:15:TYR:CD1	1:A:431:LYS:HG2	2.48	0.48
1:B:219:PHE:CE1	1:B:228:GLU:HG2	2.49	0.48
1:A:29:GLU:O	1:A:30:ILE:C	2.51	0.48
1:B:93:GLN:HG2	2:B:455:HOH:O	2.14	0.48
1:B:16:SER:OG	1:B:428:GLU:OE1	2.28	0.48
1:A:187:LYS:HE3	2:A:503:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:156:THR:O	1:A:160:ILE:HG13	2.13	0.48
1:A:304:ARG:HH11	1:A:308:GLY:HA2	1.78	0.48
1:A:343:GLY:HA3	1:A:382:LYS:C	2.34	0.48
1:A:285:ARG:HH21	1:A:285:ARG:HG2	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: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:436:GLN:HG2	1:A:436:GLN:O	2.14	0.48
1:B:228:GLU:O	1:B:231:LYS:HB3	2.14	0.47
1:A:10:ILE:HD13	1:A:172:ILE:CD1	2.43	0.47
1:B:240:GLU:O	1:B:244:MSE:HG3	2.15	0.47
1:A:332:LEU:O	1:B:103:SER:HB2	2.14	0.47
1:A:300:ILE:HG21	1:A:385:ARG:HD3	1.95	0.47
1:A:257:SER:O	1:A:260:VAL:HG22	2.14	0.47
1:B:140:ARG:HH21	1:B:401:ASP:HB2	1.79	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: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
1:B:147:GLU:CD	1:B:147:GLU:N	2.68	0.47
1:B:271:HIS:HB2	2:B:512:HOH:O	2.15	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:A:37:GLU:HG3	1:A:130:LEU:CD1	2.44	0.46
1:B:285:ARG:CD	1:B:292:LEU:HD12	2.45	0.46
1:A:213:THR:HG21	1:A:236:ARG:NH2	2.31	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:B:215:ASN:H	1:B:215:ASN:ND2	2.10	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: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:154:LYS:HZ1	1:A:158:ASP:HB2	1.81	0.46
1:A:323:VAL:HG13	1:A:324:ASN:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:HG2	1:B:98:PHE:CE2	2.52	0.45
1:A:295:ALA:HB2	1:A:337:ILE:HD11	1.97	0.45
1:B:79:ILE:HG12	1:B:97:ILE:HG23	1.98	0.45
1:A:405:PRO:HB3	2:A:522:HOH:O	2.16	0.45
1:A:45:GLU:HA	1:A:45:GLU:OE1	2.16	0.45
1:B:341:LEU:HA	1:B:342:PRO:HD2	1.84	0.45
1:B:172:ILE:N	1:B:172:ILE:HD13	2.31	0.45
1:B:57:ARG:O	1:B:112:ASP:HB3	2.15	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:B:402:GLU:N	1:B:402:GLU:CD	2.67	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:373:ILE:HD13	1:A:380:SER:CA	2.47	0.45
1:A:27:ARG:NH1	1:A:33:PHE:CG	2.85	0.45
1:B:387:GLU:HG3	2:B:476:HOH:O	2.15	0.45
1:A:378:GLU:CD	1:A:378:GLU:H	2.19	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:B:373:ILE:H	1:B:373:ILE:HD12	1.82	0.45
1:A:307:VAL:HG13	1:B:109:HIS:CD2	2.52	0.45
1:A:3:VAL:HG13	1:A:4:PRO:HD2	1.98	0.45
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:A:81:VAL:HG12	1:A:95:ILE:HG22	1.98	0.44
1:B:352:ILE:N	1:B:353:PRO:HD2	2.32	0.44
1:B:401:ASP:CB	1:B:409:LYS:HB3	2.32	0.44
1:A:226:PHE:HD1	1:A:244:MSE:HE2	1.82	0.44
1:A:111:LYS:O	1:A:112:ASP:HB2	2.18	0.44
1:A:169:PHE:HD1	1:A:279:ASN:ND2	2.15	0.44
1:A:142:ILE:CG2	1:A:408:SER:HB2	2.47	0.44
1:A:41:ARG:HD3	1:A:43:GLU:OE2	2.17	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:205:PRO:O	1:A:206:PHE:HD2	2.00	0.44
1:A:187:LYS:O	1:A:191:GLU:HG3	2.17	0.44
1:A:344:TYR:CD1	1:A:344:TYR:C	2.91	0.44
1:B:30:ILE:HD13	1:B:58:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:HIS:O	1:A:243:MSE:HG3	2.18	0.44
1:A:211:GLU:HA	1:A:214:LYS:HB3	1.99	0.44
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:A:87:LYS:HG3	1:A:88:ARG:N	2.33	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:B:85:LYS:HZ2	1:B:133:ASN:HD21	1.66	0.43
1:A:307:VAL:HG12	1:A:307:VAL:O	2.18	0.43
1:A:307:VAL:HG13	1:B:109:HIS:HD2	1.83	0.43
1:B:183:HIS:CD2	1:B:183:HIS:N	2.84	0.43
1:B:172:ILE:HD13	1:B:173:GLN:N	2.31	0.43
1:A:23:GLY:HA2	1:A:432:VAL:HG11	1.99	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:128:GLY:C	1:B:130:LEU:H	2.22	0.43
1:B:294:ARG:HH12	1:B:331:LYS:HD3	1.84	0.43
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:A:265:LEU:O	1:A:266:TYR:C	2.57	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:B:259:ARG:HD2	1:B:376:PHE:CZ	2.54	0.43
1:B:19:THR:HG21	1:B:155:LYS:HB3	2.00	0.43
1:A:228:GLU:O	1:A:231:LYS:HB3	2.19	0.43
1:B:169:PHE:CB	1:B:279:ASN:ND2	2.80	0.42
1:A:341:LEU:HA	1:A:342:PRO:HD2	1.84	0.42
1:B:220:VAL:HG11	1:B:244:MSE:CE	2.50	0.42
1:B:175:PHE:O	1:B:180:PRO:HA	2.20	0.42
1:A:25:GLN:HG2	1:A:140:ARG:O	2.20	0.42
1:B:210:PRO:HB2	1:B:212:GLU:CG	2.48	0.42
1:A:3:VAL:HG22	1:A:15:TYR:CE2	2.54	0.42
1:B:209:GLU:HA	2:B:547:HOH:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ARG:HD3	1:B:327:ASN:ND2	2.35	0.42
1:B:161:LEU:HD13	1:B:161:LEU:HA	1.86	0.42
1:B:14:LEU:C	1:B:14:LEU:HD12	2.40	0.42
1:A:174:ARG:HD3	2:A:506:HOH:O	2.19	0.42
1:A:272:GLY:O	1:A:275:SER:N	2.53	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: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:122:ARG:HH21	1:B:122:ARG:HG3	1.85	0.42
1:B:3:VAL:HG11	1:B:13:ASN:O	2.20	0.42
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: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:HG12	1:B:352:ILE:H	1.72	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
1:B:305:ASN:C	1:B:307:VAL:N	2.71	0.41
1:B:236:ARG:CZ	1:B:236:ARG:HA	2.49	0.41
1:A:181:VAL:O	1:A:185:VAL:HG23	2.20	0.41
1:B:227:LYS:CA	1:B:227:LYS:HE3	2.46	0.41
1:B:121:SER:OG	1:B:122:ARG:N	2.54	0.41
1:A:26:LEU:HD23	1:A:139:VAL:HA	2.03	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:259:ARG:NH1	1:B:378:GLU:OE1	2.54	0.41
1:B:163:GLN:O	1:B:293:ASN:HB3	2.21	0.41
1:A:157:THR:O	1:A:160:ILE:HB	2.21	0.41
1:A:40:ASN:HB2	1:B:110:LEU:HD22	2.03	0.41
1:A:376:PHE:O	1:A:379:MSE:HB3	2.21	0.41
1:B:203:ALA:O	1:B:217:ARG:CD	2.67	0.41
1:B:320:SER:O	1:B:323:VAL:HG12	2.21	0.41
1:B:178:VAL:HG23	1:B:179:ARG:H	1.86	0.41
1:A:373:ILE:HB	1:A:376:PHE:O	2.20	0.40
1:B:247:LEU:CD1	1:B:257:SER:HB3	2.45	0.40
1:A:142:ILE:C	1:A:144:ASN:H	2.24	0.40
1:B:212:GLU:HG3	1:B:212:GLU:H	1.54	0.40
1:A:29:GLU:HG3	1:A:403:LEU:HD21	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LYS:NZ	1:B:362:LYS:HB2	2.36	0.40
1:B:39:THR:HG22	1:B:94:LYS:NZ	2.36	0.40
1:A:87:LYS:O	1:A:89:ALA:N	2.53	0.40
1:B:323:VAL:HG13	1:B:324:ASN:N	2.35	0.40
1:B:54:LEU:O	1:B:92:THR:HA	2.22	0.40
1:B:327:ASN:O	1:B:331:LYS:HG2	2.21	0.40
1:B:49:TYR:CZ	1:B:124:SER:HB2	2.56	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:68:LEU:HA	1:B:68:LEU:HD22	1.94	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	11	21
1	B	435/446 (98%)	397 (91%)	33 (8%)	5 (1%)	17	36
All	All	870/892 (98%)	777 (89%)	80 (9%)	13 (2%)	13	26

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	360 (94%)	22 (6%)	25	49
1	B	382/382 (100%)	351 (92%)	31 (8%)	15	28
All	All	764/764 (100%)	711 (93%)	53 (7%)	19	38

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

Mol	Chain	Res	Type
1	A	27	ARG
1	A	41	ARG
1	A	62	HIS
1	A	64	LEU
1	A	79	ILE
1	A	106	GLU
1	A	141	ASN
1	A	158	ASP
1	A	211	GLU
1	A	218	GLN
1	A	222	ASP
1	A	259	ARG
1	A	263	GLN
1	A	264	ASN
1	A	282	LEU
1	A	293	ASN

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Mol	Chain	Res	Type
1	A	314	LYS
1	A	382	LYS
1	A	384	THR
1	A	385	ARG
1	A	387	GLU
1	A	416	LEU
1	B	14	LEU
1	B	48	LYS
1	B	68	LEU
1	B	94	LYS
1	B	101	ASP
1	B	105	ILE
1	B	123	LYS
1	B	130	LEU
1	B	137	ILE
1	B	169	PHE
1	B	172	ILE
1	B	173	GLN
1	B	179	ARG
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	259	ARG
1	B	266	TYR
1	B	292	LEU
1	B	294	ARG
1	B	318	VAL
1	B	327	ASN
1	B	367	SER
1	B	376	PHE
1	B	402	GLU
1	B	426	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN

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Mol	Chain	Res	Type
1	A	25	GLN
1	A	109	HIS
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	327	ASN
1	A	345	ASN
1	B	9	GLN
1	B	25	GLN
1	B	109	HIS
1	B	133	ASN
1	B	144	ASN
1	B	183	HIS
1	B	215	ASN
1	B	218	GLN
1	B	250	ASN
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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.11	9 (2%) 67 61	12, 49, 76, 83	0
1	B	428/446 (95%)	-0.08	6 (1%) 78 74	14, 36, 66, 77	0
All	All	856/892 (95%)	0.02	15 (1%) 71 66	12, 41, 74, 83	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	LEU	3.0
1	A	345	ASN	2.9
1	B	178	VAL	2.9
1	B	219	PHE	2.8
1	A	266	TYR	2.8
1	B	98	PHE	2.7
1	B	177	SER	2.7
1	A	305	ASN	2.6
1	A	332	LEU	2.6
1	A	314	LYS	2.4
1	B	223	THR	2.3
1	A	196	LYS	2.3
1	B	2	GLU	2.2
1	A	309	LEU	2.1
1	A	224	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.