



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:48 PM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

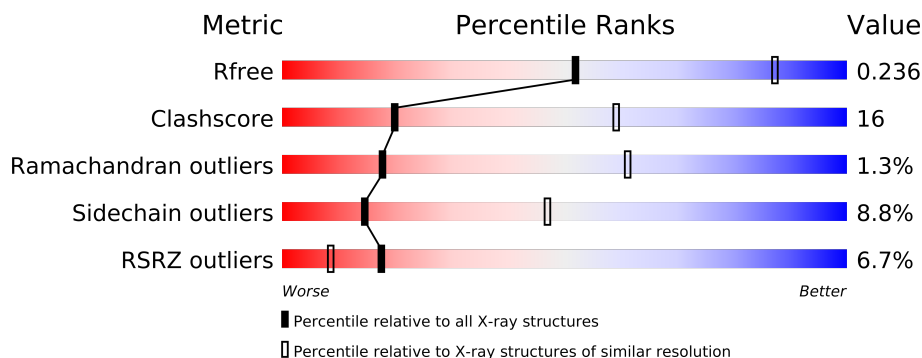
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1468 (3.00-2.96)
Clashscore	79885	1894 (3.00-2.96)
Ramachandran outliers	78287	1826 (3.00-2.96)
Sidechain outliers	78261	1829 (3.00-2.96)
RSRZ outliers	66119	1469 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	392	
1	B	392	
1	C	392	
1	D	392	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11278 atoms, of which 0 are hydrogen and 0 are deuterium.

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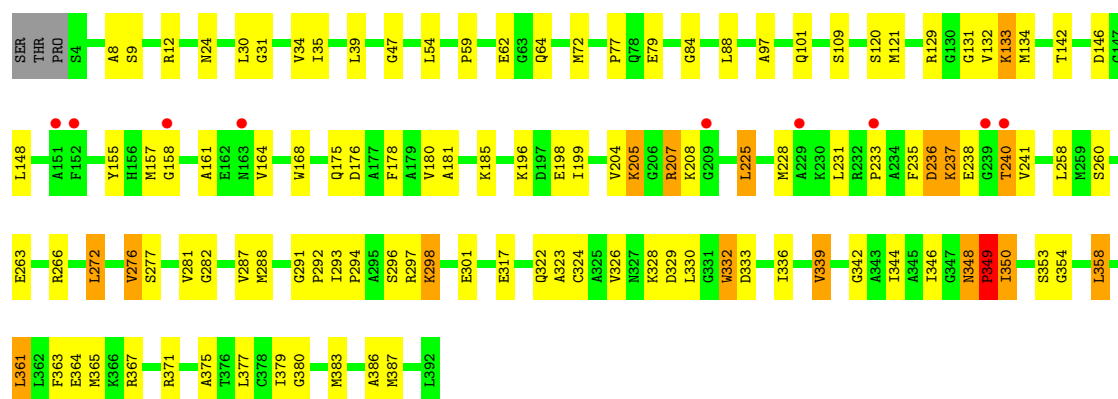
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	3	Total	O	0	0
			3	3		
2	D	5	Total	O	0	0
			5	5		

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.

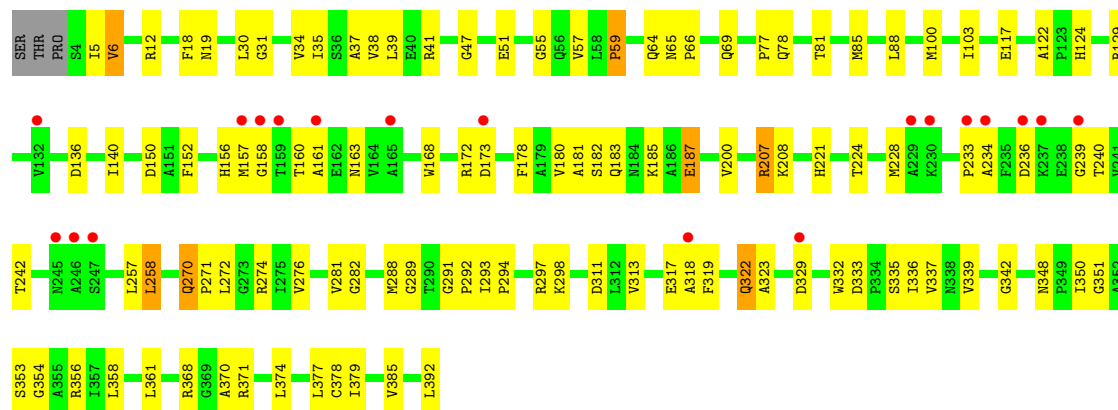
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain A: 



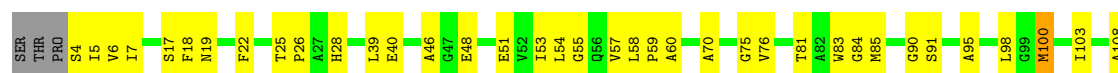
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

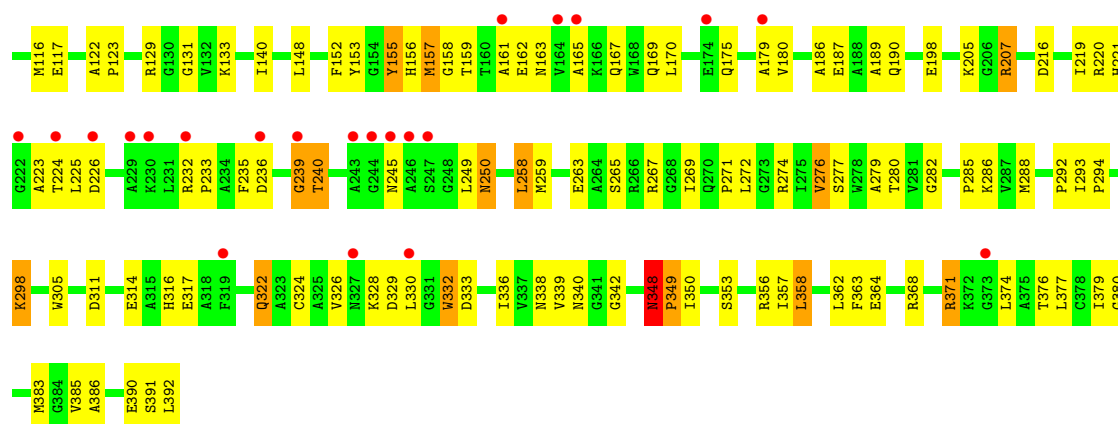
Chain B: 



• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

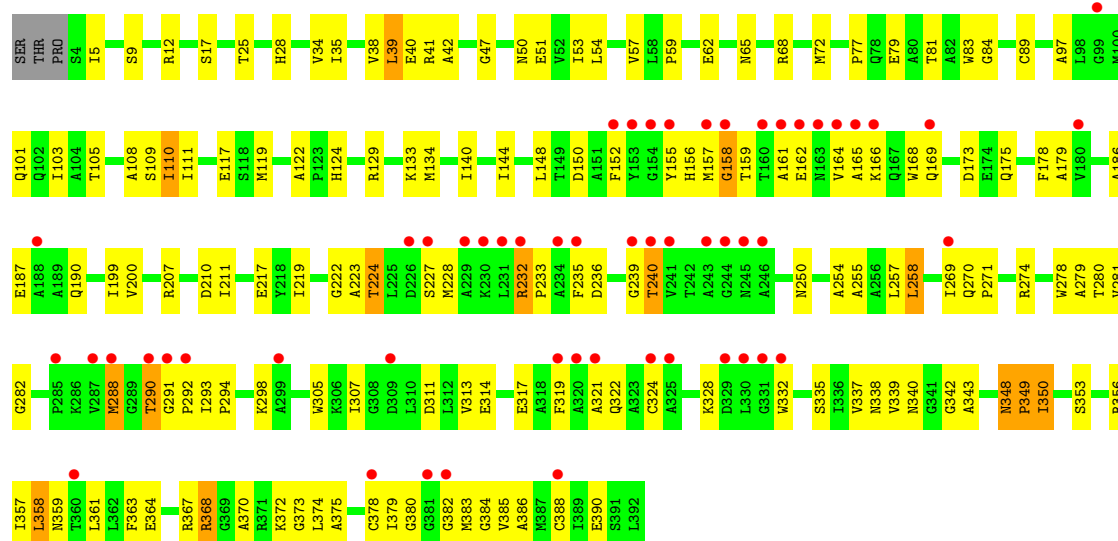
Chain C: 





● Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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 0.206 , 0.236	Depositor DCC
R_{free} test set	1974 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 9.6	EDS
Estimated twinning fraction	0.176 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	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 ²)	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.*

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (361) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:B:168:TRP:HH2	1:B:329:ASP:HB2	1.64	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/392 (99%)	345 (89%)	37 (10%)	5 (1%)	18	61
1	B	387/392 (99%)	354 (92%)	31 (8%)	2 (0%)	38	83
1	C	387/392 (99%)	337 (87%)	44 (11%)	6 (2%)	14	55
1	D	387/392 (99%)	330 (85%)	50 (13%)	7 (2%)	13	51
All	All	1548/1568 (99%)	1366 (88%)	162 (10%)	20 (1%)	18	61

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	PRO
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

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Mol	Chain	Res	Type
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%)	15	48
1	B	276/279 (99%)	259 (94%)	17 (6%)	26	67
1	C	276/279 (99%)	246 (89%)	30 (11%)	9	33
1	D	276/279 (99%)	250 (91%)	26 (9%)	13	43
All	All	1104/1116 (99%)	1007 (91%)	97 (9%)	14	47

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

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/392 (99%)	0.10	9 (2%) 57 23	2, 12, 41, 48	0
1	B	389/392 (99%)	0.17	19 (4%) 28 13	2, 11, 45, 50	0
1	C	389/392 (99%)	0.54	22 (5%) 23 11	19, 32, 49, 57	0
1	D	389/392 (99%)	0.82	55 (14%) 3 2	16, 39, 66, 71	0
All	All	1556/1568 (99%)	0.41	105 (6%) 17 8	2, 27, 54, 71	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	246	ALA	6.9
1	D	243	ALA	6.1
1	D	161	ALA	5.2
1	B	234	ALA	5.2
1	D	163	ASN	5.2
1	D	290	THR	5.1
1	D	232	ARG	5.1
1	D	226	ASP	5.1
1	D	319	PHE	4.8
1	D	154	GLY	4.8
1	C	229	ALA	4.7
1	D	320	ALA	4.7
1	C	246	ALA	4.6
1	C	161	ALA	4.5
1	D	155	TYR	4.5
1	D	164	VAL	4.4
1	B	236	ASP	4.3
1	D	288	MET	4.3
1	D	239	GLY	4.2
1	D	153	TYR	4.2
1	A	158	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	164	VAL	4.0
1	D	331	GLY	3.9
1	C	330	LEU	3.9
1	D	329	ASP	3.9
1	D	330	LEU	3.8
1	D	165	ALA	3.8
1	C	239	GLY	3.8
1	D	321	ALA	3.7
1	C	179	ALA	3.6
1	C	222	GLY	3.6
1	C	224	THR	3.5
1	B	158	GLY	3.4
1	D	180	VAL	3.4
1	B	230	LYS	3.3
1	D	231	LEU	3.3
1	D	381	GLY	3.2
1	C	236	ASP	3.2
1	A	229	ALA	3.1
1	D	285	PRO	3.1
1	D	240	THR	3.1
1	D	388	CYS	3.1
1	A	151	ALA	3.1
1	D	157	MET	3.0
1	D	325	ALA	3.0
1	D	241	VAL	2.9
1	C	244	GLY	2.9
1	D	291	GLY	2.9
1	D	235	PHE	2.9
1	D	378	CYS	2.9
1	B	247	SER	2.9
1	D	269	ILE	2.9
1	D	229	ALA	2.8
1	C	327	ASN	2.8
1	C	243	ALA	2.8
1	D	292	PRO	2.7
1	D	244	GLY	2.7
1	D	158	GLY	2.6
1	D	287	VAL	2.6
1	C	232	ARG	2.6
1	B	237	LYS	2.6
1	B	229	ALA	2.5
1	D	332	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	159	THR	2.5
1	A	233	PRO	2.5
1	A	239	GLY	2.5
1	B	161	ALA	2.5
1	B	246	ALA	2.5
1	A	163	ASN	2.4
1	D	169	GLN	2.4
1	B	245	ASN	2.4
1	B	132	VAL	2.4
1	B	233	PRO	2.4
1	C	226	ASP	2.4
1	D	309	ASP	2.4
1	D	230	LYS	2.3
1	D	382	GLY	2.3
1	D	227	SER	2.3
1	D	234	ALA	2.3
1	D	166	LYS	2.3
1	D	160	THR	2.3
1	D	360	THR	2.3
1	D	245	ASN	2.3
1	B	173	ASP	2.2
1	D	162	GLU	2.2
1	D	299	ALA	2.2
1	A	240	THR	2.2
1	C	373	GLY	2.2
1	D	324	CYS	2.2
1	D	152	PHE	2.2
1	A	209	GLY	2.2
1	B	157	MET	2.2
1	B	165	ALA	2.2
1	C	174	GLU	2.1
1	B	239	GLY	2.1
1	C	319	PHE	2.1
1	B	318	ALA	2.1
1	C	245	ASN	2.1
1	C	165	ALA	2.1
1	A	152	PHE	2.1
1	D	99	GLY	2.1
1	B	329	ASP	2.1
1	D	188	ALA	2.1
1	C	230	LYS	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 ⓘ

There are no such residues in this entry.