



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:53 AM GMT

PDB ID : 2YQ4  
Title : Crystal Structure of D-isomer specific 2-hydroxyacid dehydrogenase from *Lactobacillus delbrueckii* ssp. *bulgaricus*  
Authors : Holton, S.J.; Anandhakrishnan, M.; Geerlof, A.; Wilmanns, M.  
Deposited on : 2012-11-05  
Resolution : 3.45 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](mailto: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.

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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

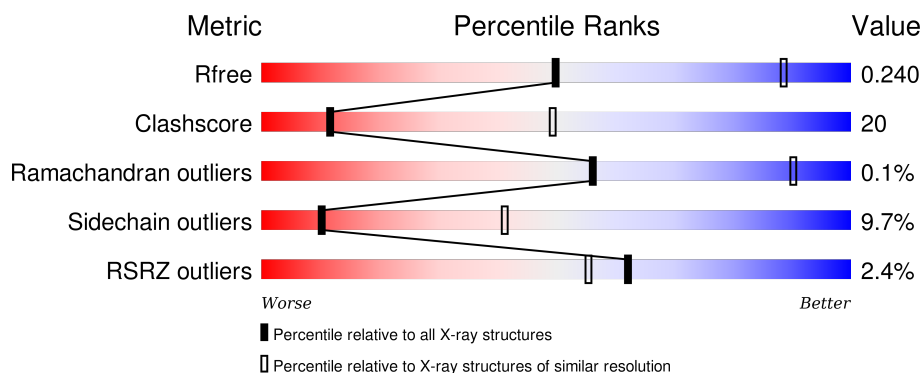
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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  $\geq 3$ , 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	343	<div> <div>2%</div> <div>67%</div> <div>25%</div> <div>• •</div> </div>
1	B	343	<div> <div>3%</div> <div>59%</div> <div>31%</div> <div>5%</div> <div>•</div> </div>
1	C	343	<div> <div>61%</div> <div>30%</div> <div>5%</div> <div>•</div> </div>
1	D	343	<div> <div>5%</div> <div>55%</div> <div>32%</div> <div>7%</div> <div>6%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10188 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 D-ISOMER SPECIFIC 2-HYDROXYACID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2545	1628	410	494	13			
1	B	328	Total	C	N	O	S	0	0	0
			2544	1626	410	495	13			
1	C	331	Total	C	N	O	S	0	0	0
			2573	1645	415	500	13			
1	D	321	Total	C	N	O	S	0	0	0
			2492	1593	399	487	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	THR	-	EXPRESSION TAG	UNP Q1GAA2
A	335	ALA	-	EXPRESSION TAG	UNP Q1GAA2
A	336	SER	-	EXPRESSION TAG	UNP Q1GAA2
A	337	GLY	-	EXPRESSION TAG	UNP Q1GAA2
A	338	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	339	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	340	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	341	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	342	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	343	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	334	THR	-	EXPRESSION TAG	UNP Q1GAA2
B	335	ALA	-	EXPRESSION TAG	UNP Q1GAA2
B	336	SER	-	EXPRESSION TAG	UNP Q1GAA2
B	337	GLY	-	EXPRESSION TAG	UNP Q1GAA2
B	338	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	339	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	340	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	341	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	342	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	343	HIS	-	EXPRESSION TAG	UNP Q1GAA2

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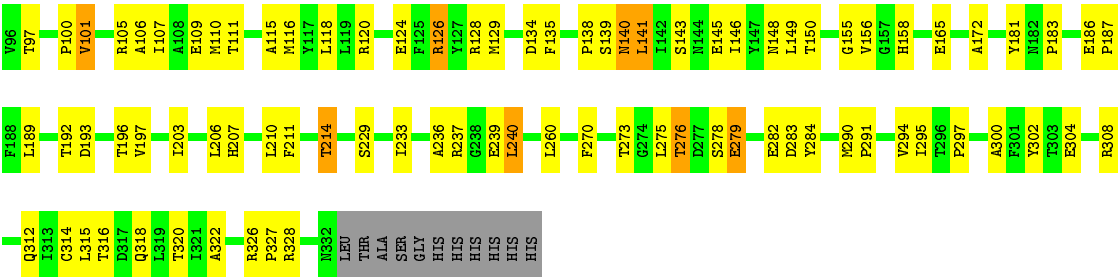
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Chain	Residue	Modelled	Actual	Comment	Reference
C	334	THR	-	EXPRESSION TAG	UNP Q1GAA2
C	335	ALA	-	EXPRESSION TAG	UNP Q1GAA2
C	336	SER	-	EXPRESSION TAG	UNP Q1GAA2
C	337	GLY	-	EXPRESSION TAG	UNP Q1GAA2
C	338	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	339	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	340	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	341	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	342	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	343	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	334	THR	-	EXPRESSION TAG	UNP Q1GAA2
D	335	ALA	-	EXPRESSION TAG	UNP Q1GAA2
D	336	SER	-	EXPRESSION TAG	UNP Q1GAA2
D	337	GLY	-	EXPRESSION TAG	UNP Q1GAA2
D	338	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	339	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	340	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	341	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	342	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	343	HIS	-	EXPRESSION TAG	UNP Q1GAA2

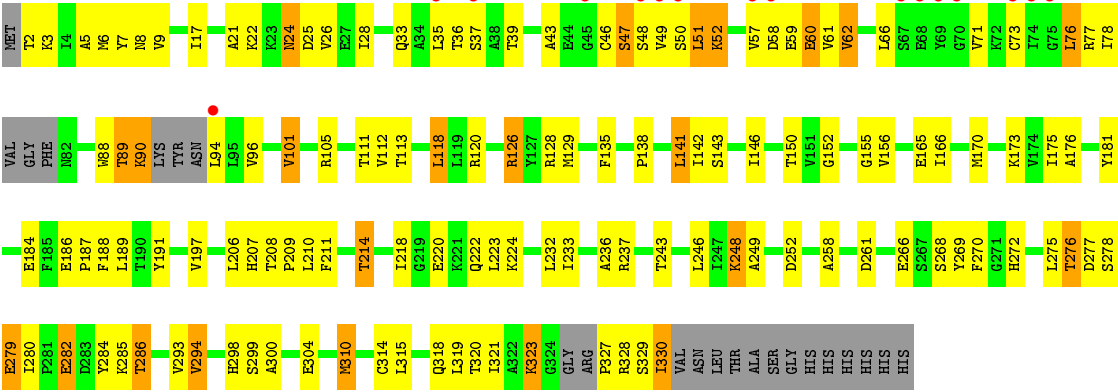
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	13	Total O 13 13	0	0
2	C	7	Total O 7 7	0	0
2	D	7	Total O 7 7	0	0





● Molecule 1: D-ISOMER SPECIFIC 2-HYDROXYACID DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.21Å 108.37Å 147.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 3.45 46.72 – 3.45	Depositor EDS
% Data completeness (in resolution range)	92.2 (44.00-3.45) 98.1 (46.72-3.45)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.179 , 0.250 0.184 , 0.240	Depositor DCC
$R_{free}$ test set	998 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 19697 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10188	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.60	0/2596	0.86	0/3528
1	B	0.63	0/2595	0.88	0/3528
1	C	0.63	0/2626	0.92	2/3571 (0.1%)
1	D	0.60	0/2540	0.85	1/3450 (0.0%)
All	All	0.62	0/10357	0.88	3/14077 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	C	156	VAL	C-N-CA	-5.51	110.73	122.30
1	D	118	LEU	CA-CB-CG	-5.20	103.33	115.30

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	2545	0	2543	86	0
1	B	2544	0	2536	121	0
1	C	2573	0	2565	111	0
1	D	2492	0	2483	117	0
2	A	7	0	0	2	0
2	B	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	7	0	0	1	0
2	D	7	0	0	3	0
All	All	10188	0	10127	411	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 20.

All (411) 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:126:ARG:HH11	1:A:126:ARG:HG2	1.05	1.16
1:B:237:ARG:HH11	1:B:237:ARG:HG2	1.02	1.10
1:B:6:MET:HE2	1:B:28:ILE:HG21	1.22	1.09
1:D:314:CYS:O	1:D:318:GLN:HG2	1.54	1.06
1:D:126:ARG:HH11	1:D:126:ARG:HG2	0.87	1.04
1:B:126:ARG:HG3	1:B:126:ARG:HH11	1.20	1.03
1:C:79:VAL:HG13	1:C:100:PRO:HA	1.41	1.02
1:B:126:ARG:CG	1:B:126:ARG:HH11	1.76	0.99
1:A:6:MET:HE1	1:A:315:LEU:HD11	1.46	0.96
1:B:237:ARG:HG2	1:B:237:ARG:NH1	1.66	0.95
1:A:126:ARG:HH11	1:A:126:ARG:CG	1.80	0.94
1:D:211:PHE:H	1:D:214:THR:HG22	1.31	0.94
1:D:126:ARG:NH1	1:D:126:ARG:HG2	1.64	0.94
1:B:237:ARG:HH11	1:B:237:ARG:CG	1.81	0.92
1:A:126:ARG:NH1	1:A:126:ARG:HG2	1.77	0.90
1:B:6:MET:CE	1:B:28:ILE:HG21	2.02	0.89
1:A:211:PHE:H	1:A:214:THR:HG22	1.37	0.89
1:B:6:MET:HE2	1:B:28:ILE:CG2	2.04	0.87
1:C:20:TRP:HE1	1:C:316:THR:CG2	1.89	0.86
1:D:276:THR:H	1:D:279:GLU:HG3	1.41	0.84
1:D:155:GLY:O	1:D:207:HIS:HB2	1.78	0.84
1:C:3:LYS:HE3	1:C:29:LYS:HE2	1.60	0.84
1:A:211:PHE:H	1:A:214:THR:CG2	1.90	0.83
1:B:20:TRP:HE1	1:B:316:THR:HG23	1.43	0.82
1:C:140:ASN:HD22	1:C:140:ASN:H	1.24	0.81
1:D:128:ARG:HD3	2:D:2003:HOH:O	1.79	0.81
1:C:6:MET:HE1	1:C:17:ILE:HG12	1.61	0.81
1:C:79:VAL:CG1	1:C:100:PRO:HA	2.11	0.80
1:A:183:PRO:HG2	1:D:101:VAL:HG22	1.67	0.77
1:D:211:PHE:H	1:D:214:THR:CG2	1.98	0.76
1:C:20:TRP:HE1	1:C:316:THR:HG23	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LYS:HE3	1:C:90:LYS:HA	1.67	0.75
1:B:59:GLU:O	1:B:62:VAL:HG22	1.87	0.74
1:C:210:LEU:HA	1:C:214:THR:HG21	1.68	0.74
1:D:3:LYS:O	1:D:46:CYS:HA	1.88	0.74
1:C:211:PHE:H	1:C:214:THR:CG2	2.01	0.73
1:C:72:LYS:HE2	1:C:322:ALA:HA	1.69	0.73
1:B:60:GLU:HG3	1:B:88:TRP:CZ3	2.23	0.73
1:B:211:PHE:H	1:B:214:THR:CG2	2.02	0.73
1:C:37:SER:OG	1:C:59:GLU:OE1	2.05	0.73
1:D:6:MET:HE1	1:D:315:LEU:HD11	1.70	0.72
1:D:138:PRO:HG2	1:D:141:LEU:HB2	1.71	0.71
1:B:211:PHE:H	1:B:214:THR:HG22	1.53	0.71
1:D:57:VAL:O	1:D:57:VAL:HG12	1.91	0.71
1:B:126:ARG:HG3	1:B:126:ARG:NH1	1.99	0.71
1:D:126:ARG:HH11	1:D:126:ARG:CG	1.83	0.70
1:C:6:MET:CE	1:C:17:ILE:HG23	2.21	0.70
1:B:66:LEU:HB3	1:B:71:VAL:CG2	2.21	0.70
1:A:104:PRO:HG2	1:D:184:GLU:HB3	1.72	0.69
1:C:211:PHE:H	1:C:214:THR:HG22	1.55	0.68
1:B:14:VAL:HB	1:B:15:PRO:HD3	1.75	0.68
1:D:280:ILE:O	1:D:285:LYS:HE3	1.94	0.68
1:D:155:GLY:HA3	1:D:208:THR:HG22	1.76	0.67
1:C:276:THR:H	1:C:279:GLU:HG3	1.59	0.67
1:D:77:ARG:O	1:D:310:MET:HG2	1.93	0.67
1:C:21:ALA:HB2	1:C:28:ILE:HD12	1.75	0.67
1:D:52:LYS:HB3	1:D:77:ARG:NH2	2.09	0.67
1:B:20:TRP:HE1	1:B:316:THR:CG2	2.08	0.67
1:C:129:MET:HG2	1:C:135:PHE:CE2	2.30	0.66
1:C:20:TRP:HE1	1:C:316:THR:HG22	1.61	0.66
1:D:76:LEU:CD2	1:D:76:LEU:N	2.58	0.66
1:D:209:PRO:O	1:D:214:THR:HG21	1.95	0.66
1:A:20:TRP:CE3	1:A:315:LEU:HD13	2.31	0.66
1:C:140:ASN:N	1:C:140:ASN:HD22	1.94	0.66
1:D:89:THR:HG21	1:D:96:VAL:HG23	1.78	0.66
1:D:282:GLU:O	1:D:286:THR:OG1	2.12	0.66
1:D:7:TYR:CE2	1:D:35:LEU:HD13	2.31	0.66
1:C:126:ARG:HH11	1:C:126:ARG:CG	2.08	0.66
1:A:82:ASN:H	1:A:82:ASN:HD22	1.43	0.65
1:A:150:THR:CG2	2:A:2004:HOH:O	2.44	0.65
1:B:126:ARG:CG	1:B:126:ARG:NH1	2.43	0.65
1:C:6:MET:HE3	1:C:17:ILE:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:CYS:O	1:C:318:GLN:HG2	1.95	0.65
1:C:6:MET:HE3	1:C:17:ILE:CG2	2.27	0.65
1:A:327:PRO:O	1:A:330:ILE:HG12	1.97	0.65
1:A:150:THR:HG23	2:A:2004:HOH:O	1.97	0.65
1:D:2:THR:O	1:D:26:VAL:HG13	1.96	0.65
1:B:20:TRP:NE1	1:B:316:THR:HG23	2.11	0.65
1:B:181:TYR:CE2	1:B:183:PRO:HD3	2.32	0.64
1:D:48:SER:HA	1:D:71:VAL:HG13	1.79	0.64
1:D:7:TYR:CZ	1:D:35:LEU:HD13	2.31	0.64
1:A:113:THR:OG1	1:B:116:MET:HB3	1.98	0.64
1:D:76:LEU:HD23	1:D:76:LEU:H	1.63	0.64
1:D:89:THR:HG22	1:D:94:LEU:O	1.98	0.63
1:A:275:LEU:HA	1:A:279:GLU:OE1	1.99	0.63
1:B:210:LEU:HA	1:B:214:THR:HG21	1.81	0.63
1:B:21:ALA:HB2	1:B:28:ILE:HG13	1.82	0.62
1:B:6:MET:HG2	1:B:50:SER:HB3	1.81	0.61
1:A:97:THR:HA	1:A:329:SER:O	1.99	0.61
1:D:166:ILE:CG2	1:D:170:MET:HE2	2.29	0.61
1:B:280:ILE:O	1:B:285:LYS:HE3	2.01	0.61
1:D:261:ASP:O	1:D:298:HIS:HA	2.00	0.61
1:A:128:ARG:CZ	1:A:138:PRO:HG3	2.31	0.61
1:B:211:PHE:O	1:B:214:THR:HG22	2.01	0.61
1:B:186:GLU:N	1:B:187:PRO:CD	2.64	0.61
1:D:220:GLU:HG2	1:D:224:LYS:HE2	1.83	0.60
1:D:33:GLN:HE21	1:D:39:THR:HG21	1.67	0.60
1:C:82:ASN:HD22	1:C:82:ASN:H	1.50	0.60
1:D:6:MET:HE3	1:D:28:ILE:HG21	1.84	0.60
1:C:3:LYS:CE	1:C:29:LYS:HE2	2.32	0.60
1:C:107:ILE:H	1:C:107:ILE:HD12	1.67	0.59
1:C:107:ILE:N	1:C:107:ILE:HD12	2.17	0.59
1:C:304:GLU:HG2	1:D:142:ILE:HD13	1.84	0.59
1:A:209:PRO:O	1:A:214:THR:HG21	2.02	0.59
1:C:155:GLY:O	1:C:207:HIS:HB2	2.03	0.58
1:C:3:LYS:HG3	1:C:27:GLU:HB3	1.84	0.58
1:C:210:LEU:HA	1:C:214:THR:CG2	2.33	0.58
1:D:211:PHE:O	1:D:214:THR:N	2.34	0.58
1:B:60:GLU:HB2	1:B:88:TRP:CD2	2.38	0.58
1:C:126:ARG:HH11	1:C:126:ARG:CB	2.17	0.58
1:C:82:ASN:ND2	1:C:82:ASN:H	2.01	0.58
1:D:276:THR:N	1:D:279:GLU:HG3	2.15	0.58
1:C:129:MET:HG2	1:C:135:PHE:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:HD12	1:C:149:LEU:N	2.19	0.58
1:B:50:SER:HA	1:B:75:GLY:O	2.04	0.57
1:C:126:ARG:HG2	1:C:126:ARG:NH1	2.18	0.57
1:B:138:PRO:HG2	1:B:141:LEU:HB2	1.86	0.57
1:D:50:SER:C	1:D:51:LEU:HD23	2.25	0.57
1:D:59:GLU:O	1:D:62:VAL:CG2	2.53	0.57
1:A:325:GLY:O	1:A:326:ARG:HG2	2.04	0.57
1:C:7:TYR:CZ	1:C:35:LEU:HD13	2.39	0.56
1:B:66:LEU:HB3	1:B:71:VAL:HG21	1.87	0.56
1:C:211:PHE:O	1:C:214:THR:HG22	2.06	0.56
1:A:140:ASN:H	1:A:140:ASN:HD22	1.53	0.55
1:B:128:ARG:HD2	1:B:141:LEU:CD2	2.35	0.55
1:A:206:LEU:HD21	1:A:218:ILE:HG13	1.87	0.55
1:B:84:ILE:N	1:B:84:ILE:HD12	2.22	0.55
1:D:210:LEU:HA	1:D:214:THR:HG21	1.87	0.55
1:D:8:ASN:HD22	1:D:52:LYS:H	1.55	0.55
1:A:154:ILE:O	1:A:208:THR:HG23	2.06	0.55
1:B:66:LEU:HB3	1:B:71:VAL:HG22	1.88	0.55
1:D:284:TYR:CD1	1:D:284:TYR:C	2.79	0.55
1:B:192:THR:OG1	1:B:193:ASP:N	2.39	0.55
1:C:6:MET:CE	1:C:17:ILE:HG12	2.35	0.55
1:C:126:ARG:CG	1:C:126:ARG:NH1	2.69	0.55
1:D:232:LEU:O	1:D:258:ALA:HA	2.06	0.55
1:B:76:LEU:HD21	1:B:84:ILE:HD11	1.89	0.54
1:B:8:ASN:HB2	1:B:52:LYS:H	1.72	0.54
1:B:33:GLN:HE21	1:B:39:THR:CG2	2.20	0.54
1:B:101:VAL:O	1:B:101:VAL:HG22	2.06	0.54
1:B:12:ILE:O	1:B:15:PRO:HD2	2.06	0.54
1:D:318:GLN:HA	1:D:318:GLN:OE1	2.08	0.54
1:D:21:ALA:HB2	1:D:28:ILE:HD12	1.90	0.54
1:A:155:GLY:HA3	1:A:208:THR:HG22	1.89	0.54
1:A:276:THR:N	1:A:279:GLU:OE1	2.35	0.54
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.21	0.54
1:B:82:ASN:H	1:B:82:ASN:HD22	1.54	0.54
1:B:82:ASN:ND2	1:B:82:ASN:H	2.06	0.54
1:B:126:ARG:HG2	1:B:126:ARG:NH1	2.22	0.54
1:A:6:MET:CE	1:A:315:LEU:HD11	2.31	0.53
1:C:211:PHE:N	1:C:214:THR:HG22	2.22	0.53
1:A:47:SER:OG	1:A:72:LYS:HE2	2.07	0.53
1:B:184:GLU:HG2	1:C:158:HIS:CD2	2.43	0.53
1:A:308:ARG:O	1:A:312:GLN:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:HB2	1:B:88:TRP:CE2	2.43	0.53
1:C:126:ARG:HH11	1:C:126:ARG:HB3	1.74	0.53
1:D:24:ASN:N	1:D:24:ASN:HD22	2.07	0.53
1:A:88:TRP:O	1:A:91:LYS:HG2	2.09	0.53
1:D:49:VAL:HG11	1:D:66:LEU:HD21	1.90	0.52
1:B:8:ASN:HD22	1:B:51:LEU:HB3	1.74	0.52
1:C:110:MET:HE2	1:C:300:ALA:HA	1.92	0.52
1:A:14:VAL:HB	1:A:15:PRO:HD3	1.92	0.52
1:B:152:GLY:HA2	1:B:175:ILE:O	2.10	0.52
1:A:187:PRO:HG3	1:D:105:ARG:HG3	1.90	0.52
1:D:320:THR:OG1	1:D:327:PRO:HG3	2.09	0.52
1:A:36:THR:HG22	1:A:59:GLU:OE1	2.09	0.52
1:A:261:ASP:CG	1:A:298:HIS:HA	2.29	0.52
1:A:320:THR:HG22	1:A:325:GLY:HA3	1.90	0.52
1:B:184:GLU:HG2	1:C:158:HIS:HD2	1.73	0.52
1:B:6:MET:HE1	1:B:17:ILE:HG23	1.92	0.52
1:D:155:GLY:CA	1:D:208:THR:HG22	2.39	0.52
1:B:124:GLU:O	1:B:128:ARG:HG3	2.09	0.52
1:D:5:ALA:HB2	1:D:46:CYS:SG	2.49	0.52
1:D:165:GLU:HG2	1:D:188:PHE:CE1	2.45	0.52
1:B:119:LEU:HD13	1:B:149:LEU:HD21	1.92	0.52
1:C:302:TYR:CE2	1:D:142:ILE:HA	2.45	0.52
1:A:155:GLY:CA	1:A:208:THR:HG22	2.40	0.52
1:C:270:PHE:CE2	1:C:297:PRO:HA	2.45	0.52
1:A:126:ARG:NH1	1:A:126:ARG:CG	2.50	0.51
1:A:182:ASN:HB3	1:A:184:GLU:OE2	2.10	0.51
1:D:25:ASP:CG	1:D:25:ASP:O	2.48	0.51
1:A:6:MET:HE1	1:A:315:LEU:CD1	2.31	0.51
1:C:90:LYS:HA	1:C:90:LYS:CE	2.38	0.51
1:B:150:THR:HB	1:B:173:LYS:HB3	1.92	0.51
1:D:112:VAL:HG11	1:D:170:MET:HE1	1.92	0.51
1:B:119:LEU:CD1	1:B:149:LEU:HD21	2.41	0.51
1:D:73:CYS:SG	1:D:321:ILE:HD12	2.50	0.51
1:A:104:PRO:HG2	1:D:184:GLU:CB	2.41	0.51
1:B:206:LEU:O	1:B:236:ALA:HB2	2.10	0.51
1:D:266:GLU:O	1:D:270:PHE:HB2	2.10	0.51
1:C:320:THR:OG1	1:C:327:PRO:HG3	2.11	0.51
1:C:20:TRP:O	1:C:24:ASN:ND2	2.33	0.50
1:B:22:LYS:HB2	1:B:22:LYS:NZ	2.26	0.50
1:D:176:ALA:HB3	1:D:189:LEU:HD13	1.92	0.50
1:D:152:GLY:HA2	1:D:175:ILE:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:TYR:CZ	1:B:310:MET:HE3	2.47	0.50
1:D:126:ARG:NH1	1:D:126:ARG:CG	2.52	0.50
1:D:76:LEU:HD23	1:D:76:LEU:N	2.21	0.50
1:C:126:ARG:HH11	1:C:126:ARG:HG2	1.72	0.50
1:B:61:VAL:HG12	1:B:65:LYS:HG3	1.94	0.50
1:D:181:TYR:HD1	1:D:191:TYR:CE2	2.30	0.50
1:C:308:ARG:O	1:C:312:GLN:HG3	2.12	0.50
1:D:218:ILE:HD13	1:D:222:GLN:HG2	1.93	0.50
1:B:269:TYR:CD1	1:B:269:TYR:N	2.79	0.50
1:B:187:PRO:HG3	1:C:105:ARG:HG3	1.92	0.50
1:B:8:ASN:ND2	1:B:51:LEU:HB3	2.27	0.50
1:B:261:ASP:OD2	1:B:298:HIS:HA	2.12	0.50
1:C:120:ARG:HD2	1:C:143:SER:OG	2.11	0.50
1:D:8:ASN:ND2	1:D:52:LYS:H	2.10	0.49
1:C:134:ASP:OD1	1:C:134:ASP:C	2.51	0.49
1:A:5:ALA:HB1	1:A:42:LEU:CD1	2.43	0.49
1:D:277:ASP:O	1:D:285:LYS:NZ	2.36	0.49
1:D:96:VAL:O	1:D:330:ILE:HA	2.13	0.49
1:A:140:ASN:N	1:A:140:ASN:HD22	2.10	0.49
1:B:284:TYR:C	1:B:284:TYR:CD1	2.85	0.49
1:D:166:ILE:HG22	1:D:170:MET:HE2	1.93	0.49
1:C:111:THR:HG23	1:C:233:ILE:HG21	1.95	0.49
1:C:189:LEU:C	1:C:189:LEU:HD12	2.33	0.49
1:D:211:PHE:N	1:D:214:THR:HG22	2.13	0.48
1:B:181:TYR:CD2	1:B:183:PRO:HD3	2.47	0.48
1:C:181:TYR:CE2	1:C:183:PRO:HD3	2.49	0.48
1:D:52:LYS:O	1:D:52:LYS:HG3	2.12	0.48
1:B:86:PHE:HA	1:B:89:THR:OG1	2.12	0.48
1:D:59:GLU:O	1:D:62:VAL:HG23	2.13	0.48
1:C:328:ARG:HB3	1:C:328:ARG:CZ	2.42	0.48
1:C:50:SER:HA	1:C:75:GLY:O	2.14	0.48
1:B:84:ILE:N	1:B:84:ILE:CD1	2.77	0.48
1:D:90:LYS:CE	1:D:90:LYS:HA	2.44	0.48
1:D:186:GLU:N	1:D:187:PRO:CD	2.77	0.48
1:B:126:ARG:HG2	1:B:126:ARG:HH11	1.70	0.47
1:A:72:LYS:HE3	1:A:322:ALA:HA	1.96	0.47
1:B:3:LYS:HD2	1:B:27:GLU:CD	2.34	0.47
1:B:89:THR:C	1:B:90:LYS:HD2	2.35	0.47
1:C:146:ILE:HG13	1:C:172:ALA:HB2	1.94	0.47
1:B:4:ILE:HD13	1:B:315:LEU:HD22	1.96	0.47
1:A:6:MET:HG2	1:A:50:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:THR:HG23	1:D:233:ILE:HG21	1.95	0.47
1:B:101:VAL:HG22	1:C:183:PRO:HG2	1.97	0.47
1:B:259:GLY:HA2	1:B:294:VAL:HG13	1.95	0.47
1:D:243:THR:O	1:D:246:LEU:HB3	2.14	0.47
1:A:221:LYS:HE3	1:A:222:GLN:HE21	1.78	0.47
1:A:261:ASP:OD2	1:A:298:HIS:HA	2.15	0.47
1:D:60:GLU:HB3	1:D:88:TRP:CD2	2.49	0.47
1:D:210:LEU:HA	1:D:214:THR:CG2	2.45	0.47
1:D:261:ASP:OD2	1:D:300:ALA:CB	2.62	0.47
1:A:221:LYS:O	1:A:225:GLU:HG3	2.15	0.47
1:A:221:LYS:HB3	1:A:222:GLN:NE2	2.30	0.47
1:C:124:GLU:O	1:C:128:ARG:HG3	2.15	0.47
1:A:90:LYS:HA	1:A:90:LYS:CE	2.44	0.47
1:A:269:TYR:N	1:A:269:TYR:CD1	2.81	0.47
1:B:6:MET:HE3	1:B:17:ILE:HD13	1.97	0.46
1:C:24:ASN:O	1:C:25:ASP:CB	2.63	0.46
1:B:21:ALA:CB	1:B:28:ILE:HG13	2.46	0.46
1:B:48:SER:OG	1:B:318:GLN:NE2	2.48	0.46
1:A:211:PHE:O	1:A:214:THR:HG22	2.16	0.46
1:D:6:MET:CE	1:D:17:ILE:HG23	2.45	0.46
1:D:319:LEU:O	1:D:323:LYS:HE2	2.15	0.46
1:C:148:ASN:C	1:C:149:LEU:HD12	2.36	0.46
1:B:309:ASN:HB3	1:B:313:ILE:HD12	1.97	0.46
1:D:293:VAL:CG1	1:D:294:VAL:N	2.79	0.46
1:C:52:LYS:HE2	2:C:2001:HOH:O	2.14	0.46
1:B:183:PRO:HG2	1:C:101:VAL:HG22	1.98	0.46
1:D:6:MET:HE3	1:D:17:ILE:HG23	1.97	0.46
1:D:272:HIS:HB2	1:D:275:LEU:HD11	1.97	0.46
1:C:210:LEU:HD22	1:C:239:GLU:HB2	1.97	0.46
1:D:52:LYS:HB3	1:D:77:ARG:CZ	2.45	0.46
1:B:77:ARG:O	1:B:310:MET:HG2	2.15	0.46
1:A:241:VAL:HG11	1:A:246:LEU:HD22	1.97	0.45
1:C:140:ASN:H	1:C:140:ASN:ND2	2.03	0.45
1:D:248:LYS:HD3	1:D:252:ASP:OD2	2.15	0.45
1:D:223:LEU:HD13	1:D:249:ALA:HB2	1.98	0.45
1:C:275:LEU:HD22	1:C:279:GLU:HB2	1.97	0.45
1:D:118:LEU:HA	1:D:118:LEU:HD23	1.65	0.45
1:D:52:LYS:CG	1:D:52:LYS:O	2.65	0.45
1:D:60:GLU:HB3	1:D:88:TRP:CE2	2.51	0.45
1:C:33:GLN:HE21	1:C:39:THR:HG21	1.82	0.45
1:C:316:THR:O	1:C:320:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:TYR:O	1:A:8:ASN:HB2	2.17	0.45
1:D:7:TYR:CD2	1:D:35:LEU:HB2	2.51	0.45
1:C:72:LYS:CE	1:C:322:ALA:HA	2.44	0.45
1:D:261:ASP:OD1	1:D:299:SER:N	2.44	0.45
1:B:62:VAL:O	1:B:66:LEU:HD12	2.17	0.44
1:A:82:ASN:H	1:A:82:ASN:ND2	2.14	0.44
1:D:120:ARG:HD2	1:D:143:SER:OG	2.17	0.44
1:A:122:ILE:HG12	1:B:296:THR:HG21	1.99	0.44
1:A:21:ALA:HB2	1:A:28:ILE:HD13	1.99	0.44
1:B:27:GLU:C	1:B:28:ILE:HG12	2.38	0.44
1:D:90:LYS:HA	1:D:90:LYS:HE3	1.98	0.44
1:C:6:MET:HE1	1:C:315:LEU:HD11	1.99	0.44
1:B:63:TYR:CG	1:B:88:TRP:HB3	2.53	0.44
1:A:5:ALA:HB1	1:A:42:LEU:HD12	1.99	0.44
1:A:143:SER:OG	1:A:144:ASN:N	2.51	0.44
1:C:31:THR:OG1	1:C:33:GLN:HG3	2.17	0.44
1:B:155:GLY:CA	1:B:208:THR:HG22	2.48	0.44
1:D:166:ILE:HG22	1:D:170:MET:CE	2.47	0.44
1:C:302:TYR:CD2	1:D:142:ILE:HA	2.53	0.44
1:B:165:GLU:OE2	1:C:165:GLU:OE2	2.35	0.44
1:A:232:LEU:O	1:A:233:ILE:HD13	2.17	0.44
1:B:19:ASP:O	1:B:23:LYS:HB2	2.17	0.44
1:D:268:SER:HB2	1:D:269:TYR:HD1	1.83	0.44
1:C:297:PRO:HG3	1:D:129:MET:SD	2.58	0.44
1:D:173:LYS:HE2	1:D:175:ILE:CG2	2.47	0.44
1:A:227:LYS:HB2	1:A:230:ALA:HB2	2.00	0.44
1:D:43:ALA:HA	1:D:46:CYS:SG	2.58	0.43
1:D:330:ILE:HG12	1:D:330:ILE:H	1.31	0.43
1:D:33:GLN:HE21	1:D:39:THR:CG2	2.31	0.43
1:C:24:ASN:O	1:C:25:ASP:HB3	2.16	0.43
1:C:145:GLU:O	1:C:149:LEU:HD13	2.18	0.43
1:C:109:GLU:CD	1:D:146:ILE:HG22	2.39	0.43
1:B:3:LYS:HG3	1:B:27:GLU:HB3	2.00	0.43
1:A:320:THR:HB	1:A:327:PRO:HG3	1.99	0.43
1:A:33:GLN:H	1:A:33:GLN:HG2	1.67	0.43
1:C:149:LEU:CD1	1:C:149:LEU:N	2.81	0.43
1:C:115:ALA:HB1	1:C:203:ILE:HD13	2.00	0.43
1:C:7:TYR:O	1:C:8:ASN:HB2	2.19	0.43
1:B:153:LEU:HD22	1:B:205:SER:HB3	2.01	0.43
1:C:73:CYS:HB2	1:C:95:LEU:HB2	2.01	0.43
1:B:242:ASP:HB3	1:B:245:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HD13	1:B:197:VAL:HG11	2.01	0.43
1:D:272:HIS:CB	1:D:275:LEU:HD11	2.49	0.43
1:B:79:VAL:HA	1:B:98:ASN:HD22	1.84	0.43
1:D:211:PHE:O	1:D:214:THR:HG22	2.19	0.43
1:A:266:GLU:OE2	1:A:298:HIS:ND1	2.49	0.43
1:B:229:SER:HA	1:B:256:ALA:HB2	2.00	0.43
1:D:128:ARG:HB2	2:D:2003:HOH:O	2.18	0.43
1:C:75:GLY:HA2	1:C:97:THR:OG1	2.19	0.43
1:A:211:PHE:H	1:A:214:THR:HG21	1.79	0.42
1:C:40:VAL:HG11	1:C:65:LYS:HD2	2.01	0.42
1:A:120:ARG:HA	1:A:120:ARG:HD2	1.73	0.42
1:A:6:MET:CE	1:A:315:LEU:HD21	2.49	0.42
1:B:121:LYS:HD2	1:B:141:LEU:HA	2.01	0.42
1:D:60:GLU:CB	1:D:88:TRP:CE2	3.01	0.42
1:D:66:LEU:HD22	1:D:71:VAL:HG11	2.01	0.42
1:B:7:TYR:O	1:B:8:ASN:HB2	2.19	0.42
1:A:268:SER:HB2	1:A:269:TYR:HD1	1.84	0.42
1:A:35:LEU:HG	1:A:62:VAL:HG11	2.01	0.42
1:C:290:MET:HA	1:C:291:PRO:HD3	1.83	0.42
1:B:88:TRP:C	1:B:90:LYS:H	2.21	0.42
1:B:266:GLU:HB2	1:B:270:PHE:CD2	2.54	0.42
1:A:73:CYS:HB2	1:A:95:LEU:HB2	2.02	0.42
1:A:239:GLU:N	1:A:239:GLU:OE1	2.49	0.42
1:C:240:LEU:HD23	1:C:240:LEU:HA	1.81	0.42
1:C:105:ARG:O	1:C:106:ALA:C	2.55	0.42
1:D:152:GLY:HA3	1:D:197:VAL:HG13	2.01	0.42
1:D:236:ALA:C	1:D:237:ARG:HG2	2.40	0.42
1:D:3:LYS:O	1:D:47:SER:N	2.48	0.42
1:B:7:TYR:CZ	1:B:35:LEU:CD1	3.03	0.42
1:B:182:ASN:HB2	1:B:185:PHE:CD2	2.55	0.42
1:B:66:LEU:HD22	1:B:71:VAL:HG21	2.01	0.42
1:B:33:GLN:HG3	1:B:39:THR:HG21	2.02	0.42
1:B:13:GLU:O	1:B:14:VAL:C	2.58	0.42
1:B:7:TYR:CE1	1:B:35:LEU:HD13	2.54	0.42
1:A:109:GLU:OE2	1:B:146:ILE:HG22	2.20	0.42
1:A:6:MET:HE1	1:A:315:LEU:HD21	2.01	0.42
1:B:60:GLU:HB2	1:B:88:TRP:CE3	2.54	0.42
1:A:186:GLU:N	1:A:187:PRO:CD	2.83	0.42
1:C:196:THR:O	1:C:197:VAL:C	2.58	0.42
1:C:6:MET:CE	1:C:17:ILE:CG2	2.91	0.41
1:C:118:LEU:HA	1:C:118:LEU:HD23	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:VAL:HG21	1:B:176:ALA:HB1	2.01	0.41
1:A:6:MET:HE3	1:A:17:ILE:HG23	2.02	0.41
1:A:320:THR:HG21	1:A:327:PRO:HG3	2.02	0.41
1:C:138:PRO:HG2	1:C:141:LEU:HB2	2.01	0.41
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.66	0.41
1:C:186:GLU:N	1:C:187:PRO:CD	2.83	0.41
1:A:20:TRP:CZ2	1:A:315:LEU:HB3	2.55	0.41
1:C:6:MET:HE3	1:C:17:ILE:HG21	2.02	0.41
1:A:187:PRO:CG	1:D:105:ARG:HG3	2.51	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.79	0.41
1:A:301:PHE:HE1	1:B:137:TRP:CZ2	2.38	0.41
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.85	0.41
1:B:314:CYS:O	1:B:318:GLN:HG2	2.21	0.41
1:B:102:TYR:CE2	1:B:310:MET:HE2	2.56	0.41
1:C:120:ARG:HH11	1:C:120:ARG:HD3	1.69	0.41
1:B:26:VAL:HG12	1:B:27:GLU:O	2.20	0.41
1:B:120:ARG:HD3	1:B:120:ARG:HH11	1.70	0.41
1:A:16:TYR:OH	1:A:304:GLU:HB3	2.20	0.41
1:C:106:ALA:HB3	1:C:107:ILE:HD12	2.03	0.41
1:D:129:MET:HG2	1:D:135:PHE:CD2	2.56	0.41
1:A:3:LYS:HG3	1:A:27:GLU:HB3	2.02	0.41
1:C:284:TYR:C	1:C:284:TYR:CD1	2.94	0.41
1:D:128:ARG:CB	2:D:2003:HOH:O	2.68	0.41
1:A:155:GLY:HA3	1:A:208:THR:CG2	2.51	0.41
1:A:154:ILE:CG2	1:A:217:MET:HE1	2.50	0.41
1:A:109:GLU:CD	1:B:146:ILE:HG22	2.41	0.41
1:C:260:LEU:O	1:C:295:ILE:HA	2.21	0.41
1:B:33:GLN:CG	1:B:39:THR:HG21	2.50	0.41
1:D:60:GLU:HG2	1:D:88:TRP:CE2	2.55	0.41
1:D:120:ARG:HD2	1:D:120:ARG:HA	1.74	0.41
1:B:105:ARG:HG3	1:C:187:PRO:HG3	2.02	0.41
1:B:97:THR:HA	1:B:329:SER:O	2.20	0.41
1:C:140:ASN:N	1:C:140:ASN:ND2	2.65	0.41
1:C:236:ALA:C	1:C:237:ARG:HG2	2.42	0.41
1:A:107:ILE:HD12	1:A:107:ILE:N	2.36	0.41
1:C:192:THR:OG1	1:C:193:ASP:N	2.54	0.41
1:C:22:LYS:HG3	1:C:23:LYS:N	2.33	0.40
1:C:116:MET:HB3	1:D:113:THR:OG1	2.21	0.40
1:B:238:GLY:C	1:B:240:LEU:H	2.23	0.40
1:C:210:LEU:CD2	1:C:239:GLU:HB2	2.51	0.40
1:B:211:PHE:H	1:B:214:THR:HG21	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:PRO:HG2	1:C:101:VAL:HG12	2.03	0.40
1:B:238:GLY:C	1:B:240:LEU:N	2.74	0.40
1:B:189:LEU:C	1:B:189:LEU:HD12	2.41	0.40
1:A:135:PHE:HB2	1:B:269:TYR:O	2.21	0.40
1:B:283:ASP:OD1	1:B:284:TYR:N	2.55	0.40
1:A:89:THR:O	1:A:90:LYS:HE3	2.22	0.40
1:C:10:SER:O	1:C:11:PRO:C	2.60	0.40
1:C:91:LYS:HE2	1:C:92:TYR:CZ	2.57	0.40
1:D:128:ARG:HD2	1:D:141:LEU:CD2	2.51	0.40
1:B:258:ALA:O	1:B:293:VAL:HA	2.21	0.40
1:B:95:LEU:HD22	1:B:330:ILE:HG21	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	324/343 (94%)	309 (95%)	15 (5%)	0	100	100
1	B	324/343 (94%)	309 (95%)	14 (4%)	1 (0%)	46	84
1	C	329/343 (96%)	316 (96%)	13 (4%)	0	100	100
1	D	313/343 (91%)	296 (95%)	17 (5%)	0	100	100
All	All	1290/1372 (94%)	1230 (95%)	59 (5%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	GLU

### 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	281/294 (96%)	260 (92%)	21 (8%)	17	55
1	B	281/294 (96%)	258 (92%)	23 (8%)	14	50
1	C	284/294 (97%)	255 (90%)	29 (10%)	9	39
1	D	276/294 (94%)	240 (87%)	36 (13%)	5	26
All	All	1122/1176 (95%)	1013 (90%)	109 (10%)	10	41

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	LYS
1	A	22	LYS
1	A	36	THR
1	A	42	LEU
1	A	54	LEU
1	A	82	ASN
1	A	101	VAL
1	A	126	ARG
1	A	140	ASN
1	A	141	LEU
1	A	149	LEU
1	A	150	THR
1	A	184	GLU
1	A	206	LEU
1	A	214	THR
1	A	269	TYR
1	A	273	THR
1	A	289	LYS
1	A	294	VAL
1	A	298	HIS
1	B	19	ASP
1	B	22	LYS
1	B	23	LYS

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Mol	Chain	Res	Type
1	B	28	ILE
1	B	48	SER
1	B	51	LEU
1	B	54	LEU
1	B	60	GLU
1	B	82	ASN
1	B	87	ASP
1	B	101	VAL
1	B	121	LYS
1	B	126	ARG
1	B	150	THR
1	B	206	LEU
1	B	214	THR
1	B	227	LYS
1	B	237	ARG
1	B	243	THR
1	B	248	LYS
1	B	269	TYR
1	B	289	LYS
1	B	298	HIS
1	C	2	THR
1	C	3	LYS
1	C	22	LYS
1	C	24	ASN
1	C	37	SER
1	C	48	SER
1	C	59	GLU
1	C	65	LYS
1	C	79	VAL
1	C	82	ASN
1	C	90	LYS
1	C	91	LYS
1	C	101	VAL
1	C	126	ARG
1	C	139	SER
1	C	140	ASN
1	C	141	LEU
1	C	150	THR
1	C	206	LEU
1	C	214	THR
1	C	229	SER
1	C	273	THR

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Mol	Chain	Res	Type
1	C	276	THR
1	C	278	SER
1	C	279	GLU
1	C	282	GLU
1	C	283	ASP
1	C	294	VAL
1	C	326	ARG
1	D	9	VAL
1	D	22	LYS
1	D	24	ASN
1	D	36	THR
1	D	37	SER
1	D	47	SER
1	D	51	LEU
1	D	52	LYS
1	D	58	ASP
1	D	60	GLU
1	D	61	VAL
1	D	62	VAL
1	D	76	LEU
1	D	78	ILE
1	D	89	THR
1	D	90	LYS
1	D	101	VAL
1	D	126	ARG
1	D	141	LEU
1	D	150	THR
1	D	156	VAL
1	D	206	LEU
1	D	214	THR
1	D	248	LYS
1	D	276	THR
1	D	278	SER
1	D	279	GLU
1	D	282	GLU
1	D	286	THR
1	D	294	VAL
1	D	304	GLU
1	D	310	MET
1	D	323	LYS
1	D	328	ARG
1	D	329	SER

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Mol	Chain	Res	Type
1	D	330	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	82	ASN
1	A	140	ASN
1	A	158	HIS
1	B	8	ASN
1	B	33	GLN
1	B	82	ASN
1	B	158	HIS
1	B	318	GLN
1	C	8	ASN
1	C	33	GLN
1	C	82	ASN
1	C	140	ASN
1	C	158	HIS
1	D	8	ASN
1	D	24	ASN
1	D	33	GLN
1	D	140	ASN
1	D	272	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	328/343 (95%)	-0.01	6 (1%) 71 64	25, 50, 88, 104	0
1	B	328/343 (95%)	-0.08	10 (3%) 54 47	22, 45, 98, 114	0
1	C	331/343 (96%)	-0.27	0 100 100	24, 43, 64, 73	0
1	D	321/343 (93%)	0.13	16 (4%) 32 27	28, 56, 94, 111	0
All	All	1308/1372 (95%)	-0.06	32 (2%) 62 55	22, 48, 92, 114	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	69	TYR	3.3
1	D	73	CYS	3.2
1	D	67	SER	3.2
1	D	35	LEU	3.1
1	A	45	GLY	3.0
1	B	45	GLY	3.0
1	A	2	THR	2.9
1	D	70	GLY	2.9
1	D	49	VAL	2.9
1	A	72	LYS	2.8
1	D	50	SER	2.7
1	B	73	CYS	2.7
1	D	74	ILE	2.7
1	B	46	CYS	2.7
1	D	45	GLY	2.6
1	D	48	SER	2.6
1	B	3	LYS	2.6
1	D	75	GLY	2.5
1	D	57	VAL	2.5
1	B	72	LYS	2.5
1	D	37	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	68	GLU	2.4
1	B	35	LEU	2.3
1	D	58	ASP	2.3
1	B	4	ILE	2.2
1	A	3	LYS	2.2
1	A	66	LEU	2.1
1	D	94	LEU	2.1
1	B	71	VAL	2.1
1	A	27	GLU	2.1
1	B	2	THR	2.0
1	B	94	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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.