



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:17 AM GMT

PDB ID : 2WL6  
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. THE N316H-H348N MUTANT.  
Authors : Merilainen, G.; Poikela, V.; Kursula, P.; Wierenga, R.K.  
Deposited on : 2009-06-22  
Resolution : 2.98 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

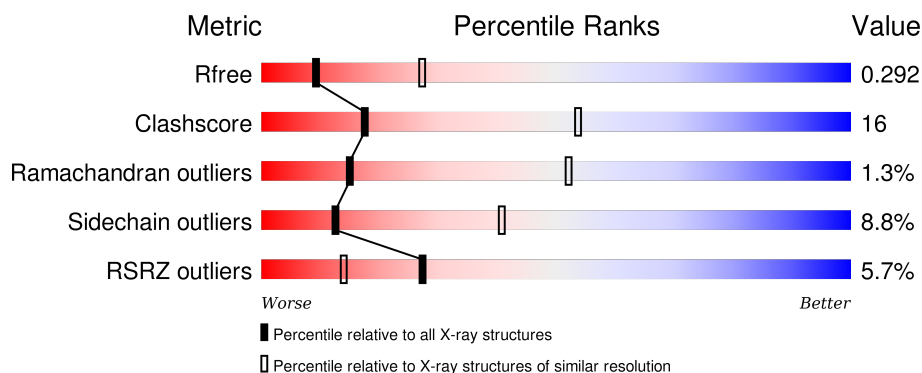
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	392	<div> <div>2%</div> <div>70%</div> <div>25%</div> <div>..</div> </div>
1	B	392	<div> <div>3%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>
1	C	392	<div> <div>5%</div> <div>61%</div> <div>34%</div> <div>..</div> </div>
1	D	392	<div> <div>13%</div> <div>60%</div> <div>36%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11278 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 ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	B	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	C	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	D	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
A	316	HIS	ASN	ENGINEERED MUTATION	UNP P07097
A	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	316	HIS	ASN	ENGINEERED MUTATION	UNP P07097
B	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	316	HIS	ASN	ENGINEERED MUTATION	UNP P07097
C	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097
D	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	316	HIS	ASN	ENGINEERED MUTATION	UNP P07097
D	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	8	Total	O	0	0
			8	8		

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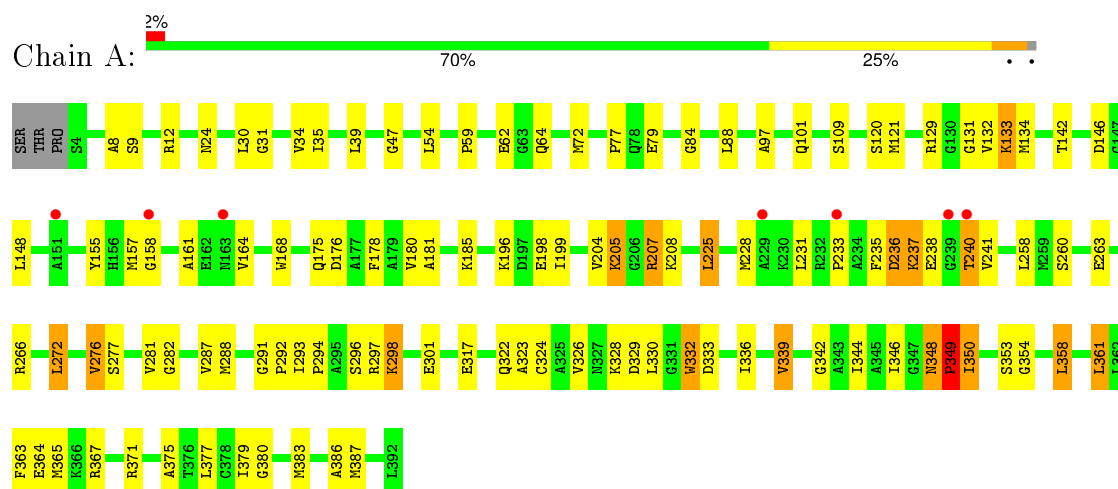
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	3	Total	O	0	0
			3	3		
2	D	5	Total	O	0	0
			5	5		

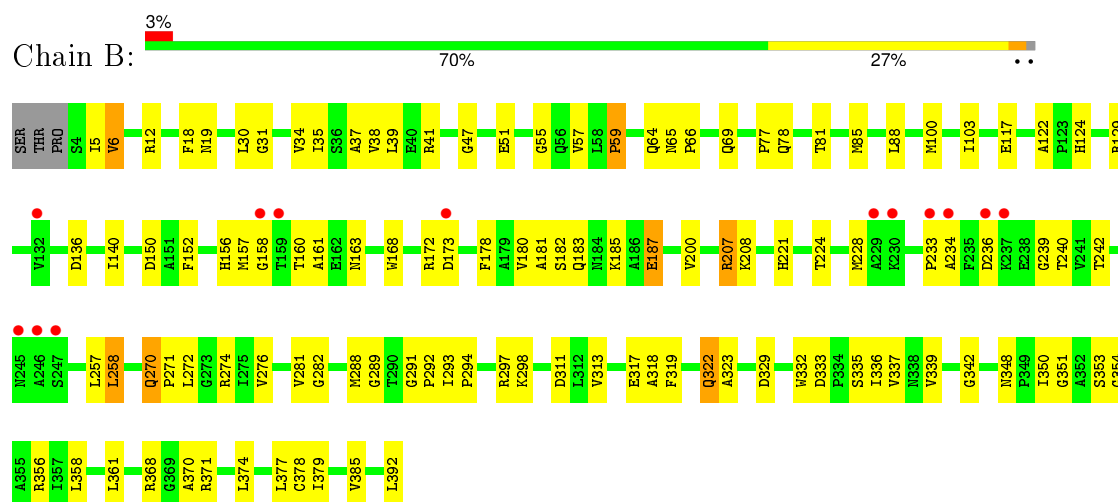
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

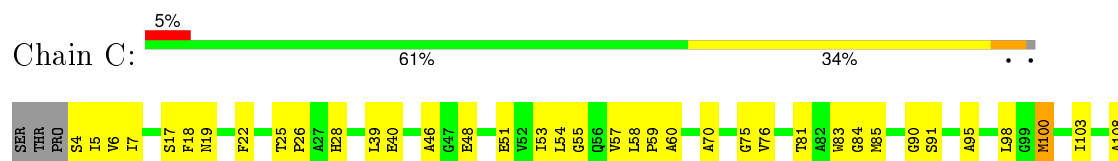
#### • Molecule 1: ACETYL-COA ACETYLTRANSFERASE

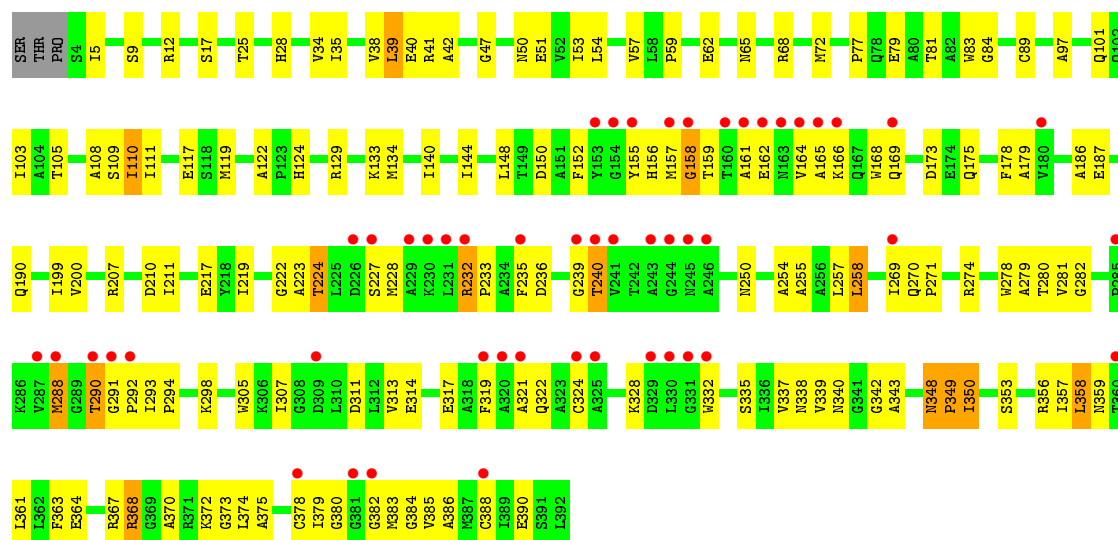


#### • Molecule 1: ACETYL-COA ACETYLTRANSFERASE



#### • Molecule 1: ACETYL-COA ACETYLTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.23Å 79.87Å 149.92Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	37.42 – 2.98 37.43 – 2.98	Depositor EDS
% Data completeness (in resolution range)	95.9 (37.42-2.98) 82.8 (37.43-2.98)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.232 , 0.291 0.233 , 0.292	Depositor DCC
$R_{free}$ test set	1974 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 11.5	EDS
Estimated twinning fraction	0.176 for h,-k,-l	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	1 of 39192 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	11278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</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	0.61	0/2854	0.72	2/3853 (0.1%)
1	B	0.60	0/2854	0.71	1/3853 (0.0%)
1	C	0.53	0/2854	0.80	2/3853 (0.1%)
1	D	0.54	0/2854	0.72	2/3853 (0.1%)
All	All	0.57	0/11416	0.74	7/15412 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	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	C	348	ASN	C-N-CD	-24.17	67.42	120.60
1	D	348	ASN	C-N-CD	-11.40	95.53	120.60
1	A	348	ASN	C-N-CD	-10.05	98.50	120.60
1	D	348	ASN	C-N-CA	-10.05	79.80	122.00
1	C	348	ASN	C-N-CA	-8.67	85.57	122.00
1	A	348	ASN	C-N-CA	-7.54	90.31	122.00
1	B	6	VAL	CB-CA-C	-5.41	101.13	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	PRO	Peptide



## 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	2813	0	2819	81	0
1	B	2813	0	2819	78	0
1	C	2813	0	2819	103	0
1	D	2813	0	2819	113	0
2	A	10	0	0	0	0
2	B	8	0	0	1	0
2	C	3	0	0	0	0
2	D	5	0	0	1	0
All	All	11278	0	11276	361	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 16.

All (361) 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:C:348:ASN:O	1:C:349:PRO:C	1.65	1.16
1:C:207:ARG:HH11	1:C:207:ARG:HG2	0.88	1.04
1:D:17:SER:OG	1:D:217:GLU:HG3	1.63	0.99
1:C:207:ARG:NH1	1:C:207:ARG:HG2	1.68	0.95
1:D:9:SER:HB3	1:D:42:ALA:HB2	1.48	0.94
1:C:348:ASN:OD1	1:C:349:PRO:N	2.03	0.93
1:C:250:ASN:HB2	1:C:349:PRO:HD3	1.54	0.89
1:C:207:ARG:HH11	1:C:207:ARG:CG	1.82	0.89
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.58	0.84
1:D:41:ARG:HH21	1:D:200:VAL:HB	1.43	0.84
1:B:348:ASN:OD1	1:B:353:SER:OG	1.98	0.82
1:D:175:GLN:HE22	1:D:240:THR:CG2	1.94	0.81
1:D:47:GLY:HA2	1:D:77:PRO:HG3	1.63	0.80
1:A:132:VAL:O	1:C:129:ARG:HA	1.83	0.78
1:C:348:ASN:O	1:C:349:PRO:O	2.02	0.77
1:D:288:MET:SD	1:D:380:GLY:HA2	2.25	0.75
1:B:354:GLY:HA2	1:B:377:LEU:HD11	1.69	0.75
1:B:207:ARG:H	1:B:207:ARG:HD3	1.52	0.74
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:HB	1:B:294:PRO:HD3	1.68	0.74
1:B:293:ILE:HB	1:B:294:PRO:CD	2.17	0.74
1:A:64:GLN:HG2	1:B:88:LEU:HD21	1.69	0.73
1:B:281:VAL:HG12	1:B:282:GLY:N	2.06	0.71
1:C:236:ASP:HB3	1:C:239:GLY:HA3	1.71	0.71
1:D:236:ASP:HB3	1:D:239:GLY:CA	2.20	0.70
1:A:131:GLY:HA2	1:C:131:GLY:HA3	1.75	0.69
1:A:348:ASN:O	1:A:348:ASN:OD1	2.11	0.69
1:C:348:ASN:O	1:C:349:PRO:CB	2.22	0.69
1:A:348:ASN:C	1:A:348:ASN:OD1	2.30	0.68
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.28	0.68
1:C:333:ASP:O	1:C:336:ILE:HG12	1.94	0.68
1:C:179:ALA:HB2	1:C:245:ASN:HB3	1.76	0.68
1:B:51:GLU:OE2	1:B:81:THR:OG1	2.13	0.67
1:D:17:SER:HG	1:D:217:GLU:HG3	1.59	0.67
1:C:95:ALA:HA	1:C:98:LEU:HD12	1.78	0.66
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.58	0.66
1:D:348:ASN:OD1	1:D:348:ASN:C	2.34	0.66
1:D:175:GLN:HE22	1:D:240:THR:HG23	1.60	0.65
1:D:5:ILE:HD12	1:D:103:ILE:CG2	2.27	0.65
1:C:54:LEU:O	1:C:84:GLY:HA2	1.96	0.65
1:D:97:ALA:O	1:D:101:GLN:HG3	1.97	0.65
1:C:198:GLU:HB3	1:C:363:PHE:CD2	2.32	0.64
1:C:162:GLU:OE2	1:C:240:THR:N	2.29	0.64
1:A:133:LYS:O	1:A:134:MET:HB3	1.96	0.64
1:D:101:GLN:O	1:D:105:THR:HG23	1.97	0.63
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.18	0.63
1:A:180:VAL:HG21	1:A:225:LEU:HA	1.80	0.63
1:A:292:PRO:O	1:A:296:SER:OG	2.12	0.63
1:D:150:ASP:OD2	1:D:152:PHE:HB2	1.99	0.62
1:A:348:ASN:HB2	1:A:353:SER:OG	1.99	0.62
1:C:358:LEU:HD22	1:C:362:LEU:HG	1.82	0.62
1:C:348:ASN:C	1:C:348:ASN:OD1	2.38	0.62
1:D:5:ILE:HD12	1:D:103:ILE:HG21	1.82	0.62
1:C:148:LEU:O	1:C:157:MET:HG2	1.99	0.62
1:D:190:GLN:HE21	1:D:219:ILE:HD12	1.64	0.61
1:A:148:LEU:O	1:A:157:MET:HG2	2.01	0.61
1:B:157:MET:HA	1:B:157:MET:HE2	1.82	0.61
1:D:41:ARG:NH2	1:D:200:VAL:HB	2.15	0.61
1:A:88:LEU:HD12	1:A:380:GLY:O	2.01	0.61
1:A:129:ARG:HH21	1:B:122:ALA:HB3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TRP:HH2	1:B:329:ASP:HB2	1.64	0.60
1:C:280:THR:HG23	1:D:81:THR:HG21	1.83	0.60
1:C:364:GLU:O	1:C:368:ARG:HG2	2.02	0.60
1:B:293:ILE:O	1:B:297:ARG:HG3	2.03	0.59
1:C:282:GLY:O	1:D:79:GLU:HA	2.02	0.59
1:B:356:ARG:HD2	1:B:356:ARG:O	2.03	0.58
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.38	0.58
1:B:258:LEU:N	1:B:258:LEU:HD22	2.18	0.58
1:A:142:THR:O	1:A:146:ASP:HB2	2.04	0.58
1:C:162:GLU:OE1	1:C:240:THR:HG22	2.04	0.57
1:B:371:ARG:NH2	2:B:2008:HOH:O	2.37	0.57
1:A:281:VAL:HG12	1:A:282:GLY:N	2.19	0.57
1:B:356:ARG:HD2	1:B:356:ARG:C	2.25	0.56
1:B:313:VAL:HB	1:B:337:VAL:HG22	1.87	0.56
1:D:53:ILE:HD13	1:D:83:TRP:CZ2	2.40	0.56
1:D:179:ALA:HB3	1:D:228:MET:SD	2.45	0.56
1:B:180:VAL:HG22	1:B:228:MET:HE2	1.88	0.55
1:A:258:LEU:HD22	1:A:258:LEU:N	2.22	0.55
1:B:12:ARG:O	1:B:200:VAL:HG12	2.07	0.55
1:D:165:ALA:O	1:D:169:GLN:N	2.39	0.55
1:C:53:ILE:HD13	1:C:83:TRP:CZ2	2.42	0.55
1:D:269:ILE:O	1:D:271:PRO:HD3	2.06	0.55
1:A:317:GLU:CD	1:A:342:GLY:HA3	2.27	0.55
1:A:361:LEU:O	1:A:365:MET:HG3	2.07	0.55
1:C:57:VAL:O	1:C:59:PRO:HD3	2.08	0.54
1:B:158:GLY:O	1:B:161:ALA:HB3	2.08	0.54
1:C:339:VAL:HG11	1:C:368:ARG:NH2	2.22	0.54
1:D:313:VAL:CG1	1:D:314:GLU:N	2.69	0.54
1:A:263:GLU:HA	1:A:266:ARG:NH1	2.23	0.54
1:C:348:ASN:OD1	1:C:349:PRO:CA	2.56	0.54
1:D:155:TYR:CD1	1:D:159:THR:HB	2.43	0.54
1:D:57:VAL:O	1:D:59:PRO:HD3	2.07	0.54
1:D:367:ARG:O	1:D:367:ARG:HG2	2.08	0.54
1:D:34:VAL:CG1	1:D:255:ALA:HB3	2.38	0.54
1:D:258:LEU:N	1:D:258:LEU:HD22	2.22	0.54
1:D:313:VAL:HG12	1:D:337:VAL:HG13	1.89	0.53
1:A:30:LEU:O	1:A:34:VAL:HG23	2.08	0.53
1:B:281:VAL:CG1	1:B:282:GLY:N	2.71	0.53
1:C:54:LEU:HD13	1:C:116:MET:CE	2.37	0.53
1:A:291:GLY:O	1:A:294:PRO:HD2	2.07	0.53
1:D:109:SER:O	1:D:110:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:PRO:HA	1:B:242:THR:HG22	1.91	0.53
1:D:379:ILE:HD11	1:D:385:VAL:HG12	1.90	0.52
1:C:207:ARG:NH1	1:C:207:ARG:CG	2.53	0.52
1:D:158:GLY:HA3	1:D:235:PHE:CG	2.44	0.52
1:B:281:VAL:HG12	1:B:282:GLY:H	1.71	0.52
1:A:236:ASP:C	1:A:236:ASP:OD1	2.47	0.52
1:D:156:HIS:ND1	1:D:157:MET:N	2.57	0.52
1:A:164:VAL:O	1:A:168:TRP:HB2	2.09	0.52
1:D:348:ASN:OD1	1:D:349:PRO:N	2.43	0.51
1:C:322:GLN:O	1:C:326:VAL:HG23	2.09	0.51
1:A:77:PRO:HB2	1:A:79:GLU:OE1	2.09	0.51
1:A:358:LEU:HD11	1:A:387:MET:CE	2.40	0.51
1:D:162:GLU:HB3	1:D:166:LYS:HE3	1.92	0.51
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.23	0.51
1:A:47:GLY:HA2	1:A:77:PRO:HD3	1.92	0.51
1:B:236:ASP:O	1:B:239:GLY:N	2.44	0.51
1:B:172:ARG:NH2	1:B:242:THR:HG21	2.25	0.51
1:A:158:GLY:O	1:A:161:ALA:HB3	2.11	0.51
1:D:348:ASN:OD1	1:D:349:PRO:CA	2.59	0.51
1:C:122:ALA:HB3	1:D:129:ARG:HH21	1.75	0.51
1:D:292:PRO:HD3	1:D:378:CYS:HA	1.91	0.51
1:D:290:THR:O	1:D:294:PRO:HD2	2.11	0.51
1:A:12:ARG:O	1:A:199:ILE:HA	2.10	0.51
1:D:307:ILE:HD12	1:D:307:ILE:H	1.76	0.51
1:B:117:GLU:OE1	1:B:351:GLY:N	2.43	0.51
1:B:157:MET:CE	1:B:157:MET:HA	2.41	0.51
1:B:183:GLN:HA	1:B:183:GLN:OE1	2.10	0.51
1:D:51:GLU:HB3	1:D:111:ILE:HD12	1.93	0.51
1:D:65:ASN:O	1:D:68:ARG:HB3	2.10	0.51
1:A:9:SER:HA	1:A:272:LEU:HD22	1.93	0.50
1:D:54:LEU:O	1:D:84:GLY:HA2	2.11	0.50
1:C:385:VAL:HG22	1:C:386:ALA:N	2.25	0.50
1:C:269:ILE:O	1:C:271:PRO:HD3	2.11	0.50
1:C:316:HIS:CG	1:C:377:LEU:HD23	2.46	0.50
1:A:276:VAL:O	1:A:277:SER:HB3	2.11	0.50
1:D:12:ARG:O	1:D:199:ILE:HA	2.12	0.50
1:D:317:GLU:CD	1:D:342:GLY:HA3	2.32	0.50
1:B:37:ALA:O	1:B:41:ARG:HG3	2.10	0.50
1:A:298:LYS:NZ	1:A:301:GLU:OE1	2.44	0.50
1:D:148:LEU:O	1:D:157:MET:HG2	2.11	0.50
1:D:12:ARG:HB2	1:D:254:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ALA:HB2	1:D:319:PHE:CD1	2.47	0.50
1:A:8:ALA:O	1:A:9:SER:HB3	2.11	0.50
1:B:333:ASP:O	1:B:336:ILE:HG12	2.12	0.49
1:C:170:LEU:HD21	1:C:328:LYS:HZ2	1.76	0.49
1:D:357:ILE:CD1	1:D:375:ALA:HB1	2.43	0.49
1:D:364:GLU:O	1:D:368:ARG:HG2	2.13	0.49
1:C:190:GLN:NE2	1:C:219:ILE:HD12	2.28	0.49
1:C:314:GLU:OE2	1:C:338:ASN:HA	2.13	0.49
1:D:293:ILE:HB	1:D:294:PRO:HD3	1.95	0.49
1:B:374:LEU:HD23	1:B:374:LEU:C	2.33	0.49
1:C:5:ILE:HG13	1:C:100:MET:HG2	1.95	0.49
1:D:9:SER:CB	1:D:42:ALA:HB2	2.32	0.48
1:D:158:GLY:HA2	1:D:319:PHE:CE2	2.47	0.48
1:C:293:ILE:HB	1:C:294:PRO:CD	2.44	0.48
1:A:326:VAL:HG13	1:A:330:LEU:HD12	1.94	0.48
1:B:31:GLY:O	1:B:35:ILE:HG13	2.13	0.48
1:D:314:GLU:OE2	1:D:338:ASN:HA	2.14	0.48
1:B:64:GLN:O	1:B:65:ASN:C	2.50	0.48
1:B:57:VAL:O	1:B:59:PRO:HD3	2.12	0.48
1:B:47:GLY:HA2	1:B:77:PRO:HD3	1.95	0.48
1:C:103:ILE:HA	1:C:108:ALA:O	2.13	0.48
1:A:342:GLY:O	1:A:346:ILE:HD12	2.14	0.48
1:A:207:ARG:H	1:A:207:ARG:HD3	1.79	0.48
1:C:250:ASN:OD1	1:C:348:ASN:N	2.44	0.48
1:C:330:LEU:HD12	1:C:332:TRP:CZ2	2.49	0.48
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.80	0.47
1:C:153:TYR:CE2	1:C:286:LYS:HD3	2.49	0.47
1:A:180:VAL:CG2	1:A:228:MET:HG3	2.44	0.47
1:B:293:ILE:CB	1:B:294:PRO:CD	2.86	0.47
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.76	0.47
1:A:354:GLY:HA2	1:A:377:LEU:HD21	1.96	0.47
1:D:12:ARG:HD2	1:D:356:ARG:HG2	1.96	0.47
1:A:317:GLU:OE1	1:A:344:ILE:HG13	2.15	0.47
1:C:152:PHE:CE1	1:D:72:MET:HG3	2.49	0.47
1:D:119:MET:HE2	1:D:350:ILE:HD11	1.96	0.47
1:B:156:HIS:ND1	1:B:157:MET:N	2.63	0.47
1:A:282:GLY:HA2	1:A:383:MET:HA	1.97	0.47
1:A:97:ALA:O	1:A:101:GLN:HG3	2.15	0.47
1:B:274:ARG:HE	1:B:392:LEU:HD21	1.78	0.47
1:A:297:ARG:HH11	1:A:297:ARG:HG2	1.80	0.47
1:A:292:PRO:HB2	1:A:326:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PRO:O	1:A:62:GLU:HB2	2.15	0.47
1:D:233:PRO:HB2	1:D:236:ASP:O	2.14	0.46
1:D:199:ILE:HG22	1:D:200:VAL:N	2.31	0.46
1:B:12:ARG:HD2	1:B:356:ARG:HG2	1.97	0.46
1:D:278:TRP:HA	1:D:386:ALA:O	2.14	0.46
1:D:133:LYS:HA	1:D:133:LYS:HD3	1.60	0.46
1:C:156:HIS:ND1	1:C:157:MET:N	2.63	0.46
1:B:234:ALA:H	1:B:242:THR:HA	1.79	0.46
1:B:291:GLY:N	1:B:292:PRO:CD	2.79	0.46
1:C:371:ARG:HA	1:C:391:SER:OG	2.15	0.46
1:D:186:ALA:HA	1:D:340:ASN:O	2.15	0.46
1:A:198:GLU:HB3	1:A:363:PHE:CD2	2.50	0.46
1:B:207:ARG:HG2	1:B:208:LYS:H	1.81	0.46
1:A:348:ASN:HA	1:A:349:PRO:HD3	1.20	0.46
1:D:348:ASN:OD1	1:D:349:PRO:C	2.54	0.46
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.50	0.46
1:A:54:LEU:O	1:A:84:GLY:HA2	2.15	0.46
1:D:124:HIS:HA	1:D:140:ILE:O	2.16	0.46
1:C:54:LEU:HD13	1:C:116:MET:HE1	1.98	0.46
1:D:317:GLU:HB2	1:D:343:ALA:H	1.81	0.46
1:A:120:SER:O	1:B:129:ARG:HD2	2.16	0.46
1:A:31:GLY:O	1:A:35:ILE:HG13	2.16	0.46
1:B:289:GLY:HA2	1:B:378:CYS:SG	2.55	0.46
1:C:22:PHE:HB3	1:C:25:THR:HB	1.98	0.46
1:D:317:GLU:HB2	1:D:343:ALA:N	2.31	0.46
1:D:117:GLU:HA	1:D:117:GLU:OE1	2.15	0.46
1:D:28:HIS:ND1	1:D:62:GLU:OE2	2.34	0.46
1:B:281:VAL:CG1	1:B:282:GLY:H	2.29	0.45
1:C:155:TYR:CD2	1:C:159:THR:HG21	2.51	0.45
1:A:204:VAL:O	1:A:204:VAL:HG12	2.16	0.45
1:B:160:THR:HA	1:B:163:ASN:HD22	1.81	0.45
1:B:333:ASP:C	1:B:335:SER:H	2.20	0.45
1:C:379:ILE:HG21	1:C:383:MET:HE3	1.97	0.45
1:A:333:ASP:O	1:A:336:ILE:HG12	2.16	0.45
1:B:318:ALA:N	1:B:322:GLN:OE1	2.47	0.45
1:C:356:ARG:NH2	1:C:357:ILE:HG22	2.31	0.45
1:D:305:TRP:CE2	1:D:372:LYS:HD3	2.50	0.45
1:A:176:ASP:O	1:A:180:VAL:HG23	2.15	0.45
1:C:7:ILE:HA	1:C:258:LEU:HD12	1.98	0.45
1:C:186:ALA:HA	1:C:340:ASN:O	2.17	0.45
1:B:34:VAL:O	1:B:38:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ALA:CB	1:C:298:LYS:HB3	2.45	0.45
1:D:232:ARG:HE	1:D:232:ARG:H	1.65	0.45
1:C:57:VAL:HB	1:C:117:GLU:OE1	2.15	0.45
1:A:364:GLU:HA	1:A:367:ARG:HG2	1.98	0.45
1:C:205:LYS:HA	1:C:205:LYS:HD3	1.43	0.45
1:C:129:ARG:HH21	1:D:122:ALA:HB3	1.81	0.45
1:C:293:ILE:HB	1:C:294:PRO:HD2	1.98	0.45
1:D:35:ILE:O	1:D:38:VAL:HG22	2.17	0.45
1:C:276:VAL:HG21	1:C:305:TRP:CZ2	2.52	0.45
1:D:358:LEU:HD23	1:D:358:LEU:HA	1.86	0.45
1:B:207:ARG:HH11	1:B:207:ARG:HG2	1.82	0.45
1:D:357:ILE:HD12	1:D:375:ALA:HB1	1.99	0.45
1:C:60:ALA:O	1:C:123:PRO:HG3	2.17	0.45
1:D:378:CYS:C	1:D:379:ILE:HG13	2.36	0.44
1:D:359:ASN:O	1:D:363:PHE:HD1	2.00	0.44
1:B:55:GLY:HA2	1:B:85:MET:O	2.18	0.44
1:B:178:PHE:CZ	1:B:323:ALA:HB1	2.52	0.44
1:A:379:ILE:HB	1:A:383:MET:HB2	1.99	0.44
1:D:279:ALA:O	1:D:385:VAL:HA	2.16	0.44
1:A:158:GLY:HA3	1:A:235:PHE:CD2	2.52	0.44
1:C:6:VAL:HA	1:C:274:ARG:HA	1.98	0.44
1:A:233:PRO:HA	1:A:241:VAL:O	2.17	0.44
1:C:165:ALA:O	1:C:169:GLN:N	2.50	0.44
1:C:348:ASN:CG	1:C:349:PRO:N	2.69	0.44
1:D:51:GLU:HA	1:D:81:THR:O	2.16	0.44
1:D:379:ILE:HB	1:D:383:MET:HB2	2.00	0.44
1:B:30:LEU:O	1:B:34:VAL:HG23	2.18	0.44
1:A:228:MET:HA	1:A:231:LEU:HD12	2.00	0.44
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.83	0.44
1:C:18:PHE:O	1:C:19:ASN:HB2	2.18	0.44
1:B:317:GLU:CD	1:B:342:GLY:HA3	2.37	0.44
1:B:150:ASP:HB2	1:B:157:MET:HE1	1.99	0.44
1:B:379:ILE:HD11	1:B:385:VAL:HG12	2.00	0.44
1:D:236:ASP:O	1:D:239:GLY:N	2.51	0.43
1:C:57:VAL:HG12	1:C:58:LEU:HG	2.00	0.43
1:D:175:GLN:NE2	1:D:240:THR:HG23	2.30	0.43
1:C:326:VAL:O	1:C:330:LEU:HG	2.18	0.43
1:D:305:TRP:CZ3	1:D:388:CYS:HB3	2.53	0.43
1:C:158:GLY:O	1:C:161:ALA:HB3	2.18	0.43
1:C:385:VAL:CG2	1:C:386:ALA:N	2.80	0.43
1:C:271:PRO:HG2	1:C:392:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HD11	1:C:324:CYS:HB2	1.98	0.43
1:D:199:ILE:CG2	1:D:200:VAL:N	2.81	0.43
1:D:368:ARG:HB3	2:D:2004:HOH:O	2.17	0.43
1:A:181:ALA:O	1:A:185:LYS:HG3	2.19	0.43
1:D:222:GLY:O	1:D:224:THR:N	2.51	0.43
1:C:46:ALA:HB1	1:C:76:VAL:HA	1.99	0.43
1:C:292:PRO:HB3	1:C:376:THR:OG1	2.18	0.43
1:C:274:ARG:NH2	1:C:390:GLU:OE1	2.51	0.43
1:D:311:ASP:HB2	1:D:370:ALA:HB1	2.01	0.43
1:B:228:MET:HE2	1:B:228:MET:HB2	1.85	0.43
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.83	0.43
1:C:263:GLU:CD	1:C:267:ARG:HE	2.22	0.43
1:D:274:ARG:NH2	1:D:390:GLU:OE1	2.49	0.43
1:A:131:GLY:HA2	1:C:131:GLY:CA	2.46	0.43
1:D:150:ASP:HB2	1:D:157:MET:CE	2.48	0.43
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.80	0.43
1:B:66:PRO:HA	1:B:69:GLN:HG3	2.01	0.43
1:B:181:ALA:O	1:B:185:LYS:HG3	2.18	0.43
1:A:88:LEU:HB2	1:A:379:ILE:HG23	1.99	0.42
1:A:361:LEU:HD22	1:A:365:MET:HG3	2.00	0.42
1:A:358:LEU:HD11	1:A:387:MET:HE1	2.00	0.42
1:B:257:LEU:C	1:B:257:LEU:HD23	2.39	0.42
1:C:187:GLU:OE2	1:C:221:HIS:HA	2.19	0.42
1:A:349:PRO:O	1:A:350:ILE:C	2.58	0.42
1:B:18:PHE:O	1:B:19:ASN:C	2.54	0.42
1:C:90:GLY:O	1:C:91:SER:C	2.58	0.42
1:C:156:HIS:CG	1:C:235:PHE:HE1	2.37	0.42
1:C:163:ASN:O	1:C:167:GLN:HB2	2.20	0.42
1:C:28:HIS:HB2	1:C:70:ALA:HB2	2.00	0.42
1:B:158:GLY:HA2	1:B:319:PHE:CZ	2.54	0.42
1:C:379:ILE:HG21	1:C:383:MET:CE	2.48	0.42
1:D:281:VAL:HG12	1:D:282:GLY:N	2.33	0.42
1:A:293:ILE:HG21	1:A:329:ASP:OD1	2.20	0.42
1:C:7:ILE:HD12	1:C:362:LEU:HD11	2.01	0.42
1:A:204:VAL:O	1:A:205:LYS:C	2.58	0.42
1:A:281:VAL:HG12	1:A:282:GLY:H	1.84	0.42
1:D:161:ALA:HB1	1:D:321:ALA:HB3	2.01	0.42
1:D:178:PHE:HE1	1:D:317:GLU:CD	2.23	0.42
1:A:133:LYS:H	1:A:133:LYS:HG2	1.42	0.42
1:D:53:ILE:HD13	1:D:83:TRP:HZ2	1.83	0.42
1:A:375:ALA:O	1:A:386:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:MET:HA	1:D:382:GLY:HA2	2.02	0.42
1:C:51:GLU:CD	1:C:83:TRP:HE1	2.24	0.42
1:D:313:VAL:HG13	1:D:314:GLU:N	2.35	0.42
1:C:379:ILE:HG22	1:C:380:GLY:O	2.20	0.42
1:C:329:ASP:C	1:C:329:ASP:OD1	2.58	0.42
1:D:39:LEU:O	1:D:40:GLU:C	2.57	0.42
1:D:280:THR:HA	1:D:384:GLY:O	2.20	0.42
1:B:180:VAL:HG22	1:B:228:MET:CE	2.50	0.41
1:D:339:VAL:HG11	1:D:368:ARG:HH21	1.85	0.41
1:A:291:GLY:N	1:A:292:PRO:CD	2.82	0.41
1:B:78:GLN:HE21	1:B:78:GLN:HB3	1.55	0.41
1:B:6:VAL:O	1:B:6:VAL:HG23	2.18	0.41
1:D:257:LEU:HD23	1:D:258:LEU:N	2.35	0.41
1:C:293:ILE:CB	1:C:294:PRO:CD	2.98	0.41
1:C:75:GLY:O	1:C:76:VAL:C	2.59	0.41
1:B:187:GLU:HG3	1:B:221:HIS:HA	2.02	0.41
1:C:55:GLY:HA2	1:C:85:MET:O	2.20	0.41
1:B:156:HIS:ND1	1:B:158:GLY:N	2.52	0.41
1:B:291:GLY:N	1:B:292:PRO:HD2	2.35	0.41
1:D:164:VAL:O	1:D:168:TRP:HD1	2.04	0.41
1:B:124:HIS:HA	1:B:140:ILE:O	2.21	0.41
1:A:24:ASN:HA	1:A:121:MET:SD	2.60	0.41
1:B:270:GLN:HA	1:B:271:PRO:HD3	1.86	0.41
1:D:108:ALA:CB	1:D:111:ILE:HD11	2.51	0.41
1:C:81:THR:HG22	1:D:383:MET:HG2	2.03	0.41
1:C:189:ALA:HB1	1:C:340:ASN:HB3	2.02	0.41
1:A:178:PHE:CZ	1:A:323:ALA:HB1	2.56	0.41
1:B:207:ARG:HG2	1:B:207:ARG:NH1	2.36	0.41
1:A:350:ILE:HD13	1:A:350:ILE:HG21	1.73	0.41
1:D:57:VAL:C	1:D:59:PRO:HD3	2.41	0.41
1:C:25:THR:HA	1:C:26:PRO:HD3	1.72	0.41
1:A:72:MET:HG3	1:B:152:PHE:CZ	2.56	0.41
1:D:348:ASN:N	1:D:349:PRO:HD3	2.28	0.41
1:A:293:ILE:HG13	1:A:326:VAL:HG22	2.03	0.41
1:D:313:VAL:HB	1:D:337:VAL:HG22	2.03	0.41
1:D:291:GLY:N	1:D:292:PRO:HD2	2.35	0.41
1:D:158:GLY:HA3	1:D:235:PHE:CD2	2.56	0.41
1:C:189:ALA:CB	1:C:340:ASN:HB3	2.50	0.41
1:B:5:ILE:HG13	1:B:100:MET:HG2	2.02	0.41
1:B:5:ILE:HD12	1:B:103:ILE:HB	2.03	0.41
1:D:291:GLY:N	1:D:292:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:O	1:A:237:LYS:C	2.58	0.41
1:C:259:MET:HB3	1:C:259:MET:HE2	1.92	0.41
1:C:233:PRO:HB2	1:C:236:ASP:O	2.20	0.40
1:D:361:LEU:HD21	1:D:373:GLY:HA3	2.02	0.40
1:C:180:VAL:HG21	1:C:225:LEU:HA	2.03	0.40
1:B:136:ASP:OD1	1:C:140:ILE:HA	2.20	0.40
1:D:250:ASN:HB2	1:D:348:ASN:O	2.21	0.40
1:D:50:ASN:OD1	1:D:109:SER:N	2.53	0.40
1:A:158:GLY:HA3	1:A:235:PHE:CE2	2.56	0.40
1:C:153:TYR:HE1	1:C:285:PRO:HG2	1.86	0.40
1:B:311:ASP:HB2	1:B:370:ALA:HB1	2.02	0.40
1:C:7:ILE:CD1	1:C:362:LEU:HD11	2.52	0.40
1:C:153:TYR:CZ	1:C:286:LYS:CG	3.04	0.40
1:C:276:VAL:O	1:C:277:SER:HB3	2.22	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	387/392 (99%)	345 (89%)	37 (10%)	5 (1%)	15	52
1	B	387/392 (99%)	354 (92%)	31 (8%)	2 (0%)	34	75
1	C	387/392 (99%)	337 (87%)	44 (11%)	6 (2%)	12	46
1	D	387/392 (99%)	330 (85%)	50 (13%)	7 (2%)	11	43
All	All	1548/1568 (99%)	1366 (88%)	162 (10%)	20 (1%)	15	52

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	PRO

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Mol	Chain	Res	Type
1	C	348	ASN
1	C	349	PRO
1	C	350	ILE
1	D	223	ALA
1	D	349	PRO
1	D	350	ILE
1	B	350	ILE
1	C	223	ALA
1	D	240	THR
1	A	205	LYS
1	C	240	THR
1	D	335	SER
1	A	350	ILE
1	A	339	VAL
1	D	158	GLY
1	C	239	GLY
1	D	270	GLN
1	A	287	VAL
1	B	59	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/279 (99%)	252 (91%)	24 (9%)	13	41
1	B	276/279 (99%)	259 (94%)	17 (6%)	23	59
1	C	276/279 (99%)	246 (89%)	30 (11%)	8	28
1	D	276/279 (99%)	250 (91%)	26 (9%)	11	37
All	All	1104/1116 (99%)	1007 (91%)	97 (9%)	12	41

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	109	SER

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Mol	Chain	Res	Type
1	A	133	LYS
1	A	155	TYR
1	A	196	LYS
1	A	207	ARG
1	A	208	LYS
1	A	225	LEU
1	A	236	ASP
1	A	237	LYS
1	A	238	GLU
1	A	240	THR
1	A	260	SER
1	A	272	LEU
1	A	276	VAL
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	324	CYS
1	A	332	TRP
1	A	339	VAL
1	A	358	LEU
1	A	361	LEU
1	A	371	ARG
1	B	39	LEU
1	B	173	ASP
1	B	182	SER
1	B	187	GLU
1	B	207	ARG
1	B	224	THR
1	B	240	THR
1	B	258	LEU
1	B	270	GLN
1	B	272	LEU
1	B	276	VAL
1	B	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	358	LEU
1	B	361	LEU
1	C	4	SER
1	C	17	SER
1	C	39	LEU

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Mol	Chain	Res	Type
1	C	40	GLU
1	C	48	GLU
1	C	100	MET
1	C	133	LYS
1	C	155	TYR
1	C	157	MET
1	C	207	ARG
1	C	216	ASP
1	C	220	ARG
1	C	224	THR
1	C	226	ASP
1	C	232	ARG
1	C	249	LEU
1	C	250	ASN
1	C	258	LEU
1	C	265	SER
1	C	272	LEU
1	C	276	VAL
1	C	288	MET
1	C	298	LYS
1	C	311	ASP
1	C	322	GLN
1	C	332	TRP
1	C	353	SER
1	C	358	LEU
1	C	371	ARG
1	C	374	LEU
1	D	25	THR
1	D	39	LEU
1	D	89	CYS
1	D	110	ILE
1	D	134	MET
1	D	144	ILE
1	D	173	ASP
1	D	187	GLU
1	D	207	ARG
1	D	210	ASP
1	D	211	ILE
1	D	224	THR
1	D	227	SER
1	D	232	ARG
1	D	258	LEU

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Mol	Chain	Res	Type
1	D	288	MET
1	D	290	THR
1	D	298	LYS
1	D	322	GLN
1	D	324	CYS
1	D	328	LYS
1	D	332	TRP
1	D	353	SER
1	D	358	LEU
1	D	368	ARG
1	D	374	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	167	GLN
1	A	175	GLN
1	B	78	GLN
1	B	163	ASN
1	B	175	GLN
1	B	184	ASN
1	C	78	GLN
1	C	101	GLN
1	C	175	GLN
1	C	184	ASN
1	C	190	GLN
1	C	316	HIS
1	D	78	GLN
1	D	175	GLN
1	D	184	ASN
1	D	190	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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, 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	389/392 (99%)	0.04	7 (1%) 71 49	2, 12, 41, 48	0
1	B	389/392 (99%)	0.10	13 (3%) 50 29	2, 11, 45, 50	0
1	C	389/392 (99%)	0.44	18 (4%) 36 19	19, 32, 49, 57	0
1	D	389/392 (99%)	0.71	50 (12%) 5 2	16, 39, 66, 71	0
All	All	1556/1568 (99%)	0.32	88 (5%) 27 14	2, 27, 54, 71	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	246	ALA	6.0
1	D	243	ALA	5.3
1	D	290	THR	4.9
1	D	226	ASP	4.8
1	D	163	ASN	4.7
1	D	161	ALA	4.6
1	D	319	PHE	4.5
1	D	232	ARG	4.3
1	D	155	TYR	4.3
1	B	234	ALA	4.3
1	D	154	GLY	4.2
1	B	236	ASP	4.2
1	C	229	ALA	4.1
1	D	320	ALA	4.1
1	D	288	MET	4.0
1	C	246	ALA	4.0
1	D	329	ASP	4.0
1	C	161	ALA	4.0
1	D	153	TYR	3.9
1	D	239	GLY	3.8
1	D	164	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	158	GLY	3.7
1	D	330	LEU	3.6
1	C	164	VAL	3.6
1	C	330	LEU	3.6
1	D	331	GLY	3.5
1	C	239	GLY	3.4
1	C	222	GLY	3.2
1	D	165	ALA	3.2
1	C	224	THR	3.2
1	D	321	ALA	3.2
1	B	158	GLY	3.1
1	D	381	GLY	3.1
1	D	231	LEU	3.0
1	C	179	ALA	3.0
1	C	236	ASP	3.0
1	D	240	THR	3.0
1	B	230	LYS	2.9
1	D	180	VAL	2.9
1	D	291	GLY	2.9
1	B	247	SER	2.8
1	D	285	PRO	2.8
1	D	388	CYS	2.8
1	C	327	ASN	2.8
1	D	157	MET	2.8
1	A	229	ALA	2.7
1	D	378	CYS	2.7
1	A	151	ALA	2.7
1	C	244	GLY	2.7
1	D	235	PHE	2.6
1	D	269	ILE	2.6
1	D	158	GLY	2.5
1	D	241	VAL	2.5
1	D	325	ALA	2.5
1	D	229	ALA	2.5
1	D	292	PRO	2.4
1	B	237	LYS	2.4
1	D	287	VAL	2.4
1	C	243	ALA	2.4
1	A	163	ASN	2.4
1	D	244	GLY	2.3
1	D	227	SER	2.3
1	D	332	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	159	THR	2.3
1	B	245	ASN	2.2
1	A	239	GLY	2.2
1	A	233	PRO	2.2
1	B	246	ALA	2.2
1	D	382	GLY	2.2
1	D	169	GLN	2.2
1	D	245	ASN	2.2
1	C	226	ASP	2.2
1	C	232	ARG	2.2
1	D	160	THR	2.2
1	B	173	ASP	2.1
1	D	309	ASP	2.1
1	D	230	LYS	2.1
1	C	174	GLU	2.1
1	B	132	VAL	2.1
1	D	360	THR	2.1
1	D	166	LYS	2.1
1	B	229	ALA	2.1
1	D	162	GLU	2.1
1	B	233	PRO	2.1
1	C	245	ASN	2.1
1	A	240	THR	2.0
1	D	324	CYS	2.0
1	C	247	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.