



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:27 pm GMT

PDB ID : 1K1Q
Title : Crystal Structure of a DinB Family Error Prone DNA Polymerase from *Sulfolobus solfataricus*
Authors : Silvian, L.F.; Toth, E.A.; Pham, P.; Goodman, M.F.; Ellenberger, T.
Deposited on : 2001-09-25
Resolution : 2.80 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

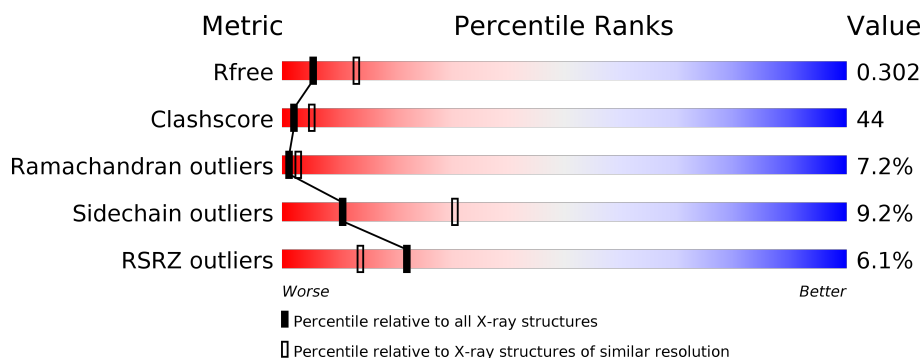
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	354	<div> <div>8%</div> <div> <div></div> <div>35%</div> <div>47%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	354	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>42%</div> <div>7%</div> <div></div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5166 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 DBH protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2517	1616	433	461	7			
1	B	341	Total	C	N	O	S	0	0	0
			2581	1661	444	469	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	SER	CYS	ENGINEERED	UNP P96022
B	31	SER	CYS	ENGINEERED	UNP P96022

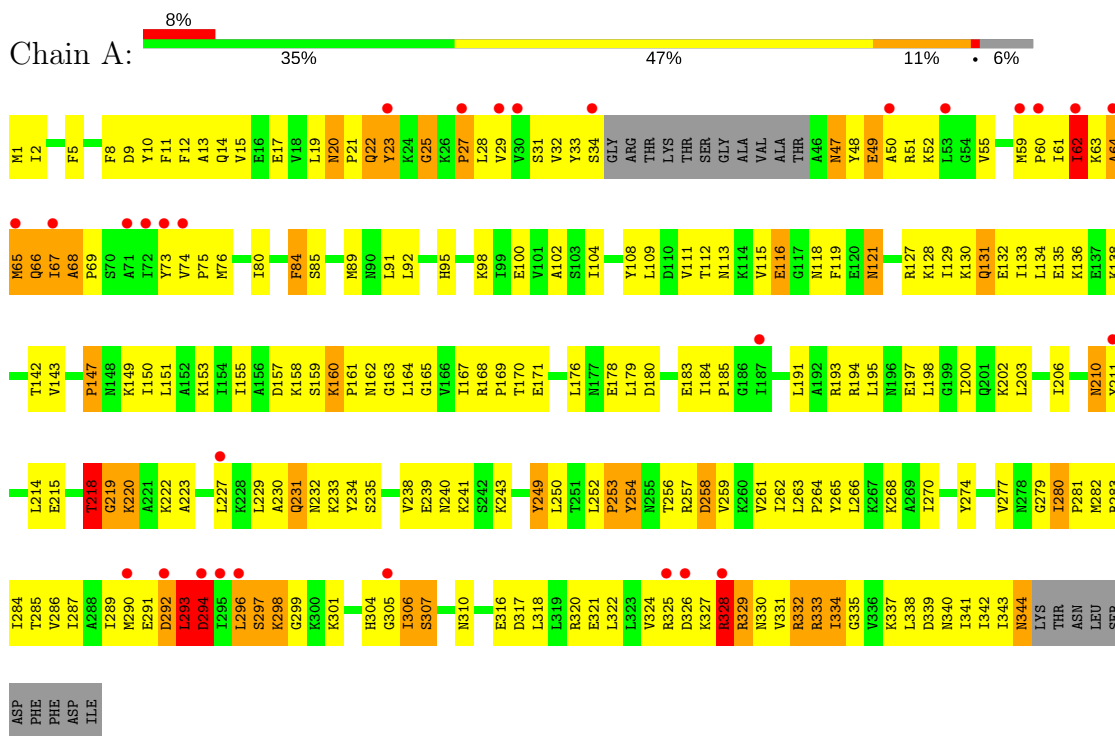
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	30	Total	O	0	0
			30	30		

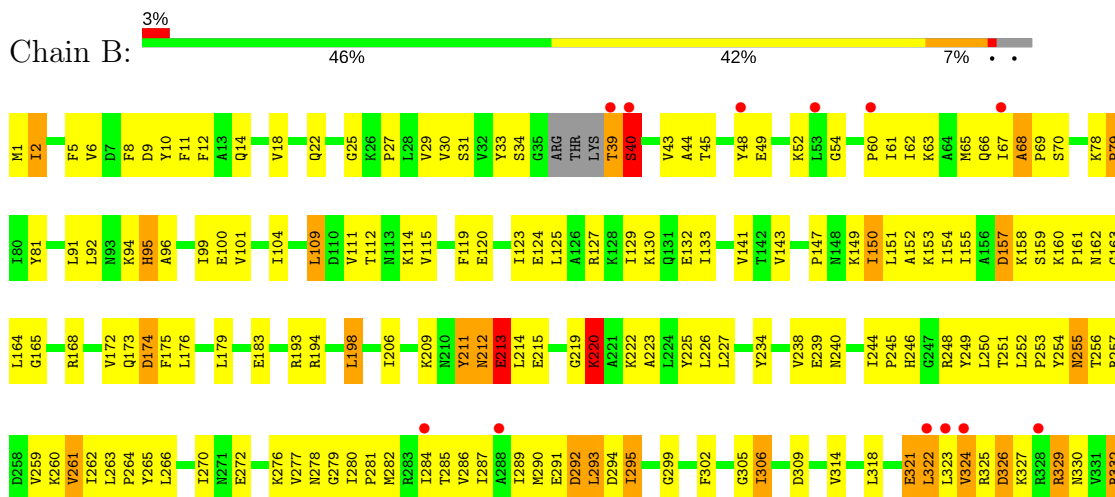
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: DBH protein



• Molecule 1: DBH protein



R333	1341	LYS	THR
1334	1342	ASN	ASN
G335	1343	LEU	LEU
V336	1344	SER	SER
K337		ASP	ASP
L338		PHE	PHE
		PHE	PHE
		ASP	ASP
		ILE	ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	111.72Å 111.72Å 132.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.10 – 2.80 40.10 – 2.81	Depositor EDS
% Data completeness (in resolution range)	94.0 (40.10-2.80) 94.1 (40.10-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.263 , 0.306 0.257 , 0.302	Depositor DCC
R_{free} test set	2141 reflections (9.93%)	DCC
Wilson B-factor (Å ²)	84.9	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5166	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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	0/2552	0.86	4/3464 (0.1%)
1	B	0.46	0/2618	0.77	3/3553 (0.1%)
All	All	0.48	0/5170	0.81	7/7017 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	LEU	N-CA-C	-12.99	75.92	111.00
1	B	213	GLU	N-CA-C	-8.07	89.21	111.00
1	B	261	VAL	N-CA-C	-7.20	91.56	111.00
1	A	329	ARG	CB-CG-CD	-5.44	97.47	111.60
1	A	220	LYS	N-CA-C	-5.39	96.43	111.00
1	A	66	GLN	N-CA-C	-5.38	96.48	111.00
1	B	109	LEU	CA-CB-CG	5.23	127.33	115.30

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	2517	0	2538	243	0
1	B	2581	0	2614	207	0
2	A	38	0	0	31	0
2	B	30	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5166	0	5152	450	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 44.

All (450) 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:293:LEU:O	1:A:294:ASP:HB3	1.50	1.12
1:B:252:LEU:HD11	1:B:262:ILE:HD12	1.31	1.08
1:A:218:THR:HG23	1:A:222:LYS:HB2	1.32	1.07
1:B:278:ASN:HB2	1:B:343:ILE:HD11	1.40	1.01
1:A:28:LEU:HD11	1:A:74:VAL:HG22	1.42	1.01
1:A:296:LEU:HD22	1:A:322:LEU:HD22	1.42	1.00
1:B:289:ILE:HG12	2:B:367:HOH:O	1.62	0.98
1:B:291:GLU:OE2	1:B:330:ASN:HB2	1.62	0.98
1:B:194:ARG:HH21	1:B:198:LEU:CD2	1.77	0.97
1:A:127:ARG:HD2	2:A:359:HOH:O	1.65	0.96
1:A:326:ASP:OD2	1:A:329:ARG:HD2	1.65	0.96
1:A:159:SER:HB3	2:A:383:HOH:O	1.64	0.95
1:A:218:THR:CG2	1:A:222:LYS:HB2	1.94	0.95
1:A:27:PRO:HG3	1:A:49:GLU:HB3	1.48	0.95
1:A:290:MET:CE	1:A:296:LEU:HD12	1.98	0.93
1:B:194:ARG:HH21	1:B:198:LEU:HD21	1.33	0.92
1:B:292:ASP:C	1:B:293:LEU:HD22	1.92	0.89
1:B:150:ILE:H	1:B:150:ILE:HD13	1.39	0.88
1:B:62:ILE:O	1:B:66:GLN:HG3	1.74	0.87
1:A:334:ILE:HD12	1:A:334:ILE:H	1.40	0.86
1:B:1:MET:HG3	1:B:147:PRO:O	1.75	0.86
1:A:306:ILE:HG22	1:A:307:SER:H	1.42	0.84
1:A:142:THR:HG21	1:A:160:LYS:HA	1.57	0.84
1:A:290:MET:HE1	1:A:296:LEU:HD12	1.58	0.84
1:B:284:ILE:HD11	1:B:314:VAL:CG1	2.07	0.84
1:B:260:LYS:HD2	2:B:380:HOH:O	1.76	0.83
1:B:220:LYS:HA	1:B:223:ALA:HB3	1.61	0.83
1:A:332:ARG:HA	2:A:356:HOH:O	1.79	0.82
1:A:306:ILE:HG22	1:A:307:SER:N	1.95	0.82
1:B:277:VAL:HG13	1:B:341:ILE:HG12	1.61	0.82
1:B:290:MET:HG3	1:B:329:ARG:NH1	1.95	0.82
1:A:66:GLN:O	1:A:69:PRO:HD3	1.80	0.81
1:B:62:ILE:HG13	1:B:63:LYS:N	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ILE:HD11	1:B:314:VAL:HG11	1.60	0.80
1:A:326:ASP:OD2	1:A:329:ARG:NH1	2.14	0.80
1:A:153:LYS:HE2	2:A:364:HOH:O	1.81	0.80
1:A:249:TYR:CD2	1:A:335:GLY:HA3	2.18	0.79
1:B:31:SER:HB3	1:B:61:ILE:HD11	1.64	0.78
1:A:194:ARG:HH21	1:A:198:LEU:HD21	1.50	0.77
1:A:320:ARG:O	1:A:324:VAL:HG23	1.83	0.77
1:A:258:ASP:HB3	2:A:370:HOH:O	1.85	0.77
1:A:28:LEU:HD11	1:A:74:VAL:CG2	2.13	0.76
1:B:343:ILE:HG23	1:B:344:ASN:N	2.01	0.75
1:A:51:ARG:HA	1:A:55:VAL:HB	1.69	0.75
1:A:326:ASP:CG	1:A:329:ARG:HD2	2.05	0.75
1:B:39:THR:O	1:B:40:SER:HB2	1.88	0.74
1:B:252:LEU:HD11	1:B:262:ILE:CD1	2.16	0.74
1:A:290:MET:HE3	1:A:296:LEU:HD12	1.69	0.73
1:A:296:LEU:HD22	1:A:322:LEU:CD2	2.18	0.73
1:A:327:LYS:O	1:A:328:ARG:HB3	1.87	0.72
1:A:130:LYS:HE3	1:A:163:GLY:O	1.89	0.72
1:B:264:PRO:HG3	2:B:384:HOH:O	1.89	0.72
1:B:194:ARG:NH2	1:B:198:LEU:HD21	2.02	0.71
1:A:218:THR:CG2	1:A:219:GLY:N	2.54	0.71
1:A:61:ILE:HG12	2:A:373:HOH:O	1.90	0.71
1:A:218:THR:HG22	2:A:384:HOH:O	1.91	0.70
1:A:306:ILE:O	1:A:307:SER:HB3	1.91	0.70
1:B:263:LEU:HB3	1:B:264:PRO:HD3	1.73	0.70
1:B:65:MET:O	1:B:69:PRO:HG3	1.91	0.70
1:B:159:SER:O	1:B:163:GLY:HA3	1.92	0.70
1:A:157:ASP:HA	1:A:160:LYS:HG3	1.74	0.70
1:A:250:LEU:HD11	1:A:268:LYS:HD3	1.72	0.69
1:A:252:LEU:HD12	1:A:333:ARG:H	1.56	0.69
1:A:231:GLN:HB2	2:A:375:HOH:O	1.92	0.69
1:B:255:ASN:N	1:B:255:ASN:ND2	2.39	0.69
1:B:324:VAL:HG12	1:B:324:VAL:O	1.92	0.69
1:B:252:LEU:HB3	1:B:253:PRO:HD2	1.75	0.69
1:B:255:ASN:ND2	1:B:255:ASN:H	1.91	0.69
1:B:286:VAL:HG23	1:B:318:LEU:HD13	1.75	0.69
1:A:299:GLY:HA2	1:A:318:LEU:HD13	1.75	0.68
1:B:255:ASN:HD22	1:B:255:ASN:N	1.89	0.68
1:A:291:GLU:O	1:A:292:ASP:O	2.11	0.68
1:A:296:LEU:HD23	1:A:325:ARG:HH21	1.58	0.68
1:A:277:VAL:HG13	1:A:341:ILE:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLN:CG	1:B:174:ASP:N	2.57	0.68
1:B:240:ASN:OD1	1:B:343:ILE:HG22	1.93	0.67
1:A:332:ARG:O	1:A:333:ARG:HB3	1.95	0.67
1:B:265:TYR:O	1:B:334:ILE:HG21	1.94	0.67
1:B:94:LYS:HA	2:B:381:HOH:O	1.95	0.67
1:B:260:LYS:HB2	2:B:380:HOH:O	1.93	0.67
1:B:252:LEU:CD1	1:B:262:ILE:HD12	2.18	0.67
1:B:255:ASN:HB3	1:B:332:ARG:HB2	1.77	0.67
1:A:98:LYS:NZ	1:A:238:VAL:O	2.28	0.66
1:A:285:THR:HG22	1:A:287:ILE:HD12	1.77	0.66
1:A:289:ILE:HD12	1:A:333:ARG:HD2	1.78	0.66
1:A:298:LYS:NZ	1:A:321:GLU:OE2	2.28	0.66
1:A:219:GLY:HA3	2:A:389:HOH:O	1.96	0.66
1:A:257:ARG:NH1	1:A:329:ARG:O	2.27	0.66
1:A:280:ILE:H	1:A:280:ILE:HD13	1.60	0.66
1:B:211:TYR:O	1:B:212:ASN:C	2.33	0.66
1:A:284:ILE:CG1	1:A:306:ILE:HD13	2.26	0.65
1:B:130:LYS:NZ	1:B:162:ASN:OD1	2.31	0.64
1:B:293:LEU:N	1:B:293:LEU:HD13	2.11	0.64
1:B:332:ARG:HG3	1:B:332:ARG:O	1.97	0.64
1:B:206:ILE:CD1	1:B:226:LEU:HB3	2.27	0.64
1:A:262:ILE:HG13	2:A:370:HOH:O	1.98	0.64
1:B:260:LYS:CB	2:B:380:HOH:O	2.46	0.63
1:B:246:HIS:HD2	1:B:276:LYS:O	1.81	0.63
1:A:22:GLN:O	1:A:23:TYR:CB	2.46	0.63
1:A:250:LEU:O	1:A:333:ARG:HG3	1.98	0.63
1:A:252:LEU:HB2	2:A:356:HOH:O	1.98	0.63
1:A:62:ILE:HG13	1:A:63:LYS:H	1.62	0.63
1:A:334:ILE:HD12	1:A:334:ILE:N	2.12	0.63
1:B:265:TYR:O	1:B:334:ILE:CG2	2.46	0.63
1:A:65:MET:SD	1:A:73:TYR:CB	2.86	0.63
1:A:31:SER:O	1:A:76:MET:HB2	1.99	0.63
1:B:168:ARG:O	1:B:172:VAL:HG23	1.99	0.63
1:A:215:GLU:HA	2:A:384:HOH:O	1.98	0.63
1:B:6:VAL:HG22	1:B:143:VAL:HG12	1.80	0.62
1:A:85:SER:O	1:A:89:MET:HG2	1.99	0.62
1:A:218:THR:HG23	1:A:219:GLY:H	1.65	0.62
1:B:255:ASN:HB3	1:B:332:ARG:CB	2.30	0.62
1:B:329:ARG:HH11	1:B:329:ARG:CB	2.12	0.62
1:A:316:GLU:O	1:A:320:ARG:HG2	2.00	0.62
1:A:22:GLN:O	1:A:22:GLN:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ASN:HA	1:B:215:GLU:H	1.65	0.61
1:A:317:ASP:O	1:A:321:GLU:HG3	2.00	0.61
1:A:333:ARG:N	2:A:356:HOH:O	2.33	0.61
1:B:119:PHE:O	1:B:123:ILE:HG13	2.00	0.61
1:A:293:LEU:O	1:A:294:ASP:CB	2.34	0.61
1:A:341:ILE:N	1:A:341:ILE:HD12	2.16	0.61
1:B:259:VAL:O	1:B:260:LYS:HB2	2.00	0.61
1:B:14:GLN:O	1:B:18:VAL:HG23	2.00	0.60
1:A:274:TYR:CD1	1:A:338:LEU:HD11	2.36	0.60
1:B:251:THR:HA	1:B:333:ARG:HG3	1.83	0.60
1:B:155:ILE:HG13	1:B:165:GLY:HA3	1.83	0.60
1:B:173:GLN:HG2	1:B:174:ASP:H	1.66	0.60
1:B:60:PRO:HG3	2:B:373:HOH:O	2.01	0.60
1:B:111:VAL:O	1:B:115:VAL:HG22	2.02	0.60
1:A:20:ASN:O	1:A:22:GLN:O	2.20	0.60
1:B:68:ALA:H	1:B:69:PRO:HD3	1.67	0.60
1:B:294:ASP:O	1:B:295:ILE:HG12	2.02	0.60
1:B:302:PHE:CD1	1:B:306:ILE:HD11	2.37	0.60
1:A:332:ARG:HG3	1:A:332:ARG:O	2.01	0.60
1:B:96:ALA:HB2	1:B:109:LEU:CD2	2.31	0.60
1:A:193:ARG:O	1:A:197:GLU:HG3	2.00	0.60
1:A:328:ARG:O	1:A:328:ARG:HD2	2.01	0.59
1:A:292:ASP:OD2	1:A:329:ARG:NH2	2.34	0.59
1:A:191:LEU:HD21	1:A:218:THR:HA	1.84	0.59
1:A:223:ALA:HB2	2:A:384:HOH:O	2.03	0.59
1:B:173:GLN:HG2	1:B:174:ASP:N	2.18	0.59
1:B:286:VAL:HG23	1:B:318:LEU:CD1	2.33	0.59
1:A:277:VAL:CG1	1:A:341:ILE:HG12	2.31	0.59
1:B:150:ILE:HD13	1:B:150:ILE:N	2.14	0.59
1:B:211:TYR:O	1:B:213:GLU:N	2.36	0.59
1:B:343:ILE:CG2	1:B:344:ASN:N	2.65	0.59
1:A:306:ILE:O	1:A:307:SER:CB	2.51	0.58
1:B:68:ALA:N	1:B:69:PRO:HD3	2.16	0.58
1:B:92:LEU:HD21	1:B:133:ILE:HD11	1.85	0.58
1:B:254:TYR:O	1:B:254:TYR:CD1	2.57	0.58
1:A:25:GLY:O	1:A:49:GLU:HG2	2.04	0.58
1:A:239:GLU:O	1:A:241:LYS:N	2.37	0.58
1:A:113:ASN:C	1:A:115:VAL:N	2.56	0.57
1:A:339:ASP:HA	2:A:362:HOH:O	2.05	0.57
1:A:111:VAL:O	1:A:115:VAL:HG22	2.04	0.57
1:B:149:LYS:HD3	1:B:238:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLU:O	1:B:324:VAL:N	2.37	0.57
1:A:49:GLU:OE1	1:A:49:GLU:N	2.37	0.57
1:A:63:LYS:O	1:A:67:ILE:N	2.26	0.57
1:A:326:ASP:C	2:A:374:HOH:O	2.43	0.57
1:B:206:ILE:HD12	1:B:226:LEU:HB3	1.86	0.57
1:A:218:THR:HG22	1:A:219:GLY:N	2.19	0.57
1:A:296:LEU:HD23	1:A:325:ARG:NH2	2.19	0.57
1:A:283:ARG:HA	1:A:301:LYS:HA	1.86	0.57
1:A:327:LYS:O	1:A:328:ARG:CB	2.53	0.56
1:B:292:ASP:OD2	1:B:329:ARG:HD3	2.05	0.56
1:A:261:VAL:HB	2:A:370:HOH:O	2.03	0.56
1:A:149:LYS:HD3	1:A:238:VAL:HG22	1.87	0.56
1:A:50:ALA:O	1:A:55:VAL:CG2	2.53	0.56
1:B:48:TYR:OH	1:B:161:PRO:HD3	2.05	0.56
1:A:285:THR:HG22	1:A:287:ILE:CD1	2.35	0.56
1:A:292:ASP:OD2	1:A:329:ARG:NE	2.39	0.56
1:B:332:ARG:O	1:B:333:ARG:CB	2.54	0.56
1:A:155:ILE:HG13	1:A:165:GLY:HA3	1.88	0.56
1:B:9:ASP:O	1:B:10:TYR:C	2.44	0.56
1:A:66:GLN:O	1:A:69:PRO:CD	2.54	0.56
1:A:252:LEU:HD21	1:A:334:ILE:HD11	1.88	0.55
1:B:100:GLU:HB2	1:B:239:GLU:O	2.06	0.55
1:A:95:HIS:HE1	1:A:132:GLU:OE2	1.89	0.55
1:A:257:ARG:O	1:A:258:ASP:O	2.24	0.55
1:A:2:ILE:HD13	1:A:119:PHE:HA	1.88	0.55
1:A:249:TYR:CD1	1:A:249:TYR:N	2.74	0.55
1:A:131:GLN:O	1:A:135:GLU:OE1	2.23	0.55
1:B:124:GLU:O	1:B:127:ARG:HB3	2.06	0.55
1:B:96:ALA:HB2	1:B:109:LEU:HD23	1.89	0.55
1:B:293:LEU:H	1:B:293:LEU:HD13	1.70	0.54
1:B:245:PRO:HA	1:B:338:LEU:O	2.07	0.54
1:A:147:PRO:HD3	1:A:167:ILE:O	2.07	0.54
1:A:130:LYS:NZ	1:A:162:ASN:OD1	2.39	0.54
1:A:9:ASP:O	1:A:10:TYR:C	2.46	0.54
1:B:293:LEU:N	1:B:293:LEU:HD22	2.21	0.54
1:A:252:LEU:CD2	1:A:334:ILE:HD11	2.38	0.54
1:B:194:ARG:NH2	1:B:198:LEU:CD2	2.59	0.54
1:A:23:TYR:C	1:A:25:GLY:H	2.10	0.54
1:A:161:PRO:O	1:A:162:ASN:HB3	2.08	0.54
1:B:250:LEU:O	1:B:333:ARG:HG3	2.08	0.54
1:B:285:THR:HG22	1:B:287:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ALA:HB2	1:B:109:LEU:HG	1.89	0.54
1:B:246:HIS:CD2	1:B:276:LYS:O	2.61	0.54
1:A:168:ARG:HB2	1:A:171:GLU:HG2	1.90	0.54
1:A:95:HIS:ND1	1:A:129:ILE:HG12	2.23	0.53
1:B:147:PRO:HG2	1:B:172:VAL:HG21	1.89	0.53
1:B:295:ILE:HG12	2:B:367:HOH:O	2.08	0.53
1:B:67:ILE:O	1:B:68:ALA:HB2	2.08	0.53
1:A:135:GLU:OE1	1:A:135:GLU:N	2.36	0.53
1:A:284:ILE:HG12	1:A:306:ILE:HD13	1.89	0.53
1:B:211:TYR:CD2	1:B:212:ASN:N	2.76	0.53
1:B:277:VAL:HG21	1:B:338:LEU:HD12	1.90	0.53
1:B:292:ASP:CA	1:B:293:LEU:HD22	2.38	0.53
1:A:218:THR:CG2	1:A:219:GLY:H	2.20	0.53
1:A:98:LYS:CE	1:A:238:VAL:O	2.57	0.53
1:B:52:LYS:C	1:B:54:GLY:H	2.11	0.53
1:A:33:TYR:O	1:A:34:SER:HB3	2.09	0.53
1:A:282:MET:HE2	1:A:340:ASN:HB3	1.90	0.53
1:B:129:ILE:O	1:B:133:ILE:HG13	2.09	0.52
1:A:13:ALA:O	1:A:17:GLU:HG3	2.08	0.52
1:A:290:MET:CE	1:A:296:LEU:CD1	2.81	0.52
1:A:326:ASP:N	2:A:374:HOH:O	2.41	0.52
1:A:218:THR:CG2	2:A:384:HOH:O	2.52	0.52
1:B:61:ILE:CG2	1:B:61:ILE:O	2.57	0.52
1:B:292:ASP:HA	1:B:293:LEU:HD22	1.90	0.52
1:B:248:ARG:HG2	1:B:272:GLU:HB2	1.90	0.52
1:A:113:ASN:C	1:A:115:VAL:H	2.12	0.52
1:A:291:GLU:CB	2:A:360:HOH:O	2.56	0.52
1:B:285:THR:HG22	1:B:287:ILE:CD1	2.39	0.52
1:A:104:ILE:HG12	1:A:104:ILE:O	2.10	0.52
1:A:28:LEU:HD12	1:A:29:VAL:N	2.25	0.52
1:A:318:LEU:O	1:A:322:LEU:HG	2.10	0.52
1:B:150:ILE:H	1:B:150:ILE:CD1	2.06	0.52
1:B:220:LYS:HA	1:B:223:ALA:CB	2.38	0.52
1:B:289:ILE:CG2	1:B:293:LEU:HA	2.39	0.52
1:A:19:LEU:C	1:A:21:PRO:HD3	2.31	0.51
1:A:332:ARG:O	1:A:333:ARG:CB	2.58	0.51
1:B:222:LYS:HA	1:B:225:TYR:HB3	1.92	0.51
1:B:277:VAL:CG1	1:B:341:ILE:HG12	2.39	0.51
1:B:325:ARG:O	1:B:325:ARG:HG2	2.10	0.51
1:A:128:LYS:O	1:A:131:GLN:HB2	2.11	0.51
1:B:149:LYS:HB2	2:B:359:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ARG:HH21	1:B:198:LEU:CG	2.22	0.51
1:B:78:LYS:HB3	1:B:79:PRO:HD3	1.92	0.51
1:A:263:LEU:HB3	1:A:264:PRO:HD3	1.91	0.51
1:A:282:MET:HG2	1:A:342:ILE:HD11	1.91	0.51
1:B:149:LYS:O	1:B:152:ALA:N	2.44	0.51
1:B:211:TYR:CG	1:B:212:ASN:N	2.78	0.51
1:A:297:SER:O	1:A:325:ARG:NH2	2.43	0.51
1:A:66:GLN:C	1:A:68:ALA:H	2.14	0.51
1:A:8:PHE:CD2	1:A:8:PHE:N	2.78	0.51
1:B:287:ILE:N	1:B:287:ILE:HD12	2.26	0.51
1:A:13:ALA:HB1	1:A:47:ASN:HB3	1.92	0.50
1:A:65:MET:O	1:A:69:PRO:HA	2.11	0.50
1:A:159:SER:CB	2:A:383:HOH:O	2.41	0.50
1:A:227:LEU:O	1:A:231:GLN:HG3	2.11	0.50
1:A:259:VAL:N	2:A:370:HOH:O	2.44	0.50
1:B:96:ALA:HB2	1:B:109:LEU:CG	2.41	0.50
1:A:258:ASP:C	2:A:370:HOH:O	2.49	0.50
1:B:29:VAL:HG13	1:B:43:VAL:HG13	1.94	0.50
1:B:62:ILE:O	1:B:66:GLN:CG	2.54	0.49
1:A:179:LEU:HD23	1:A:184:ILE:HD11	1.94	0.49
1:B:8:PHE:HA	1:B:141:VAL:HG12	1.93	0.49
1:B:154:ILE:HD13	1:B:179:LEU:HD21	1.95	0.49
1:B:321:GLU:O	1:B:322:LEU:C	2.50	0.49
1:A:257:ARG:C	1:A:258:ASP:O	2.50	0.49
1:A:150:ILE:HD13	1:A:150:ILE:N	2.28	0.49
1:A:194:ARG:HH21	1:A:198:LEU:CD2	2.24	0.49
1:B:194:ARG:HE	1:B:198:LEU:HG	1.77	0.49
1:B:299:GLY:HA2	1:B:318:LEU:HD11	1.94	0.49
1:A:50:ALA:O	1:A:55:VAL:HG23	2.11	0.49
1:A:118:ASN:HD22	1:A:121:ASN:HB2	1.77	0.49
1:A:203:LEU:O	1:A:206:ILE:HB	2.13	0.49
1:A:290:MET:HE3	1:A:296:LEU:CD1	2.40	0.49
1:B:257:ARG:NH2	1:B:327:LYS:HA	2.28	0.49
1:A:296:LEU:HD13	1:A:322:LEU:HB3	1.93	0.49
1:A:65:MET:HE1	1:A:73:TYR:CB	2.42	0.49
1:B:175:PHE:CE2	1:B:179:LEU:HD13	2.48	0.49
1:A:292:ASP:HB2	1:A:294:ASP:OD2	2.13	0.48
1:A:281:PRO:O	1:A:305:GLY:O	2.31	0.48
1:A:158:LYS:HE2	1:A:183:GLU:OE1	2.13	0.48
1:B:124:GLU:O	1:B:127:ARG:CB	2.61	0.48
1:B:284:ILE:HD11	1:B:314:VAL:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:NZ	2:A:355:HOH:O	2.46	0.48
1:A:266:LEU:O	1:A:270:ILE:HG13	2.13	0.48
1:B:214:LEU:HD23	1:B:214:LEU:C	2.33	0.48
1:B:281:PRO:O	1:B:305:GLY:O	2.31	0.48
1:B:323:LEU:C	1:B:325:ARG:H	2.15	0.48
1:B:52:LYS:C	1:B:54:GLY:N	2.67	0.48
1:B:62:ILE:CG1	1:B:63:LYS:N	2.72	0.48
1:A:65:MET:CE	1:A:73:TYR:CB	2.91	0.48
1:B:289:ILE:HG23	1:B:293:LEU:HA	1.96	0.48
1:A:233:LYS:O	1:A:235:SER:N	2.46	0.48
1:A:280:ILE:H	1:A:280:ILE:CD1	2.20	0.48
1:B:61:ILE:O	1:B:61:ILE:HG22	2.13	0.48
1:A:285:THR:HA	1:A:299:GLY:HA3	1.96	0.48
1:B:293:LEU:HD11	1:B:332:ARG:HH12	1.78	0.48
1:A:160:LYS:N	1:A:161:PRO:CD	2.77	0.48
1:A:134:LEU:O	1:A:138:LYS:HA	2.14	0.48
1:A:32:VAL:HG13	1:A:32:VAL:O	2.14	0.48
1:A:343:ILE:O	1:A:344:ASN:HB3	2.13	0.48
1:B:31:SER:CB	1:B:61:ILE:HD11	2.40	0.48
1:A:160:LYS:N	1:A:161:PRO:HD3	2.28	0.48
1:A:210:ASN:OD1	1:A:210:ASN:C	2.52	0.48
1:A:328:ARG:C	1:A:328:ARG:HD2	2.35	0.47
1:B:263:LEU:O	1:B:266:LEU:HB3	2.14	0.47
1:A:1:MET:HA	1:A:112:THR:OG1	2.13	0.47
1:B:341:ILE:HG22	1:B:343:ILE:HD12	1.94	0.47
1:A:218:THR:HB	2:A:384:HOH:O	2.14	0.47
1:B:5:PHE:O	1:B:143:VAL:HA	2.14	0.47
1:B:277:VAL:HG12	1:B:279:GLY:H	1.78	0.47
1:B:62:ILE:HG13	1:B:63:LYS:H	1.78	0.47
1:A:168:ARG:H	1:A:171:GLU:CD	2.18	0.47
1:A:80:ILE:O	1:A:84:PHE:HB2	2.15	0.47
1:B:214:LEU:HD23	1:B:214:LEU:O	2.15	0.47
1:A:100:GLU:HG2	1:A:100:GLU:O	2.15	0.46
1:B:130:LYS:HE3	1:B:163:GLY:O	2.15	0.46
1:B:153:LYS:O	1:B:157:ASP:OD1	2.34	0.46
1:A:162:ASN:CG	1:A:162:ASN:O	2.54	0.46
1:A:249:TYR:HB2	1:A:333:ARG:HD3	1.98	0.46
1:A:10:TYR:CE1	1:A:14:GLN:HB2	2.51	0.46
1:A:151:LEU:HB3	1:A:167:ILE:HD12	1.97	0.46
1:A:98:LYS:HE3	1:A:238:VAL:O	2.15	0.46
1:B:48:TYR:CZ	1:B:161:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:O	1:A:143:VAL:HA	2.15	0.46
1:A:282:MET:HG2	1:A:342:ILE:CD1	2.45	0.46
1:B:255:ASN:HB3	1:B:332:ARG:CA	2.46	0.45
1:A:297:SER:O	1:A:298:LYS:HB2	2.16	0.45
1:A:10:TYR:O	1:A:10:TYR:CD1	2.69	0.45
1:A:130:LYS:CE	1:A:163:GLY:O	2.63	0.45
1:A:65:MET:HG3	2:A:388:HOH:O	2.17	0.45
1:B:250:LEU:N	1:B:334:ILE:O	2.49	0.45
1:B:270:ILE:HG12	1:B:336:VAL:HG21	1.97	0.45
1:A:290:MET:HE1	1:A:296:LEU:CD1	2.39	0.45
1:B:343:ILE:O	1:B:344:ASN:CB	2.64	0.45
1:A:159:SER:O	1:A:163:GLY:HA3	2.16	0.45
1:A:218:THR:CB	2:A:384:HOH:O	2.64	0.45
1:A:283:ARG:HG2	1:A:301:LYS:CB	2.47	0.45
1:A:249:TYR:CB	1:A:333:ARG:HD3	2.47	0.45
1:B:249:TYR:HE1	2:B:356:HOH:O	1.99	0.45
1:A:195:LEU:HD22	1:A:200:ILE:HD12	1.98	0.45
1:A:19:LEU:O	1:A:21:PRO:HD3	2.17	0.45
1:B:127:ARG:HH11	1:B:164:LEU:HD13	1.82	0.45
1:B:151:LEU:HD21	1:B:176:LEU:HD21	1.99	0.45
1:B:99:ILE:O	1:B:240:ASN:HA	2.17	0.45
1:B:91:LEU:HD11	1:B:132:GLU:OE1	2.18	0.44
1:A:176:LEU:CD1	1:A:232:ASN:HB2	2.47	0.44
1:A:227:LEU:O	1:A:230:ALA:HB3	2.18	0.44
1:A:68:ALA:N	1:A:69:PRO:HD3	2.30	0.44
1:A:11:PHE:O	1:A:15:VAL:HG23	2.16	0.44
1:A:214:LEU:O	1:A:214:LEU:HD23	2.17	0.44
1:A:265:TYR:HB3	1:A:334:ILE:HD13	1.99	0.44
1:B:127:ARG:HD2	1:B:164:LEU:CD1	2.48	0.44
1:A:5:PHE:CD1	1:A:108:TYR:CE2	3.06	0.44
1:A:339:ASP:CA	2:A:362:HOH:O	2.62	0.44
1:A:64:ALA:C	1:A:66:GLN:H	2.20	0.44
1:B:104:ILE:O	1:B:104:ILE:HG12	2.17	0.44
1:B:253:PRO:HG2	1:B:254:TYR:H	1.83	0.44
1:B:329:ARG:HH11	1:B:329:ARG:HB3	1.82	0.44
1:B:1:MET:O	1:B:147:PRO:HA	2.18	0.44
1:B:33:TYR:O	1:B:34:SER:HB3	2.16	0.44
1:A:291:GLU:O	1:A:292:ASP:C	2.56	0.44
1:B:2:ILE:HG23	1:B:119:PHE:CD1	2.53	0.44
1:A:252:LEU:CD1	1:A:331:VAL:HG12	2.48	0.44
1:B:92:LEU:HB3	1:B:109:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:HB2	1:B:11:PHE:HB2	1.99	0.44
1:A:250:LEU:CD1	1:A:268:LYS:HB3	2.48	0.43
1:B:326:ASP:C	1:B:326:ASP:OD1	2.56	0.43
1:B:329:ARG:HH11	1:B:329:ARG:HB2	1.83	0.43
1:A:296:LEU:CD2	1:A:325:ARG:NH2	2.81	0.43
1:B:270:ILE:CG1	1:B:336:VAL:HG21	2.48	0.43
1:B:31:SER:HB3	1:B:61:ILE:CD1	2.41	0.43
1:B:343:ILE:HG23	1:B:344:ASN:H	1.77	0.43
1:B:127:ARG:NH1	1:B:164:LEU:HD13	2.33	0.43
1:B:12:PHE:HB2	1:B:45:THR:HB	2.00	0.43
1:A:10:TYR:HD1	1:A:13:ALA:HB3	1.83	0.43
1:A:184:ILE:HD13	1:A:229:LEU:CD2	2.48	0.43
1:B:321:GLU:O	1:B:323:LEU:N	2.51	0.43
1:B:209:LYS:O	1:B:211:TYR:N	2.40	0.43
1:B:279:GLY:O	1:B:341:ILE:HG23	2.19	0.43
1:B:280:ILE:HA	1:B:281:PRO:HD3	1.73	0.43
1:B:302:PHE:HB2	1:B:306:ILE:HG13	2.00	0.43
1:A:91:LEU:HD11	1:A:136:LYS:HD2	2.00	0.43
1:B:248:ARG:HE	1:B:272:GLU:CD	2.22	0.43
1:B:324:VAL:CG1	1:B:324:VAL:O	2.62	0.43
1:B:25:GLY:HA2	1:B:49:GLU:OE2	2.19	0.43
1:A:286:VAL:HG21	1:A:318:LEU:HB2	2.00	0.43
1:B:160:LYS:HB2	1:B:161:PRO:HA	1.99	0.43
1:A:281:PRO:HG2	1:A:338:LEU:HD13	2.00	0.43
1:A:281:PRO:O	1:A:306:ILE:HD12	2.18	0.43
1:A:33:TYR:O	1:A:34:SER:CB	2.66	0.43
1:A:27:PRO:HA	1:A:49:GLU:HB2	2.00	0.43
1:A:306:ILE:CG2	1:A:307:SER:H	2.11	0.43
1:A:337:LYS:HE2	2:A:378:HOH:O	2.18	0.43
1:B:280:ILE:HD12	1:B:342:ILE:HD12	2.01	0.43
1:B:287:ILE:N	1:B:287:ILE:CD1	2.82	0.43
1:B:332:ARG:O	1:B:333:ARG:HB3	2.18	0.42
1:A:28:LEU:C	1:A:28:LEU:HD12	2.39	0.42
1:B:8:PHE:N	1:B:8:PHE:CD2	2.85	0.42
1:A:92:LEU:HD21	1:A:133:ILE:HD11	2.02	0.42
1:B:158:LYS:NZ	1:B:183:GLU:OE1	2.48	0.42
1:A:254:TYR:CD2	1:A:254:TYR:N	2.87	0.42
1:A:305:GLY:O	1:A:306:ILE:HB	2.20	0.42
1:A:250:LEU:O	1:A:333:ARG:HA	2.19	0.42
1:B:282:MET:O	1:B:302:PHE:N	2.41	0.42
1:B:150:ILE:CD1	2:B:359:HOH:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TYR:HD1	1:B:256:THR:HG23	1.83	0.42
1:A:252:LEU:O	1:A:253:PRO:C	2.57	0.42
1:A:48:TYR:CB	2:A:386:HOH:O	2.68	0.42
1:A:11:PHE:O	1:A:12:PHE:C	2.57	0.42
1:A:279:GLY:O	1:A:341:ILE:HG23	2.19	0.42
1:B:120:GLU:OE1	1:B:123:ILE:HD12	2.20	0.42
1:B:130:LYS:HE2	1:B:141:VAL:O	2.19	0.42
1:B:234:TYR:O	1:B:234:TYR:CD2	2.73	0.42
1:B:278:ASN:CB	1:B:343:ILE:HD11	2.29	0.42
1:A:132:GLU:HG3	1:A:136:LYS:HE3	2.02	0.41
1:A:119:PHE:CD1	1:A:169:PRO:HD3	2.55	0.41
1:A:180:ASP:OD1	1:A:202:LYS:HD3	2.20	0.41
1:A:222:LYS:HG3	2:A:389:HOH:O	2.20	0.41
1:A:63:LYS:O	1:A:64:ALA:C	2.58	0.41
1:B:52:LYS:O	1:B:54:GLY:N	2.53	0.41
1:A:98:LYS:HE3	1:A:238:VAL:HB	2.02	0.41
1:B:292:ASP:C	1:B:293:LEU:CD2	2.78	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD23	1.88	0.41
1:A:20:ASN:O	1:A:22:GLN:N	2.54	0.41
1:A:341:ILE:N	1:A:341:ILE:CD1	2.81	0.41
1:A:184:ILE:HA	1:A:185:PRO:HD3	1.79	0.41
1:A:281:PRO:HG2	1:A:338:LEU:HD22	2.03	0.41
1:B:95:HIS:HE1	1:B:132:GLU:OE2	2.03	0.41
1:A:20:ASN:O	1:A:21:PRO:C	2.57	0.41
1:A:296:LEU:C	1:A:296:LEU:CD2	2.88	0.41
1:A:332:ARG:CG	1:A:332:ARG:O	2.66	0.41
1:B:111:VAL:O	1:B:112:THR:C	2.58	0.41
1:B:125:LEU:C	1:B:127:ARG:H	2.24	0.41
1:A:113:ASN:O	1:A:115:VAL:N	2.54	0.41
1:B:125:LEU:C	1:B:127:ARG:N	2.74	0.41
1:B:219:GLY:O	1:B:220:LYS:CB	2.69	0.41
1:B:259:VAL:O	1:B:260:LYS:CB	2.65	0.41
1:A:257:ARG:HG2	1:A:330:ASN:HA	2.02	0.41
1:B:11:PHE:CE2	1:B:81:TYR:HB3	2.55	0.41
1:B:332:ARG:O	1:B:332:ARG:CG	2.67	0.41
1:A:33:TYR:HB2	1:A:34:SER:H	1.42	0.41
1:B:250:LEU:C	1:B:333:ARG:HG3	2.42	0.40
1:A:109:LEU:N	1:A:109:LEU:HD12	2.36	0.40
1:B:295:ILE:HG22	1:B:295:ILE:O	2.20	0.40
1:B:30:VAL:O	1:B:44:ALA:HB3	2.21	0.40
1:B:65:MET:O	1:B:69:PRO:CG	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:CD1	1:A:268:LYS:HD3	2.46	0.40
1:B:294:ASP:O	1:B:295:ILE:CG1	2.69	0.40
1:A:100:GLU:OE1	1:A:243:LYS:HE3	2.22	0.40
1:A:284:ILE:HD11	1:A:306:ILE:HD13	2.04	0.40
1:A:344:ASN:C	1:A:344:ASN:HD22	2.24	0.40
1:A:254:TYR:CE1	1:A:256:THR:HG22	2.57	0.40
1:B:101:VAL:HG11	1:B:244:ILE:HD12	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	329/354 (93%)	259 (79%)	40 (12%)	30 (9%)	1	1
1	B	337/354 (95%)	274 (81%)	45 (13%)	18 (5%)	2	7
All	All	666/708 (94%)	533 (80%)	85 (13%)	48 (7%)	1	3

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	75	PRO
1	A	116	GLU
1	A	234	TYR
1	A	240	ASN
1	A	258	ASP
1	A	292	ASP
1	A	294	ASP
1	A	307	SER
1	B	40	SER
1	B	212	ASN

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Mol	Chain	Res	Type
1	B	321	GLU
1	A	62	ILE
1	A	211	TYR
1	A	220	LYS
1	A	298	LYS
1	A	306	ILE
1	A	328	ARG
1	A	333	ARG
1	B	68	ALA
1	B	211	TYR
1	B	306	ILE
1	B	322	LEU
1	A	64	ALA
1	A	131	GLN
1	A	164	LEU
1	A	293	LEU
1	B	27	PRO
1	B	198	LEU
1	B	213	GLU
1	B	220	LYS
1	A	25	GLY
1	A	27	PRO
1	A	68	ALA
1	A	218	THR
1	A	219	GLY
1	B	114	LYS
1	B	326	ASP
1	A	67	ILE
1	A	304	HIS
1	B	95	HIS
1	B	261	VAL
1	A	60	PRO
1	A	102	ALA
1	B	295	ILE
1	B	333	ARG
1	A	253	PRO
1	B	324	VAL

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	257/309 (83%)	228 (89%)	29 (11%)	7	20
1	B	262/309 (85%)	243 (93%)	19 (7%)	16	42
All	All	519/618 (84%)	471 (91%)	48 (9%)	11	30

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	22	GLN
1	A	47	ASN
1	A	49	GLU
1	A	52	LYS
1	A	59	MET
1	A	62	ILE
1	A	65	MET
1	A	84	PHE
1	A	116	GLU
1	A	121	ASN
1	A	147	PRO
1	A	160	LYS
1	A	170	THR
1	A	178	GLU
1	A	210	ASN
1	A	218	THR
1	A	231	GLN
1	A	249	TYR
1	A	254	TYR
1	A	280	ILE
1	A	294	ASP
1	A	296	LEU
1	A	297	SER
1	A	310	ASN
1	A	328	ARG
1	A	332	ARG
1	A	334	ILE
1	A	344	ASN
1	B	2	ILE
1	B	22	GLN

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Mol	Chain	Res	Type
1	B	39	THR
1	B	40	SER
1	B	70	SER
1	B	79	PRO
1	B	150	ILE
1	B	157	ASP
1	B	174	ASP
1	B	193	ARG
1	B	220	LYS
1	B	227	LEU
1	B	255	ASN
1	B	292	ASP
1	B	293	LEU
1	B	309	ASP
1	B	329	ARG
1	B	332	ARG
1	B	343	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	90	ASN
1	A	95	HIS
1	A	118	ASN
1	A	121	ASN
1	A	212	ASN
1	A	344	ASN
1	B	22	GLN
1	B	90	ASN
1	B	95	HIS
1	B	231	GLN
1	B	255	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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	333/354 (94%)	0.49	29 (8%) 11 6	50, 71, 99, 104	0
1	B	341/354 (96%)	0.40	12 (3%) 44 33	56, 75, 92, 102	0
All	All	674/708 (95%)	0.44	41 (6%) 22 14	50, 73, 96, 104	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	PRO	4.8
1	A	73	TYR	4.8
1	A	71	ALA	4.5
1	A	23	TYR	4.3
1	A	53	LEU	4.3
1	A	64	ALA	4.1
1	B	288	ALA	4.1
1	A	34	SER	3.8
1	A	62	ILE	3.8
1	A	60	PRO	3.6
1	A	50	ALA	3.4
1	A	59	MET	3.3
1	A	296	LEU	3.3
1	B	324	VAL	3.1
1	A	211	TYR	3.1
1	A	74	VAL	3.1
1	B	323	LEU	3.1
1	A	65	MET	3.1
1	A	29	VAL	3.0
1	B	53	LEU	2.9
1	A	326	ASP	2.9
1	A	305	GLY	2.9
1	A	328	ARG	2.8
1	B	322	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	325	ARG	2.8
1	A	30	VAL	2.7
1	B	60	PRO	2.6
1	B	328	ARG	2.6
1	A	292	ASP	2.5
1	A	290	MET	2.5
1	B	48	TYR	2.4
1	B	40	SER	2.4
1	A	72	ILE	2.4
1	B	284	ILE	2.2
1	A	187	ILE	2.2
1	A	227	LEU	2.2
1	A	67	ILE	2.2
1	A	294	ASP	2.1
1	B	67	ILE	2.1
1	B	39	THR	2.0
1	A	295	ILE	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 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.