



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:59 am BST

PDB ID : 1DR8
Title : STRUCTURE OF MODIFIED 3-ISOPROPYLMALATE DEHYDROGENASE AT THE C-TERMINUS, HD177
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Deposited on : 2000-01-06
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

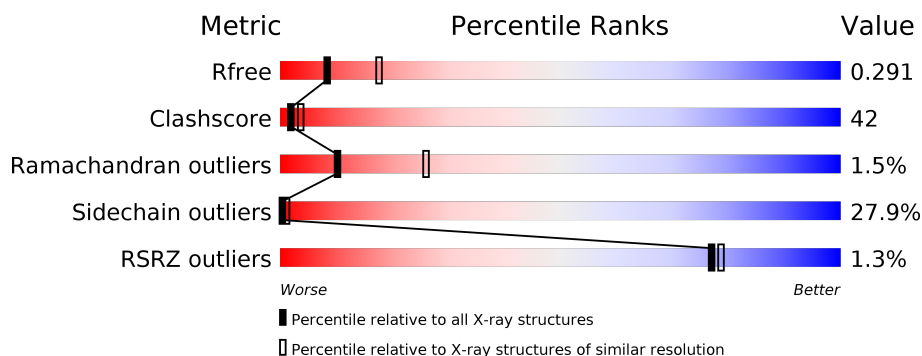
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	344	
1	B	344	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5233 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 3-ISOPROPYLMALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2580	1645	446	482	7			
1	B	344	Total	C	N	O	S	0	0	0
			2580	1645	446	482	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ARG	SER	see remark 999	UNP Q5SIY4
A	172	LEU	ALA	see remark 999	UNP Q5SIY4
A	341	GLY	LEU	see remark 999	UNP Q5SIY4
A	342	MET	ARG	see remark 999	UNP Q5SIY4
A	343	GLY	HIS	see remark 999	UNP Q5SIY4
A	344	ILE	LEU	see remark 999	UNP Q5SIY4
B	85	ARG	SER	see remark 999	UNP Q5SIY4
B	172	LEU	ALA	see remark 999	UNP Q5SIY4
B	341	GLY	LEU	see remark 999	UNP Q5SIY4
B	342	MET	ARG	see remark 999	UNP Q5SIY4
B	343	GLY	HIS	see remark 999	UNP Q5SIY4
B	344	ILE	LEU	see remark 999	UNP Q5SIY4

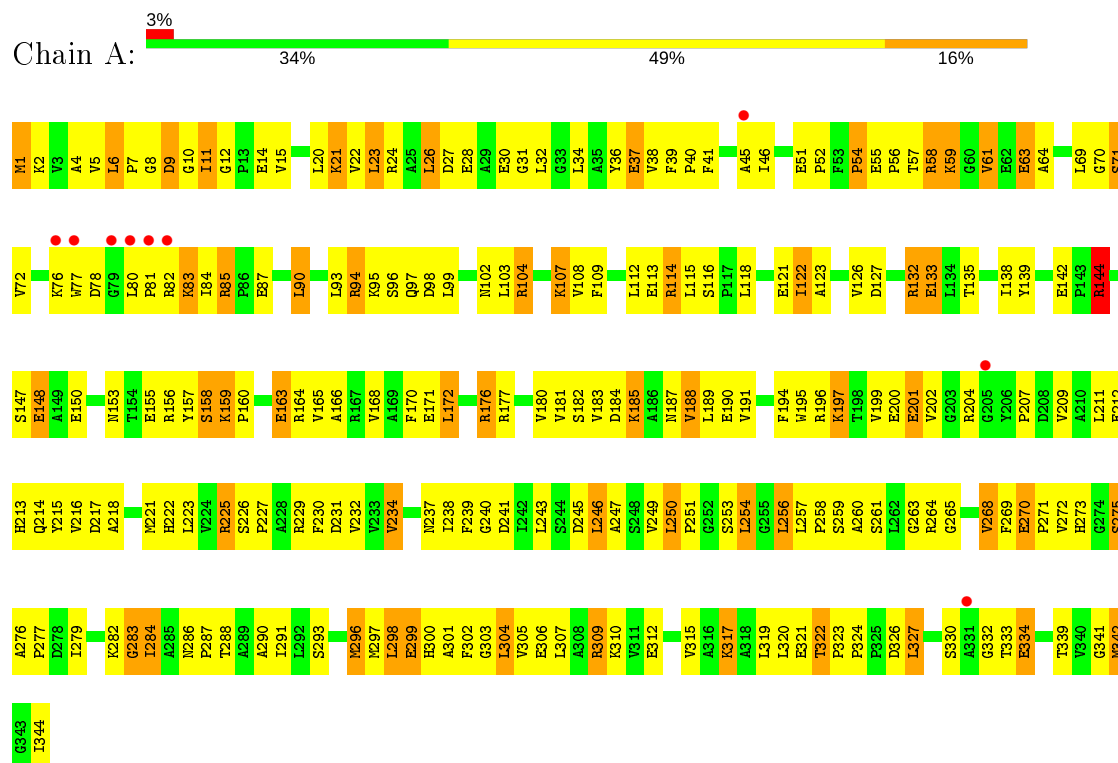
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	35	Total	O	0	0
			35	35		

3 Residue-property plots

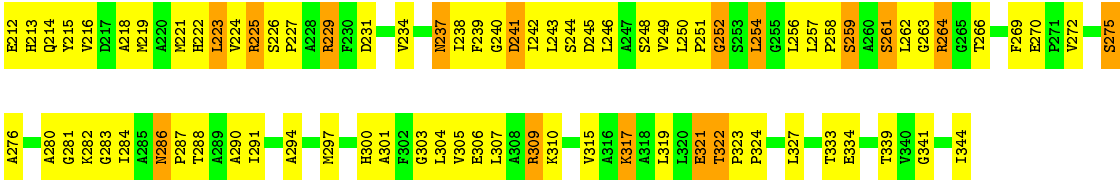
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 3-ISOPROPYLMALATE DEHYDROGENASE



• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.89Å 85.98Å 54.37Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	6.50 – 2.70 53.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	80.2 (6.50-2.70) 80.5 (53.49-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 2.69Å)	Xtriage
Refinement program	X-PLOR (ONLINE) 98.1	Depositor
R, R_{free}	0.205 , 0.302 0.197 , 0.291	Depositor DCC
R_{free} test set	1517 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5233	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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

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	0/2634	0.64	0/3573
1	B	0.41	0/2634	0.63	0/3573
All	All	0.41	0/5268	0.64	0/7146

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	2580	0	2618	260	0
1	B	2580	0	2618	201	0
2	A	38	0	0	11	0
2	B	35	0	0	10	0
All	All	5233	0	5236	435	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 42.

All (435) 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:160:PRO:HA	2:A:369:HOH:O	1.27	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:HG23	1:B:153:ASN:HD22	1.09	1.14
1:A:58:ARG:HB2	1:A:58:ARG:HH11	1.20	1.02
1:A:148:GLU:HB2	2:A:349:HOH:O	1.59	1.00
1:B:90:LEU:HG	1:B:94:ARG:HH22	1.26	0.97
1:A:132:ARG:HH11	1:A:132:ARG:HG2	1.29	0.96
1:A:164:ARG:HH11	1:A:264:ARG:HH12	1.06	0.92
1:B:103:LEU:HD21	1:B:172:LEU:HD21	1.53	0.90
1:A:196:ARG:NH1	1:A:213:HIS:HB3	1.86	0.90
1:B:185:LYS:HG2	1:B:216:VAL:HG12	1.55	0.89
1:B:188:VAL:O	1:B:189:LEU:HD23	1.71	0.89
1:A:287:PRO:O	1:A:291:ILE:HG13	1.72	0.89
1:A:191:VAL:HG23	1:B:153:ASN:ND2	1.87	0.88
1:B:115:LEU:HD21	1:B:327:LEU:HD22	1.54	0.88
1:B:115:LEU:HB3	2:B:356:HOH:O	1.75	0.86
1:A:324:PRO:HB3	2:A:368:HOH:O	1.77	0.85
1:B:181:VAL:HG13	1:B:212:GLU:HG3	1.57	0.85
1:A:55:GLU:HA	1:A:58:ARG:NH1	1.92	0.84
1:A:132:ARG:NH1	1:A:132:ARG:HG2	1.91	0.83
1:A:158:SER:OG	1:A:160:PRO:HD2	1.77	0.83
1:A:164:ARG:HH11	1:A:264:ARG:NH1	1.77	0.82
1:A:58:ARG:CB	1:A:58:ARG:HH11	1.93	0.82
1:B:109:PHE:HB2	1:B:112:LEU:HD12	1.60	0.82
1:B:90:LEU:HG	1:B:94:ARG:NH2	1.95	0.81
1:A:82:ARG:NH1	1:A:85:ARG:HH21	1.78	0.81
1:A:21:LYS:HG3	1:A:24:ARG:HH21	1.46	0.81
1:B:67:VAL:HG23	1:B:266:THR:HG21	1.64	0.80
1:A:102:ASN:HD22	1:A:132:ARG:HH12	1.28	0.78
1:B:170:PHE:HZ	1:B:211:LEU:HD22	1.48	0.78
1:B:76:LYS:HG3	1:B:76:LYS:O	1.82	0.78
1:A:200:GLU:HG2	2:A:357:HOH:O	1.84	0.78
1:A:196:ARG:HH11	1:A:196:ARG:HG3	1.48	0.78
1:A:55:GLU:HA	1:A:58:ARG:HH12	1.46	0.78
1:B:5:VAL:HG12	1:B:7:PRO:HD3	1.64	0.78
1:A:104:ARG:NH1	1:A:272:VAL:HG21	1.99	0.77
1:B:181:VAL:HG13	1:B:212:GLU:CG	2.14	0.76
1:A:288:THR:HG23	1:A:315:VAL:CG1	2.15	0.76
1:A:1:MET:HE1	1:A:32:LEU:HD23	1.68	0.76
1:A:269:PHE:CZ	1:A:297:MET:HA	2.22	0.75
1:B:218:ALA:HA	1:B:221:MET:HE2	1.68	0.75
1:A:118:LEU:HB3	1:A:122:ILE:HG12	1.67	0.75
1:B:116:SER:HB2	1:B:250:LEU:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:HG2	1:A:309:ARG:HH11	1.53	0.74
1:B:132:ARG:HB2	1:B:240:GLY:HA3	1.69	0.74
1:A:132:ARG:HB2	1:A:240:GLY:HA3	1.70	0.74
1:B:58:ARG:HG2	2:B:372:HOH:O	1.86	0.74
1:B:196:ARG:NH1	1:B:213:HIS:HB3	2.02	0.73
1:B:85:ARG:HD2	2:B:352:HOH:O	1.87	0.73
1:A:142:GLU:H	1:A:156:ARG:NH2	1.87	0.73
1:A:133:GLU:HG2	1:A:165:VAL:HG11	1.70	0.72
1:B:76:LYS:HG2	1:B:77:TRP:CE2	2.24	0.72
1:B:172:LEU:HD11	1:B:300:HIS:CD2	2.24	0.72
1:B:286:ASN:ND2	1:B:288:THR:H	1.88	0.72
1:B:115:LEU:O	1:B:252:GLY:HA2	1.90	0.72
1:A:104:ARG:HH11	1:A:272:VAL:HG21	1.54	0.71
1:A:1:MET:HG2	1:A:302:PHE:CZ	2.25	0.71
1:A:164:ARG:NH1	1:A:264:ARG:HH12	1.85	0.71
1:B:67:VAL:HG23	1:B:266:THR:CG2	2.21	0.71
1:A:21:LYS:HG3	1:A:24:ARG:NH2	2.04	0.71
1:A:309:ARG:NH1	1:A:309:ARG:HG2	2.05	0.70
1:A:102:ASN:HD22	1:A:132:ARG:NH1	1.90	0.70
1:A:102:ASN:ND2	1:A:132:ARG:HH12	1.90	0.69
1:A:6:LEU:HD12	1:A:39:PHE:HB2	1.73	0.69
1:B:107:LYS:HE2	1:B:127:ASP:OD1	1.93	0.69
1:B:115:LEU:HD21	1:B:327:LEU:CD2	2.23	0.69
1:B:118:LEU:HD11	1:B:250:LEU:HG	1.73	0.69
1:B:113:GLU:HB3	1:B:120:GLU:HG3	1.75	0.69
1:B:213:HIS:O	1:B:214:GLN:HG2	1.93	0.69
1:A:187:ASN:HB3	1:A:215:TYR:CZ	2.28	0.69
1:A:191:VAL:H	1:B:153:ASN:ND2	1.90	0.69
1:A:259:SER:HB3	1:A:270:GLU:O	1.92	0.69
1:A:309:ARG:CG	1:A:309:ARG:HH11	2.05	0.68
1:B:54:PRO:HB2	1:B:56:PRO:HD2	1.75	0.68
1:B:183:VAL:HG11	1:B:243:LEU:HD11	1.74	0.68
1:A:164:ARG:O	1:A:168:VAL:HG23	1.92	0.68
1:B:319:LEU:HD22	1:B:327:LEU:HD11	1.76	0.68
1:B:85:ARG:HB3	1:B:87:GLU:HG2	1.76	0.68
1:B:246:LEU:O	1:B:249:VAL:HG22	1.94	0.68
1:A:153:ASN:OD1	1:B:189:LEU:HD22	1.94	0.68
1:B:158:SER:C	1:B:160:PRO:HD2	2.14	0.68
1:B:132:ARG:NH2	1:B:241:ASP:OD1	2.27	0.67
1:A:196:ARG:NH1	1:A:196:ARG:HG3	2.09	0.67
1:A:103:LEU:HD21	1:A:172:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD23	1:B:35:ALA:N	2.10	0.67
1:A:249:VAL:CG1	1:B:221:MET:HG2	2.25	0.67
1:B:281:GLY:C	1:B:282:LYS:HE2	2.15	0.66
1:B:27:ASP:HA	1:B:32:LEU:HG	1.77	0.66
1:A:176:ARG:HH11	1:A:176:ARG:HB3	1.59	0.66
1:A:234:VAL:HG23	2:A:367:HOH:O	1.96	0.66
1:A:85:ARG:HB3	1:A:85:ARG:NH1	2.11	0.66
1:A:58:ARG:NH1	1:A:58:ARG:HB2	2.02	0.66
1:A:222:HIS:HA	1:A:225:ARG:HG3	1.78	0.66
1:A:170:PHE:HZ	1:A:211:LEU:HD13	1.61	0.65
1:B:309:ARG:HH11	1:B:309:ARG:HG3	1.61	0.65
1:B:103:LEU:CD2	1:B:172:LEU:HD21	2.24	0.65
1:B:259:SER:HB2	1:B:270:GLU:O	1.95	0.65
1:B:53:PHE:CZ	1:B:58:ARG:HG3	2.32	0.65
1:B:303:GLY:O	1:B:305:VAL:HG23	1.97	0.65
1:A:299:GLU:OE2	1:A:305:VAL:HG12	1.97	0.64
1:A:85:ARG:HB3	1:A:85:ARG:HH11	1.62	0.64
1:A:170:PHE:CZ	1:A:211:LEU:HD13	2.32	0.64
1:A:59:LYS:O	1:A:63:GLU:HG2	1.96	0.64
1:B:180:VAL:CG2	1:B:211:LEU:HD13	2.28	0.64
1:A:11:ILE:HD12	1:A:276:ALA:HB3	1.80	0.63
1:B:188:VAL:HG12	1:B:188:VAL:O	1.99	0.63
1:A:82:ARG:HB3	1:A:83:LYS:HE2	1.80	0.63
1:B:53:PHE:CE2	1:B:58:ARG:HG3	2.34	0.63
1:A:288:THR:HG23	1:A:315:VAL:HG11	1.80	0.62
1:A:6:LEU:CD1	1:A:39:PHE:HB2	2.28	0.62
1:A:85:ARG:HH11	1:A:85:ARG:CB	2.11	0.62
1:A:288:THR:HG21	1:A:319:LEU:HD11	1.81	0.62
1:A:57:THR:O	1:A:61:VAL:HG13	2.00	0.62
1:B:199:VAL:O	1:B:202:VAL:HG12	1.98	0.62
1:A:103:LEU:HD11	1:A:172:LEU:CD2	2.30	0.62
1:A:304:LEU:HG	1:A:307:LEU:HD22	1.81	0.62
1:B:264:ARG:HG2	1:B:264:ARG:O	1.99	0.62
1:B:254:LEU:HB2	2:B:369:HOH:O	2.01	0.61
1:A:104:ARG:NH1	1:A:272:VAL:HG11	2.15	0.61
1:A:1:MET:CE	1:A:32:LEU:HD23	2.30	0.61
1:A:246:LEU:O	1:A:249:VAL:HG22	2.00	0.61
1:B:26:LEU:HD21	1:B:307:LEU:HD22	1.81	0.61
1:A:132:ARG:CG	1:A:132:ARG:HH11	2.07	0.61
1:A:144:ARG:HD3	1:A:144:ARG:O	2.01	0.61
1:A:191:VAL:H	1:B:153:ASN:HD21	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:HD12	1:B:212:GLU:N	2.15	0.61
1:A:299:GLU:HG3	1:A:300:HIS:N	2.16	0.60
1:A:271:PRO:HB2	1:A:273:HIS:CD2	2.35	0.60
1:A:142:GLU:H	1:A:156:ARG:HH21	1.48	0.60
1:A:118:LEU:HB3	1:A:122:ILE:CG1	2.31	0.60
1:A:97:GLN:HB3	1:A:265:GLY:HA3	1.84	0.60
1:B:26:LEU:O	1:B:30:GLU:HB2	2.01	0.60
1:A:103:LEU:HD11	1:A:172:LEU:HD21	1.83	0.60
1:A:249:VAL:HG13	1:B:221:MET:HG2	1.82	0.59
1:B:319:LEU:HD22	1:B:327:LEU:CD1	2.31	0.59
1:A:51:GLU:O	1:A:54:PRO:HD3	2.02	0.59
1:B:11:ILE:O	1:B:15:VAL:HG13	2.02	0.59
1:A:190:GLU:OE2	1:A:190:GLU:N	2.34	0.59
1:B:144:ARG:HA	1:B:152:TRP:O	2.02	0.59
1:A:321:GLU:C	1:A:323:PRO:HD3	2.24	0.59
1:B:184:ASP:OD2	1:B:196:ARG:HD3	2.03	0.59
1:A:164:ARG:HD3	1:A:264:ARG:HH22	1.68	0.58
1:B:199:VAL:HG12	1:B:211:LEU:HD21	1.85	0.58
1:A:176:ARG:HH12	1:A:177:ARG:HH11	1.51	0.58
1:B:287:PRO:O	1:B:291:ILE:HD12	2.03	0.58
1:B:121:GLU:HG2	1:B:124:ARG:HH22	1.67	0.58
1:A:112:LEU:HD21	1:A:320:LEU:HG	1.85	0.58
1:A:126:VAL:HG22	1:A:227:PRO:HB2	1.86	0.58
1:A:341:GLY:HA3	2:A:352:HOH:O	2.04	0.58
1:B:55:GLU:N	1:B:56:PRO:HD2	2.19	0.58
1:A:223:LEU:HD21	1:A:247:ALA:HB2	1.85	0.58
1:A:276:ALA:HB1	1:A:279:ILE:HG12	1.86	0.57
1:B:121:GLU:HG2	1:B:124:ARG:NH2	2.19	0.57
1:A:187:ASN:OD1	1:A:188:VAL:HG12	2.04	0.57
1:A:238:ILE:HD11	1:B:239:PHE:HZ	1.68	0.57
1:A:164:ARG:CD	1:A:264:ARG:HH22	2.18	0.57
1:A:118:LEU:HG	1:A:122:ILE:HD11	1.86	0.57
1:B:146:MET:SD	1:B:147:SER:O	2.63	0.56
1:B:282:LYS:N	1:B:282:LYS:HE2	2.20	0.56
1:B:197:LYS:HE2	1:B:197:LYS:O	2.05	0.56
1:B:99:LEU:HA	1:B:263:GLY:HA3	1.88	0.56
1:A:201:GLU:HA	1:A:204:ARG:NH2	2.20	0.56
1:B:341:GLY:O	1:B:344:ILE:HB	2.06	0.56
1:A:118:LEU:CG	1:A:122:ILE:HD11	2.36	0.56
1:A:163:GLU:HG3	1:A:202:VAL:CG2	2.36	0.56
1:A:30:GLU:HB2	1:A:32:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HG3	1:A:188:VAL:CG1	2.36	0.56
1:A:269:PHE:CD1	1:A:297:MET:HB2	2.41	0.56
1:A:176:ARG:HH12	1:A:177:ARG:NH1	2.04	0.56
1:A:231:ASP:OD1	1:A:232:VAL:HG23	2.06	0.55
1:B:126:VAL:HG22	1:B:227:PRO:HB2	1.87	0.55
1:B:176:ARG:HD3	1:B:231:ASP:OD1	2.06	0.55
1:A:221:MET:HG2	1:B:249:VAL:CG1	2.37	0.55
1:A:14:GLU:OE1	1:A:283:GLY:HA2	2.07	0.55
1:A:221:MET:HG2	1:B:249:VAL:HG13	1.89	0.55
1:B:223:LEU:O	1:B:250:LEU:HD21	2.06	0.55
1:A:234:VAL:CG2	2:A:367:HOH:O	2.53	0.55
1:B:270:GLU:HG2	2:B:366:HOH:O	2.06	0.55
1:B:87:GLU:CD	1:B:87:GLU:H	2.07	0.55
1:A:138:ILE:HD13	2:B:361:HOH:O	2.07	0.55
1:A:226:SER:N	1:A:227:PRO:CD	2.70	0.55
1:A:41:PHE:CE2	1:A:72:VAL:HG11	2.42	0.55
1:A:341:GLY:CA	2:A:352:HOH:O	2.54	0.54
1:A:231:ASP:C	1:A:231:ASP:OD1	2.45	0.54
1:A:183:VAL:HG11	1:A:243:LEU:HD11	1.90	0.54
1:A:108:VAL:HG22	1:A:251:PRO:HA	1.90	0.54
1:A:99:LEU:CD1	1:A:268:VAL:HG13	2.37	0.54
1:A:185:LYS:HG3	1:A:188:VAL:HG13	1.90	0.54
1:B:269:PHE:CD1	1:B:297:MET:HB2	2.43	0.53
1:B:182:SER:HA	1:B:234:VAL:HG12	1.91	0.53
1:A:216:VAL:HG13	1:A:217:ASP:N	2.23	0.53
1:A:256:LEU:HD21	1:A:319:LEU:CD1	2.39	0.53
1:B:15:VAL:HG23	1:B:290:ALA:HB2	1.89	0.53
1:B:2:LYS:HB3	1:B:65:GLU:HG3	1.91	0.53
1:A:201:GLU:HA	1:A:204:ARG:CZ	2.39	0.53
1:B:259:SER:OG	1:B:272:VAL:CG2	2.57	0.53
1:A:1:MET:HG2	1:A:302:PHE:CE1	2.43	0.53
1:A:6:LEU:O	1:A:69:LEU:HD12	2.09	0.53
1:A:191:VAL:CG2	1:B:153:ASN:HD22	2.00	0.53
1:A:115:LEU:HD11	1:A:327:LEU:HD22	1.90	0.52
1:B:94:ARG:HG3	1:B:99:LEU:HB2	1.90	0.52
1:A:54:PRO:HB2	1:A:56:PRO:HD2	1.91	0.52
1:A:41:PHE:HE2	1:A:72:VAL:HG11	1.74	0.52
1:A:82:ARG:CZ	1:A:82:ARG:HB2	2.39	0.52
1:A:83:LYS:H	1:A:83:LYS:HE2	1.74	0.52
1:A:37:GLU:HG2	1:A:39:PHE:CZ	2.45	0.52
1:A:69:LEU:HD12	1:A:70:GLY:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LYS:O	1:A:284:ILE:HG22	2.10	0.52
1:B:136:GLY:H	1:B:237:ASN:ND2	2.07	0.52
1:B:14:GLU:OE1	1:B:283:GLY:HA2	2.10	0.52
1:A:122:ILE:HG13	1:A:123:ALA:N	2.21	0.52
1:A:322:THR:N	1:A:323:PRO:HD3	2.23	0.52
1:A:5:VAL:O	1:A:7:PRO:HD3	2.10	0.52
1:A:133:GLU:HG3	1:A:157:TYR:HE1	1.74	0.52
1:A:157:TYR:CE1	1:A:195:TRP:HZ3	2.28	0.52
1:A:80:LEU:HB3	1:A:84:ILE:HD11	1.92	0.52
1:A:160:PRO:O	1:A:164:ARG:HG2	2.10	0.51
1:A:30:GLU:HB2	1:A:32:LEU:HD11	1.92	0.51
1:B:303:GLY:O	1:B:305:VAL:N	2.42	0.51
1:B:76:LYS:HG2	1:B:77:TRP:CZ2	2.45	0.51
1:A:182:SER:HB2	1:A:199:VAL:HG11	1.92	0.51
1:A:333:THR:HG23	1:A:334:GLU:N	2.25	0.51
1:B:115:LEU:C	1:B:252:GLY:HA2	2.30	0.51
1:B:212:GLU:OE1	1:B:229:ARG:NH2	2.44	0.51
1:A:247:ALA:HA	1:A:250:LEU:HD22	1.93	0.51
1:A:317:LYS:O	1:A:321:GLU:HG3	2.11	0.51
1:B:87:GLU:OE2	1:B:87:GLU:N	2.44	0.51
1:A:216:VAL:HG22	1:B:242:ILE:HD13	1.93	0.50
1:A:197:LYS:HE3	1:B:146:MET:HE1	1.92	0.50
1:B:199:VAL:HA	1:B:202:VAL:HG12	1.93	0.50
1:B:159:LYS:HD3	1:B:163:GLU:OE1	2.11	0.50
1:B:254:LEU:CB	2:B:369:HOH:O	2.58	0.50
1:B:105:PRO:HG2	1:B:258:PRO:HG2	1.94	0.50
1:B:78:ASP:O	1:B:85:ARG:NH2	2.42	0.50
1:A:99:LEU:HD22	1:A:261:SER:O	2.12	0.50
1:A:176:ARG:HH11	1:A:176:ARG:CB	2.25	0.50
1:A:222:HIS:HB2	1:A:230:PHE:HE2	1.77	0.49
1:B:158:SER:CB	1:B:160:PRO:HD2	2.42	0.49
1:B:286:ASN:HD22	1:B:286:ASN:C	2.15	0.49
1:B:170:PHE:HD1	1:B:209:VAL:HG11	1.78	0.49
1:B:15:VAL:CG2	1:B:290:ALA:HB2	2.43	0.49
1:A:204:ARG:O	1:A:207:PRO:HD3	2.12	0.49
1:A:341:GLY:O	1:A:344:ILE:HB	2.12	0.49
1:B:185:LYS:HG2	1:B:216:VAL:CG1	2.36	0.49
1:A:324:PRO:CB	2:A:368:HOH:O	2.46	0.49
1:B:238:ILE:O	1:B:242:ILE:HG13	2.12	0.49
1:B:286:ASN:HD22	1:B:287:PRO:N	2.11	0.49
1:A:113:GLU:OE1	1:A:113:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:NH1	1:A:264:ARG:NH1	2.53	0.49
1:A:181:VAL:HA	1:A:212:GLU:O	2.13	0.49
1:B:1:MET:O	1:B:1:MET:HG2	2.12	0.49
1:B:26:LEU:CD2	1:B:307:LEU:HD22	2.42	0.49
1:B:80:LEU:HG	1:B:81:PRO:HD2	1.95	0.49
1:B:107:LYS:HG2	1:B:127:ASP:OD1	2.13	0.48
1:B:158:SER:OG	1:B:160:PRO:HD2	2.12	0.48
1:A:153:ASN:HD21	1:B:190:GLU:HB2	1.77	0.48
1:B:212:GLU:HG3	1:B:212:GLU:O	2.11	0.48
1:B:1:MET:HE2	1:B:34:LEU:HG	1.96	0.48
1:B:99:LEU:HD13	1:B:261:SER:HB3	1.94	0.48
1:B:159:LYS:O	1:B:163:GLU:HG3	2.13	0.48
1:A:238:ILE:HG23	1:A:239:PHE:N	2.28	0.48
1:B:55:GLU:N	1:B:56:PRO:CD	2.77	0.48
1:B:170:PHE:CZ	1:B:211:LEU:HD22	2.38	0.48
1:A:8:GLY:HA3	1:A:71:SER:O	2.14	0.48
1:B:45:ALA:HB1	1:B:54:PRO:HD3	1.95	0.48
1:A:11:ILE:HD13	1:A:275:SER:O	2.14	0.47
1:A:138:ILE:HB	1:A:155:GLU:HB2	1.96	0.47
1:A:212:GLU:OE2	1:A:229:ARG:NH2	2.46	0.47
1:A:258:PRO:HG2	1:A:296:MET:HE2	1.95	0.47
1:B:114:ARG:NH2	1:B:115:LEU:HD13	2.29	0.47
1:A:20:LEU:HD13	1:A:36:TYR:CZ	2.48	0.47
1:B:167:ARG:O	1:B:171:GLU:HG2	2.15	0.47
1:A:144:ARG:HE	1:B:190:GLU:CD	2.18	0.47
1:B:200:GLU:OE1	1:B:200:GLU:O	2.32	0.47
1:A:114:ARG:HA	1:B:119:LYS:HZ3	1.79	0.47
1:B:1:MET:CE	1:B:34:LEU:HG	2.44	0.47
1:A:218:ALA:HA	1:A:221:MET:HE2	1.97	0.47
1:A:4:ALA:HB2	1:A:64:ALA:HB2	1.97	0.47
1:B:100:PHE:CD1	1:B:164:ARG:HD3	2.49	0.47
1:B:211:LEU:HD12	1:B:212:GLU:H	1.79	0.47
1:A:55:GLU:CA	1:A:58:ARG:HH12	2.21	0.47
1:B:112:LEU:HB3	2:B:356:HOH:O	2.15	0.47
1:B:115:LEU:HD23	2:B:356:HOH:O	2.14	0.47
1:B:183:VAL:HG11	1:B:243:LEU:CD1	2.42	0.47
1:A:63:GLU:H	1:A:63:GLU:HG2	1.58	0.47
1:A:81:PRO:O	1:A:84:ILE:HG12	2.14	0.47
1:B:196:ARG:HD2	1:B:213:HIS:CG	2.50	0.47
1:B:7:PRO:CD	1:B:38:VAL:HG13	2.45	0.47
1:A:269:PHE:CE1	1:A:297:MET:HA	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG11	1:B:221:MET:HG2	1.96	0.46
1:B:26:LEU:CG	1:B:307:LEU:HD22	2.45	0.46
1:B:39:PHE:CZ	1:B:60:GLY:HA3	2.50	0.46
1:A:180:VAL:HG12	1:A:211:LEU:HD12	1.97	0.46
1:A:226:SER:N	1:A:227:PRO:HD2	2.30	0.46
1:B:170:PHE:HE2	1:B:202:VAL:HG13	1.80	0.46
1:B:288:THR:HG23	1:B:315:VAL:HG11	1.97	0.46
1:B:291:ILE:O	1:B:294:ALA:HB3	2.15	0.46
1:B:69:LEU:HD23	1:B:70:GLY:N	2.31	0.46
1:B:159:LYS:N	1:B:160:PRO:HD2	2.30	0.46
1:A:1:MET:HB3	1:A:34:LEU:HA	1.97	0.46
1:A:22:VAL:HG21	1:A:291:ILE:HG21	1.98	0.46
1:A:85:ARG:HD3	1:A:87:GLU:OE1	2.15	0.46
1:A:90:LEU:HD13	1:A:94:ARG:CZ	2.46	0.46
1:A:138:ILE:HG12	1:B:189:LEU:HD11	1.98	0.46
1:A:144:ARG:NE	1:B:190:GLU:OE1	2.48	0.46
1:A:26:LEU:HD12	1:A:298:LEU:HD21	1.97	0.46
1:B:259:SER:OG	1:B:272:VAL:HG22	2.16	0.46
1:A:99:LEU:HD11	1:A:268:VAL:HG13	1.97	0.46
1:B:275:SER:O	1:B:276:ALA:C	2.54	0.46
1:A:303:GLY:O	1:A:305:VAL:N	2.48	0.46
1:A:333:THR:HG23	1:A:334:GLU:H	1.81	0.46
1:B:139:TYR:HE1	1:B:238:ILE:HD12	1.81	0.46
1:B:10:GLY:C	1:B:12:GLY:H	2.19	0.45
1:B:21:LYS:NZ	1:B:334:GLU:OE2	2.49	0.45
1:A:104:ARG:CZ	1:A:272:VAL:HG11	2.46	0.45
1:A:20:LEU:HD13	1:A:36:TYR:CE1	2.51	0.45
1:A:98:ASP:O	1:A:263:GLY:HA3	2.16	0.45
1:B:47:ASP:OD2	1:B:76:LYS:NZ	2.37	0.45
1:A:322:THR:OG1	1:A:339:THR:HG21	2.16	0.45
1:B:222:HIS:HA	1:B:225:ARG:HG2	1.97	0.45
1:A:108:VAL:CG2	1:A:251:PRO:HA	2.47	0.45
1:A:276:ALA:N	1:A:277:PRO:HD3	2.32	0.45
1:A:9:ASP:OD2	1:A:9:ASP:N	2.49	0.45
1:B:2:LYS:NZ	1:B:2:LYS:CB	2.80	0.45
1:B:1:MET:HB3	1:B:34:LEU:HA	1.98	0.45
1:A:127:ASP:O	1:A:177:ARG:NH1	2.47	0.45
1:A:94:ARG:HH11	1:A:94:ARG:CG	2.30	0.45
1:B:193:GLU:HA	2:B:351:HOH:O	2.16	0.45
1:B:280:ALA:O	1:B:282:LYS:HE3	2.16	0.44
1:B:82:ARG:O	1:B:84:ILE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:MET:SD	1:B:223:LEU:HD23	2.57	0.44
1:A:103:LEU:HB2	1:A:260:ALA:HB3	1.99	0.44
1:A:132:ARG:HD3	1:A:240:GLY:HA3	1.99	0.44
1:A:45:ALA:HB1	1:A:54:PRO:CD	2.48	0.44
1:A:69:LEU:HD12	1:A:70:GLY:N	2.32	0.44
1:A:250:LEU:N	1:A:251:PRO:CD	2.81	0.44
1:B:181:VAL:HA	1:B:212:GLU:O	2.16	0.44
1:B:226:SER:N	1:B:227:PRO:CD	2.80	0.44
1:A:99:LEU:HA	1:A:263:GLY:HA3	2.00	0.44
1:B:159:LYS:N	1:B:160:PRO:CD	2.80	0.44
1:A:118:LEU:HD22	1:A:118:LEU:N	2.32	0.44
1:A:201:GLU:HA	1:A:204:ARG:NE	2.32	0.44
1:A:187:ASN:HB3	1:A:215:TYR:OH	2.18	0.44
1:A:21:LYS:HE3	1:A:21:LYS:HB2	1.64	0.44
1:A:194:PHE:CD1	1:B:151:ALA:HB2	2.53	0.44
1:A:103:LEU:HD11	1:A:172:LEU:HD23	2.00	0.43
1:B:180:VAL:HG13	1:B:209:VAL:CG1	2.48	0.43
1:A:283:GLY:O	1:A:333:THR:HG22	2.18	0.43
1:A:112:LEU:HD12	1:A:115:LEU:HD22	2.00	0.43
1:A:269:PHE:CE2	1:A:297:MET:HA	2.53	0.43
1:A:139:TYR:HB2	1:A:237:ASN:ND2	2.34	0.43
1:A:132:ARG:HD2	1:A:237:ASN:O	2.19	0.43
1:A:94:ARG:HG2	1:A:94:ARG:NH1	2.33	0.43
1:B:141:GLY:O	1:B:144:ARG:HD2	2.18	0.43
1:B:187:ASN:HB3	1:B:215:TYR:CE1	2.53	0.43
1:A:118:LEU:HD12	1:A:122:ILE:HD11	2.01	0.43
1:A:188:VAL:O	1:A:188:VAL:HG22	2.17	0.43
1:A:222:HIS:HB2	1:A:230:PHE:CE2	2.54	0.43
1:A:166:ALA:O	1:A:170:PHE:HD2	2.02	0.43
1:A:196:ARG:CG	1:A:196:ARG:HH11	2.25	0.43
1:B:7:PRO:CG	1:B:38:VAL:HG13	2.49	0.43
1:A:133:GLU:HG3	1:A:157:TYR:CE1	2.53	0.43
1:A:286:ASN:ND2	1:A:288:THR:OG1	2.49	0.43
1:A:320:LEU:O	1:A:323:PRO:HD3	2.18	0.43
1:B:146:MET:SD	1:B:147:SER:N	2.91	0.42
1:A:238:ILE:HG23	1:A:239:PHE:CD1	2.54	0.42
1:B:181:VAL:HG13	1:B:212:GLU:CD	2.40	0.42
1:B:43:GLY:HA2	1:B:46:ILE:HD12	2.01	0.42
1:A:246:LEU:HD21	1:B:224:VAL:HG21	2.00	0.42
1:A:324:PRO:CA	2:A:368:HOH:O	2.65	0.42
1:A:94:ARG:HA	1:A:99:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ILE:HD12	1:B:244:SER:HA	2.01	0.42
1:A:11:ILE:O	1:A:15:VAL:HG22	2.19	0.42
1:B:223:LEU:HA	1:B:223:LEU:HD22	1.92	0.42
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.84	0.42
1:B:176:ARG:HB3	1:B:177:ARG:H	1.66	0.42
1:A:52:PRO:O	1:A:54:PRO:HD2	2.19	0.42
1:A:46:ILE:HD11	1:A:84:ILE:O	2.20	0.42
1:B:164:ARG:HG3	1:B:164:ARG:H	1.68	0.42
1:A:5:VAL:HG21	1:A:20:LEU:HD11	2.01	0.42
1:A:20:LEU:O	1:A:24:ARG:HG3	2.20	0.42
1:A:51:GLU:OE2	1:A:54:PRO:HA	2.20	0.42
1:A:58:ARG:HH11	1:A:58:ARG:CG	2.28	0.42
1:B:170:PHE:CE2	1:B:202:VAL:HG13	2.54	0.42
1:A:107:LYS:HD3	1:A:109:PHE:CE1	2.55	0.42
1:A:153:ASN:ND2	1:B:190:GLU:HB2	2.35	0.42
1:A:317:LYS:HA	1:A:317:LYS:NZ	2.34	0.42
1:A:40:PRO:C	1:A:45:ALA:HB2	2.40	0.41
1:B:172:LEU:HD11	1:B:300:HIS:HD2	1.78	0.41
1:A:226:SER:CB	2:A:361:HOH:O	2.68	0.41
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.82	0.41
1:B:34:LEU:C	1:B:34:LEU:HD23	2.40	0.41
1:B:61:VAL:HG22	1:B:67:VAL:HG21	2.01	0.41
1:A:256:LEU:HD21	1:A:319:LEU:HD13	2.03	0.41
1:A:172:LEU:HD11	1:A:300:HIS:NE2	2.34	0.41
1:A:45:ALA:HB1	1:A:54:PRO:HG3	2.02	0.41
1:A:116:SER:HB2	1:A:250:LEU:O	2.20	0.41
1:A:159:LYS:O	1:A:163:GLU:HB2	2.20	0.41
1:A:15:VAL:HB	1:A:290:ALA:HB2	2.01	0.41
1:A:319:LEU:HD23	1:A:324:PRO:CD	2.50	0.41
1:A:58:ARG:NH1	1:A:58:ARG:CG	2.83	0.41
1:B:160:PRO:O	1:B:164:ARG:HG3	2.21	0.41
1:B:297:MET:O	1:B:301:ALA:HB3	2.20	0.41
1:A:254:LEU:C	1:A:256:LEU:H	2.24	0.41
1:B:262:LEU:HA	1:B:262:LEU:HD13	1.86	0.41
1:B:94:ARG:HD3	1:B:99:LEU:HD12	2.02	0.41
1:A:118:LEU:HD12	1:A:122:ILE:CD1	2.50	0.41
1:A:189:LEU:HD21	1:B:138:ILE:HG23	2.02	0.41
1:A:189:LEU:HD21	1:B:138:ILE:O	2.21	0.41
1:A:190:GLU:HB2	1:B:153:ASN:HD21	1.85	0.41
1:B:323:PRO:HA	1:B:324:PRO:HD3	1.75	0.41
1:A:188:VAL:CG2	1:A:188:VAL:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:THR:HG23	1:A:342:MET:HE2	2.02	0.41
1:A:6:LEU:HG	1:A:41:PHE:HB2	2.03	0.41
1:A:20:LEU:HD23	1:A:23:LEU:HD23	2.02	0.41
1:B:6:LEU:HD12	1:B:39:PHE:HB2	2.03	0.41
1:B:93:LEU:HD13	1:B:94:ARG:NH1	2.35	0.41
1:A:133:GLU:HB3	1:A:157:TYR:OH	2.21	0.41
1:A:165:VAL:HG23	1:A:166:ALA:N	2.35	0.41
1:A:231:ASP:OD1	1:A:232:VAL:N	2.54	0.41
1:B:309:ARG:HH11	1:B:309:ARG:CG	2.28	0.41
1:B:250:LEU:N	1:B:251:PRO:CD	2.84	0.40
1:B:317:LYS:HG2	1:B:321:GLU:OE2	2.21	0.40
1:B:322:THR:OG1	1:B:339:THR:HG21	2.21	0.40
1:A:10:GLY:HA3	1:A:275:SER:O	2.21	0.40
1:B:286:ASN:ND2	1:B:286:ASN:C	2.74	0.40
1:A:184:ASP:O	1:A:215:TYR:HA	2.22	0.40
1:A:170:PHE:CD1	1:A:209:VAL:HG11	2.56	0.40
1:A:153:ASN:HD22	1:B:191:VAL:HG22	1.87	0.40
1:A:290:ALA:O	1:A:293:SER:HB2	2.22	0.40
1:A:10:GLY:C	1:A:12:GLY:H	2.25	0.40
1:A:301:ALA:O	1:A:302:PHE:CD1	2.74	0.40
1:A:82:ARG:HA	1:A:85:ARG:CZ	2.51	0.40
1:B:136:GLY:H	1:B:237:ASN:HD21	1.68	0.40
1:B:254:LEU:HG	1:B:254:LEU:H	1.67	0.40
1:B:309:ARG:CG	1:B:309:ARG:NH1	2.85	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	342/344 (99%)	300 (88%)	36 (10%)	6 (2%)	8 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	342/344 (99%)	298 (87%)	40 (12%)	4 (1%)	13	32
All	All	684/688 (99%)	598 (87%)	76 (11%)	10 (2%)	10	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLY
1	A	283	GLY
1	B	31	GLY
1	A	144	ARG
1	B	83	LYS
1	B	188	VAL
1	B	252	GLY
1	A	332	GLY
1	A	54	PRO
1	A	188	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	265/265 (100%)	187 (71%)	78 (29%)	0	1
1	B	265/265 (100%)	195 (74%)	70 (26%)	0	1
All	All	530/530 (100%)	382 (72%)	148 (28%)	0	1

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	6	LEU
1	A	9	ASP
1	A	11	ILE
1	A	21	LYS

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Mol	Chain	Res	Type
1	A	23	LEU
1	A	26	LEU
1	A	27	ASP
1	A	28	GLU
1	A	37	GLU
1	A	38	VAL
1	A	58	ARG
1	A	59	LYS
1	A	61	VAL
1	A	63	GLU
1	A	71	SER
1	A	76	LYS
1	A	77	TRP
1	A	78	ASP
1	A	83	LYS
1	A	85	ARG
1	A	90	LEU
1	A	93	LEU
1	A	94	ARG
1	A	95	LYS
1	A	96	SER
1	A	104	ARG
1	A	107	LYS
1	A	114	ARG
1	A	121	GLU
1	A	122	ILE
1	A	132	ARG
1	A	133	GLU
1	A	135	THR
1	A	144	ARG
1	A	147	SER
1	A	148	GLU
1	A	150	GLU
1	A	158	SER
1	A	159	LYS
1	A	163	GLU
1	A	171	GLU
1	A	172	LEU
1	A	176	ARG
1	A	185	LYS
1	A	197	LYS
1	A	201	GLU

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Mol	Chain	Res	Type
1	A	214	GLN
1	A	225	ARG
1	A	234	VAL
1	A	241	ASP
1	A	245	ASP
1	A	246	LEU
1	A	250	LEU
1	A	253	SER
1	A	254	LEU
1	A	256	LEU
1	A	257	LEU
1	A	268	VAL
1	A	270	GLU
1	A	275	SER
1	A	284	ILE
1	A	296	MET
1	A	298	LEU
1	A	299	GLU
1	A	304	LEU
1	A	306	GLU
1	A	309	ARG
1	A	310	LYS
1	A	312	GLU
1	A	317	LYS
1	A	322	THR
1	A	326	ASP
1	A	327	LEU
1	A	330	SER
1	A	334	GLU
1	A	342	MET
1	B	2	LYS
1	B	9	ASP
1	B	17	GLU
1	B	24	ARG
1	B	27	ASP
1	B	30	GLU
1	B	37	GLU
1	B	51	GLU
1	B	55	GLU
1	B	58	ARG
1	B	62	GLU
1	B	76	LYS

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Mol	Chain	Res	Type
1	B	85	ARG
1	B	87	GLU
1	B	90	LEU
1	B	93	LEU
1	B	94	ARG
1	B	95	LYS
1	B	96	SER
1	B	114	ARG
1	B	116	SER
1	B	118	LEU
1	B	119	LYS
1	B	120	GLU
1	B	121	GLU
1	B	132	ARG
1	B	134	LEU
1	B	138	ILE
1	B	146	MET
1	B	147	SER
1	B	150	GLU
1	B	157	TYR
1	B	159	LYS
1	B	161	GLU
1	B	164	ARG
1	B	172	LEU
1	B	174	ARG
1	B	178	LYS
1	B	180	VAL
1	B	181	VAL
1	B	182	SER
1	B	191	VAL
1	B	196	ARG
1	B	197	LYS
1	B	201	GLU
1	B	204	ARG
1	B	223	LEU
1	B	225	ARG
1	B	229	ARG
1	B	237	ASN
1	B	241	ASP
1	B	245	ASP
1	B	248	SER
1	B	254	LEU

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Mol	Chain	Res	Type
1	B	256	LEU
1	B	257	LEU
1	B	259	SER
1	B	261	SER
1	B	264	ARG
1	B	275	SER
1	B	284	ILE
1	B	286	ASN
1	B	304	LEU
1	B	306	GLU
1	B	309	ARG
1	B	310	LYS
1	B	317	LYS
1	B	321	GLU
1	B	322	THR
1	B	333	THR

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

Mol	Chain	Res	Type
1	A	102	ASN
1	A	153	ASN
1	A	214	GLN
1	B	153	ASN
1	B	214	GLN
1	B	222	HIS
1	B	237	ASN
1	B	286	ASN

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	344/344 (100%)	-0.13	9 (2%) 56 57	6, 33, 57, 84	0
1	B	344/344 (100%)	-0.24	0 100 100	3, 31, 49, 57	0
All	All	688/688 (100%)	-0.18	9 (1%) 77 78	3, 32, 53, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	3.3
1	A	82	ARG	3.0
1	A	76	LYS	2.7
1	A	81	PRO	2.6
1	A	79	GLY	2.6
1	A	205	GLY	2.2
1	A	45	ALA	2.1
1	A	77	TRP	2.1
1	A	331	ALA	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.