



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:02 AM GMT

PDB ID : 1HQF
Title : CRYSTAL STRUCTURE OF THE BINUCLEAR MANGANESE MET-
ALLOENZYME ARGINASE COMPLEXED WITH N-HYDROXY-L-
ARGININE
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Deposited on : 2000-12-16
Resolution : 2.90 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>

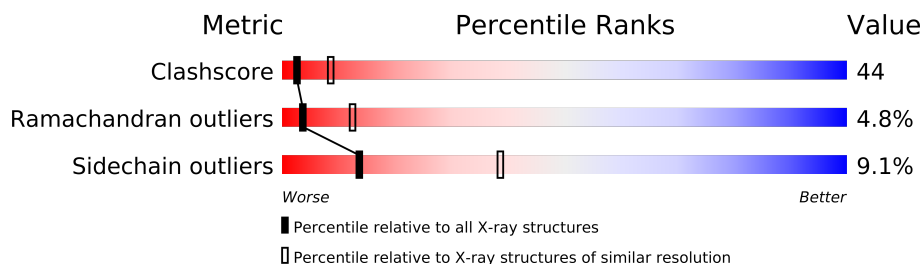
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.90 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))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	
1	C	323	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7245 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.

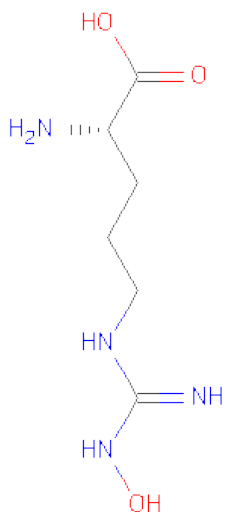
- Molecule 1 is a protein called ARGINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			
1	B	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			
1	C	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is N-OMEGA-HYDROXY-L-ARGININE (three-letter code: HAR) (formula: C₆H₁₄N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	6	4	3		
3	B	1	Total	C	N	O	0	0
			13	6	4	3		
3	C	1	Total	C	N	O	0	0
			13	6	4	3		

- Molecule 4 is water.

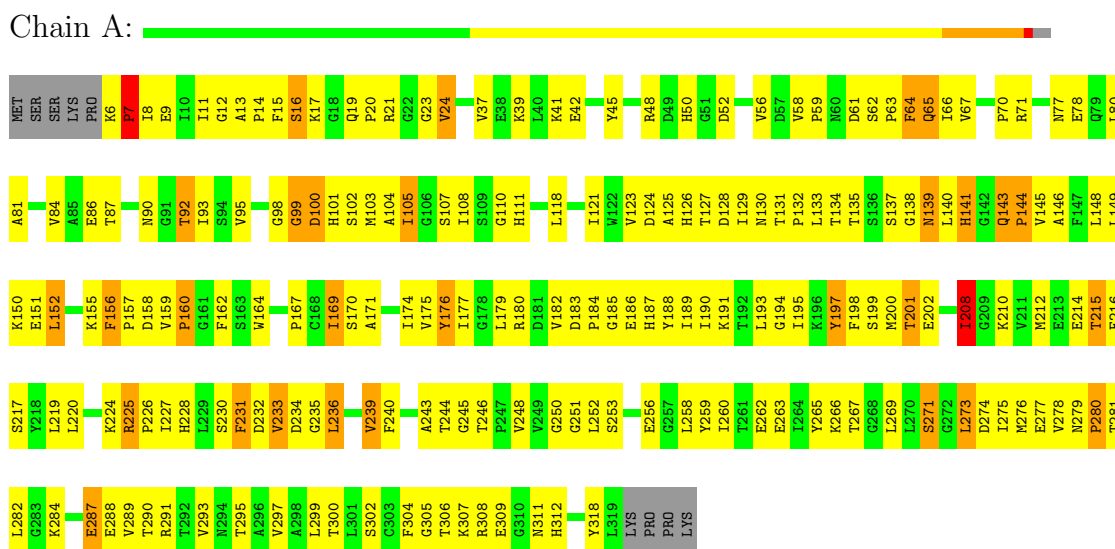
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	5	Total	O	0	0
			5	5		
4	C	5	Total	O	0	0
			5	5		

3 Residue-property plots

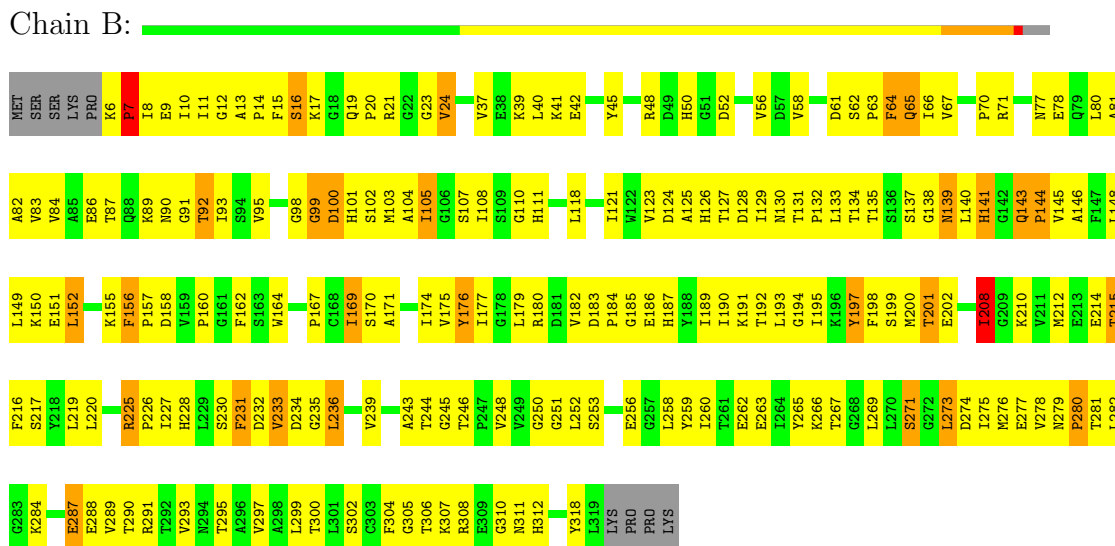
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: ARGINASE 1



• Molecule 1: ARGINASE 1



• Molecule 1: ARGINASE 1

Chain C:



L282	S217	K150	A81	Met
G283	Y218	E151	E84	Ser
G284	L220	L152	E86	Lys
E287		K155	T87	Pro
E288	K224	F156		K6
V289	R225	P157	N90	P7
T290	P226	D158	G91	I8
T291	T227	V159	T92	E9
T292	H228	P160	G92	I10
V293	L229	G161	I93	I11
M294	S230	F162	S94	G12
A296	F231	S163	V95	A13
V297	V232	W164		P14
A298	D234	P167	G98	F15
L299	D235	C168	G99	S16
T300	L236	I169	D100	K17
L301		S170	H101	G18
S302	V239	A171	M103	Q19
C303	F240		A104	P20
F304	A243	I174	I105	G22
G305	T244	V175	G106	G23
T306	G245	Y176	S107	V24
K307	T246	I177	I108	
R308	T247	L178	S109	V37
E309	V248	L179	G110	E38
G310	V249	R180	H111	K39
N311	G250	D181		L40
H312	G251	V182	L118	K41
D317	L252	D183	I121	E42
Y318	S253	P184	W122	Y45
L319		G185	V123	N46
Lys	E256	E186	D124	V47
Pro	G257	H187	A125	R48
Pro	L258	I189	L126	D49
Lys	Y259	I190	T127	H50
	L260	K191	D128	G51
	T261	T192	I129	D52
	E262	L193	N130	
	E263	G194	T131	V56
	L264	K196	P132	D57
	T265	Y197	L133	V58
	T266	F198	T134	
	T267	S199	T135	D61
	G268	M200	S136	S62
	L269	T201	S137	P63
	L270	E202	G138	F64
	S271		N139	Q65
	G272		L140	I66
	L273	T203	H141	V67
	D274	G209	G142	
	L275	K210	Q143	P70
	E276	V211	P144	R71
	E277	M212	V145	
	V278	E213	A146	N77
	N279	E214	F147	E78
	P280	T215	L148	G79

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	88.00Å 88.00Å 112.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7245	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HAR, MN

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	0.42	0/2448	0.71	1/3325 (0.0%)
1	B	0.42	0/2448	0.71	1/3325 (0.0%)
1	C	0.42	0/2448	0.71	1/3325 (0.0%)
All	All	0.42	0/7344	0.71	3/9975 (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
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	GLY	N-CA-C	-6.78	96.16	113.10
1	C	99	GLY	N-CA-C	-6.77	96.18	113.10
1	B	99	GLY	N-CA-C	-6.76	96.21	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	176	TYR	Sidechain
1	C	176	TYR	Sidechain

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	2395	0	2420	217	0
1	B	2395	0	2420	219	0
1	C	2395	0	2420	224	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	13	0	11	2	0
3	B	13	0	11	2	0
3	C	13	0	11	2	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
All	All	7245	0	7293	645	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 44.

All (645) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:6:LYS:HD3	1:B:7:PRO:HD2	1.23	1.15
1:A:6:LYS:HD3	1:A:7:PRO:HD2	1.23	1.14
1:C:6:LYS:HD3	1:C:7:PRO:HD2	1.23	1.08
1:B:82:ALA:O	1:B:86:GLU:HG2	1.53	1.07
1:A:37:VAL:HG23	4:A:602:HOH:O	1.61	1.00
1:C:37:VAL:HG23	4:C:612:HOH:O	1.61	0.99
1:B:37:VAL:HG23	4:B:607:HOH:O	1.61	0.97
1:B:258:LEU:HD23	1:B:299:LEU:HD23	1.52	0.92
1:A:258:LEU:HD23	1:A:299:LEU:HD23	1.52	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:306:THR:HA	1:B:311:ASN:HD21	1.34	0.91
1:C:7:PRO:HG2	1:C:92:THR:HA	1.50	0.91
1:A:7:PRO:HG2	1:A:92:THR:HA	1.50	0.91
1:A:306:THR:HA	1:A:311:ASN:HD21	1.34	0.91
1:C:143:GLN:H	1:C:144:PRO:HD3	1.36	0.90
1:B:7:PRO:HG2	1:B:92:THR:HA	1.50	0.90
1:C:258:LEU:HD23	1:C:299:LEU:HD23	1.52	0.90
1:A:143:GLN:H	1:A:144:PRO:HD3	1.36	0.90
1:B:143:GLN:H	1:B:144:PRO:HD3	1.36	0.89
1:C:306:THR:HA	1:C:311:ASN:HD21	1.34	0.88
1:A:143:GLN:H	1:A:144:PRO:CD	1.88	0.86
1:C:143:GLN:H	1:C:144:PRO:CD	1.88	0.86
1:B:143:GLN:H	1:B:144:PRO:CD	1.88	0.86
1:A:230:SER:HA	1:A:274:ASP:HB2	1.58	0.85
1:C:6:LYS:HD3	1:C:7:PRO:CD	2.07	0.84
1:C:230:SER:HA	1:C:274:ASP:HB2	1.58	0.84
1:A:234:ASP:HB3	1:A:244:THR:HG21	1.57	0.84
1:B:230:SER:HA	1:B:274:ASP:HB2	1.58	0.84
1:B:6:LYS:HD3	1:B:7:PRO:CD	2.07	0.81
1:A:6:LYS:HD3	1:A:7:PRO:CD	2.07	0.81
1:C:287:GLU:CG	1:C:291:ARG:HH21	1.92	0.81
1:B:287:GLU:CG	1:B:291:ARG:HH21	1.92	0.81
1:A:287:GLU:CG	1:A:291:ARG:HH21	1.92	0.80
1:B:6:LYS:CD	1:B:7:PRO:HD2	2.11	0.80
1:A:210:LYS:HE3	1:A:214:GLU:OE2	1.81	0.79
1:B:210:LYS:HE3	1:B:214:GLU:OE2	1.81	0.79
1:C:210:LYS:HE3	1:C:214:GLU:OE2	1.81	0.79
1:A:244:THR:HG22	1:A:245:GLY:H	1.48	0.79
1:A:67:VAL:HA	1:A:138:GLY:CA	2.13	0.78
1:B:306:THR:HA	1:B:311:ASN:ND2	1.98	0.78
1:B:67:VAL:HA	1:B:138:GLY:CA	2.13	0.78
1:C:244:THR:HG22	1:C:245:GLY:H	1.48	0.78
1:A:306:THR:HA	1:A:311:ASN:ND2	1.98	0.78
1:C:67:VAL:HA	1:C:138:GLY:CA	2.13	0.78
1:A:6:LYS:CD	1:A:7:PRO:HD2	2.11	0.78
1:B:244:THR:HG22	1:B:245:GLY:H	1.48	0.77
1:B:234:ASP:HB3	1:B:244:THR:HG21	1.66	0.77
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.67	0.77
1:A:201:THR:HG22	1:C:308:ARG:HB2	1.66	0.76
1:C:234:ASP:HB3	1:C:244:THR:HG21	1.66	0.76
1:A:188:TYR:CD2	1:C:318:TYR:HB2	2.20	0.76
1:C:306:THR:HA	1:C:311:ASN:ND2	1.98	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:19:GLN:HB2	1:C:20:PRO:HD2	1.67	0.75
1:C:6:LYS:CD	1:C:7:PRO:HD2	2.11	0.75
1:A:137:SER:HB2	1:A:139:ASN:OD1	1.87	0.75
1:C:137:SER:HB2	1:C:139:ASN:OD1	1.87	0.75
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.67	0.75
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.68	0.75
1:B:137:SER:HB2	1:B:139:ASN:OD1	1.87	0.74
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.68	0.74
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.68	0.74
1:B:308:ARG:HB2	1:C:201:THR:HG22	1.68	0.74
1:A:146:ALA:HA	1:A:152:LEU:HD23	1.71	0.73
1:A:220:LEU:HD13	1:A:269:LEU:HD12	1.71	0.73
1:C:146:ALA:HA	1:C:152:LEU:HD23	1.71	0.72
1:C:143:GLN:N	1:C:144:PRO:CD	2.52	0.72
1:A:140:LEU:O	1:A:144:PRO:HD3	1.90	0.72
1:C:220:LEU:HD13	1:C:269:LEU:HD12	1.71	0.72
1:C:258:LEU:O	1:C:262:GLU:HG3	1.90	0.72
1:B:146:ALA:HA	1:B:152:LEU:HD23	1.71	0.72
1:A:67:VAL:HA	1:A:138:GLY:HA3	1.72	0.72
1:B:258:LEU:O	1:B:262:GLU:HG3	1.90	0.71
1:B:220:LEU:HD13	1:B:269:LEU:HD12	1.71	0.71
1:C:140:LEU:O	1:C:144:PRO:HD3	1.90	0.71
1:A:143:GLN:N	1:A:144:PRO:CD	2.52	0.71
1:B:140:LEU:O	1:B:144:PRO:HD3	1.90	0.71
1:A:258:LEU:O	1:A:262:GLU:HG3	1.90	0.70
1:A:187:HIS:O	1:A:191:LYS:HG2	1.91	0.70
1:B:187:HIS:O	1:B:191:LYS:HG2	1.91	0.70
1:C:187:HIS:O	1:C:191:LYS:HG2	1.91	0.70
1:C:212:MET:HE1	1:C:260:ILE:HG23	1.73	0.70
1:C:67:VAL:HA	1:C:138:GLY:HA3	1.72	0.70
1:C:258:LEU:CD2	1:C:299:LEU:HD23	2.22	0.70
1:B:143:GLN:N	1:B:144:PRO:CD	2.52	0.70
1:A:212:MET:HE1	1:A:260:ILE:HG23	1.74	0.70
1:B:67:VAL:HA	1:B:138:GLY:HA3	1.72	0.69
1:B:180:ARG:CZ	1:B:251:GLY:HA3	2.23	0.69
1:A:258:LEU:CD2	1:A:299:LEU:HD23	2.22	0.69
1:B:212:MET:HE1	1:B:260:ILE:HG23	1.74	0.69
1:C:175:VAL:HG11	1:C:215:THR:HG22	1.74	0.69
1:C:180:ARG:CZ	1:C:251:GLY:HA3	2.22	0.69
1:A:12:GLY:HA3	1:A:52:ASP:OD1	1.93	0.69
1:B:86:GLU:O	1:B:89:LYS:HG2	1.92	0.68
1:A:7:PRO:HG2	1:A:92:THR:CA	2.24	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:175:VAL:HG11	1:A:215:THR:HG22	1.74	0.68
1:A:180:ARG:CZ	1:A:251:GLY:HA3	2.22	0.68
1:C:12:GLY:HA3	1:C:52:ASP:OD1	1.93	0.68
1:B:258:LEU:CD2	1:B:299:LEU:HD23	2.22	0.68
1:C:129:ILE:CG2	1:C:186:GLU:HG2	2.24	0.68
1:A:129:ILE:CG2	1:A:186:GLU:HG2	2.24	0.68
1:B:287:GLU:OE1	1:B:291:ARG:HB2	1.94	0.67
1:B:175:VAL:HG11	1:B:215:THR:HG22	1.74	0.67
1:B:12:GLY:HA3	1:B:52:ASP:OD1	1.93	0.67
1:C:169:ILE:HD13	1:C:169:ILE:H	1.60	0.67
1:C:287:GLU:OE1	1:C:291:ARG:HB2	1.94	0.67
1:B:278:VAL:HG12	1:B:280:PRO:HD3	1.76	0.67
1:A:135:THR:HB	1:A:137:SER:O	1.94	0.67
1:A:287:GLU:OE1	1:A:291:ARG:HB2	1.94	0.67
1:B:7:PRO:HG2	1:B:92:THR:CA	2.24	0.67
1:B:135:THR:HB	1:B:137:SER:O	1.94	0.67
1:C:135:THR:HB	1:C:137:SER:O	1.94	0.66
1:B:129:ILE:CG2	1:B:186:GLU:HG2	2.24	0.66
1:A:169:ILE:H	1:A:169:ILE:HD13	1.60	0.66
1:C:278:VAL:HG12	1:C:280:PRO:HD3	1.76	0.66
1:A:278:VAL:HG12	1:A:280:PRO:HD3	1.76	0.66
1:B:169:ILE:H	1:B:169:ILE:HD13	1.60	0.65
1:B:180:ARG:NH1	1:B:248:VAL:O	2.28	0.65
1:C:7:PRO:HG2	1:C:92:THR:CA	2.24	0.65
1:A:129:ILE:HG23	1:A:186:GLU:HG2	1.78	0.65
1:C:129:ILE:HG23	1:C:186:GLU:HG2	1.78	0.65
1:B:199:SER:OG	1:B:201:THR:HG23	1.97	0.65
1:B:129:ILE:HG23	1:B:186:GLU:HG2	1.78	0.65
1:C:180:ARG:NH1	1:C:248:VAL:O	2.28	0.65
1:A:111:HIS:CE1	1:A:271:SER:HB3	2.33	0.64
1:B:111:HIS:CE1	1:B:271:SER:HB3	2.33	0.64
1:A:180:ARG:NH1	1:A:248:VAL:O	2.28	0.64
1:C:199:SER:OG	1:C:201:THR:HG23	1.97	0.64
1:A:87:THR:HG22	1:A:92:THR:OG1	1.98	0.64
1:B:87:THR:HG22	1:B:92:THR:OG1	1.98	0.64
1:B:83:VAL:O	1:B:86:GLU:HB2	1.97	0.63
1:C:185:GLY:O	1:C:189:ILE:HG13	1.98	0.63
1:A:185:GLY:O	1:A:189:ILE:HG13	1.99	0.63
1:A:232:ASP:O	1:A:234:ASP:N	2.32	0.63
1:C:111:HIS:CE1	1:C:271:SER:HB3	2.33	0.63
1:A:199:SER:OG	1:A:201:THR:HG23	1.97	0.63
1:A:188:TYR:OH	1:C:317:ASP:HA	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:185:GLY:O	1:B:189:ILE:HG13	1.98	0.63
1:C:253:SER:OG	1:C:256:GLU:HG3	1.99	0.63
1:B:232:ASP:O	1:B:234:ASP:N	2.32	0.63
1:A:309:GLU:OE2	1:B:187:HIS:NE2	2.32	0.62
1:B:253:SER:OG	1:B:256:GLU:HG3	1.99	0.62
1:C:232:ASP:O	1:C:234:ASP:N	2.32	0.62
1:A:253:SER:OG	1:A:256:GLU:HG3	1.99	0.62
1:C:87:THR:HG22	1:C:92:THR:OG1	1.98	0.61
1:C:169:ILE:HD13	1:C:169:ILE:N	2.15	0.61
1:B:67:VAL:HA	1:B:138:GLY:HA2	1.82	0.61
1:C:67:VAL:HA	1:C:138:GLY:HA2	1.82	0.61
1:A:67:VAL:HA	1:A:138:GLY:HA2	1.82	0.61
1:B:169:ILE:HD13	1:B:169:ILE:N	2.15	0.61
1:A:169:ILE:HD13	1:A:169:ILE:N	2.15	0.61
1:B:262:GLU:OE1	1:C:201:THR:HB	2.00	0.60
1:B:244:THR:HG22	1:B:245:GLY:N	2.16	0.60
1:C:244:THR:HG22	1:C:245:GLY:N	2.16	0.60
1:A:188:TYR:CG	1:C:318:TYR:HB2	2.36	0.60
1:B:130:ASN:HB3	1:B:135:THR:HG23	1.84	0.59
1:B:244:THR:HG23	1:B:277:GLU:O	2.02	0.59
1:A:84:VAL:HG21	1:A:107:SER:HA	1.83	0.59
1:C:24:VAL:O	1:C:99:GLY:HA2	2.02	0.59
1:A:244:THR:HG23	1:A:277:GLU:O	2.02	0.59
1:A:24:VAL:O	1:A:99:GLY:HA2	2.02	0.59
1:C:244:THR:HG23	1:C:277:GLU:O	2.02	0.59
1:A:287:GLU:CD	1:A:291:ARG:HH21	2.05	0.59
1:B:24:VAL:O	1:B:99:GLY:HA2	2.02	0.59
1:B:232:ASP:OD2	1:B:234:ASP:OD2	2.20	0.59
1:A:133:LEU:HD21	1:A:157:PRO:HD2	1.85	0.59
1:C:11:ILE:HD13	1:C:50:HIS:HB3	1.84	0.59
1:C:287:GLU:CD	1:C:291:ARG:HH21	2.05	0.59
1:C:273:LEU:HD13	1:C:275:ILE:HD11	1.85	0.59
1:B:84:VAL:HG21	1:B:107:SER:HA	1.83	0.59
1:B:11:ILE:HD13	1:B:50:HIS:HB3	1.84	0.59
1:C:84:VAL:HG21	1:C:107:SER:HA	1.83	0.59
1:C:133:LEU:HD21	1:C:157:PRO:HD2	1.85	0.59
1:A:11:ILE:HD13	1:A:50:HIS:HB3	1.84	0.59
1:A:273:LEU:HD13	1:A:275:ILE:HD11	1.85	0.59
1:A:244:THR:HG22	1:A:245:GLY:N	2.16	0.58
1:C:232:ASP:OD2	1:C:234:ASP:OD2	2.21	0.58
1:B:133:LEU:HD21	1:B:157:PRO:HD2	1.85	0.58
1:A:130:ASN:HB3	1:A:135:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:130:ASN:HB3	1:C:135:THR:HG23	1.84	0.58
1:C:105:ILE:HG22	1:C:148:LEU:HD21	1.84	0.58
1:C:129:ILE:HD13	1:C:145:VAL:CG1	2.34	0.58
1:A:129:ILE:O	1:A:129:ILE:HG13	2.04	0.58
1:A:105:ILE:HG22	1:A:148:LEU:HD21	1.84	0.58
1:B:287:GLU:CD	1:B:291:ARG:HH21	2.05	0.58
1:C:129:ILE:HG13	1:C:129:ILE:O	2.04	0.58
1:A:263:GLU:O	1:A:267:THR:HG23	2.04	0.58
1:B:129:ILE:HD13	1:B:145:VAL:CG1	2.34	0.58
1:B:105:ILE:HG22	1:B:148:LEU:HD21	1.84	0.57
1:C:263:GLU:O	1:C:267:THR:HG23	2.04	0.57
1:B:263:GLU:O	1:B:267:THR:HG23	2.04	0.57
1:B:273:LEU:HD13	1:B:275:ILE:HD11	1.85	0.57
1:B:19:GLN:NE2	1:B:24:VAL:HG21	2.20	0.57
1:C:312:HIS:HB2	1:C:318:TYR:CE2	2.40	0.57
1:B:129:ILE:HG13	1:B:129:ILE:O	2.04	0.57
1:C:127:THR:HB	1:C:129:ILE:HG22	1.87	0.57
1:A:129:ILE:HD13	1:A:145:VAL:CG1	2.34	0.56
1:A:312:HIS:HB2	1:A:318:TYR:CE2	2.40	0.56
1:B:9:GLU:OE1	1:B:50:HIS:HB2	2.06	0.56
1:A:127:THR:HB	1:A:129:ILE:HG22	1.87	0.56
1:A:19:GLN:NE2	1:A:24:VAL:HG21	2.20	0.56
1:A:9:GLU:OE1	1:A:50:HIS:HB2	2.06	0.56
1:C:19:GLN:NE2	1:C:24:VAL:HG21	2.20	0.56
1:C:16:SER:CB	1:C:24:VAL:HG23	2.36	0.56
1:C:9:GLU:OE1	1:C:50:HIS:HB2	2.06	0.56
1:B:126:HIS:HB2	1:B:128:ASP:OD1	2.06	0.56
1:A:78:GLU:HB2	1:A:164:TRP:CE2	2.41	0.56
1:C:287:GLU:CG	1:C:291:ARG:NH2	2.68	0.55
1:B:127:THR:HB	1:B:129:ILE:HG22	1.87	0.55
1:A:212:MET:HE2	1:A:260:ILE:HA	1.87	0.55
1:C:78:GLU:HB2	1:C:164:TRP:CE2	2.41	0.55
1:C:129:ILE:HD13	1:C:145:VAL:HB	1.89	0.55
1:B:16:SER:CB	1:B:24:VAL:HG23	2.36	0.55
1:B:312:HIS:HB2	1:B:318:TYR:CE2	2.40	0.55
1:B:212:MET:CE	1:B:260:ILE:HG23	2.37	0.55
1:C:212:MET:CE	1:C:260:ILE:HG23	2.37	0.55
1:C:212:MET:HE2	1:C:260:ILE:HA	1.88	0.55
1:A:212:MET:CE	1:A:260:ILE:HG23	2.37	0.55
1:A:305:GLY:O	1:A:307:LYS:HG3	2.07	0.55
1:A:16:SER:CB	1:A:24:VAL:HG23	2.36	0.55
1:C:64:PHE:HZ	1:C:157:PRO:HB2	1.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:ILE:HD13	1:B:145:VAL:HB	1.88	0.55
1:A:287:GLU:HG3	1:A:291:ARG:HH21	1.71	0.55
1:A:236:LEU:HD12	1:A:252:LEU:HB2	1.89	0.55
1:B:78:GLU:HB2	1:B:164:TRP:CE2	2.42	0.55
1:C:279:ASN:O	1:C:281:THR:N	2.40	0.55
1:B:265:TYR:CZ	1:B:305:GLY:HA2	2.42	0.54
1:B:212:MET:HE2	1:B:260:ILE:HA	1.87	0.54
1:A:64:PHE:HZ	1:A:157:PRO:HB2	1.72	0.54
1:A:126:HIS:HB2	1:A:128:ASP:OD1	2.06	0.54
1:B:287:GLU:CG	1:B:291:ARG:NH2	2.68	0.54
1:B:64:PHE:HZ	1:B:157:PRO:HB2	1.72	0.54
1:B:65:GLN:HE22	1:B:157:PRO:HG3	1.73	0.54
1:C:199:SER:O	1:C:202:GLU:N	2.41	0.54
1:C:305:GLY:O	1:C:307:LYS:HG3	2.07	0.54
1:C:126:HIS:HB2	1:C:128:ASP:OD1	2.06	0.54
1:A:265:TYR:CZ	1:A:305:GLY:HA2	2.42	0.54
1:A:129:ILE:HD13	1:A:145:VAL:HB	1.89	0.54
1:B:121:ILE:HD12	1:B:121:ILE:N	2.23	0.54
1:B:236:LEU:HD12	1:B:252:LEU:HB2	1.89	0.54
1:C:186:GLU:O	1:C:190:ILE:HG12	2.08	0.54
1:A:199:SER:O	1:A:202:GLU:N	2.41	0.54
1:C:65:GLN:HE22	1:C:157:PRO:HG3	1.72	0.54
1:B:279:ASN:O	1:B:281:THR:N	2.40	0.54
1:B:305:GLY:O	1:B:307:LYS:HG3	2.07	0.54
1:C:265:TYR:CZ	1:C:305:GLY:HA2	2.42	0.54
1:A:180:ARG:NH2	1:A:251:GLY:HA3	2.23	0.54
1:A:279:ASN:O	1:A:281:THR:N	2.40	0.54
1:A:121:ILE:N	1:A:121:ILE:HD12	2.23	0.54
1:A:105:ILE:HA	1:A:148:LEU:HD21	1.90	0.53
1:B:105:ILE:HA	1:B:148:LEU:HD21	1.90	0.53
1:C:236:LEU:HD12	1:C:252:LEU:HB2	1.89	0.53
1:B:100:ASP:OD1	1:B:102:SER:N	2.34	0.53
1:C:180:ARG:NH2	1:C:251:GLY:HA3	2.23	0.53
1:C:287:GLU:HG3	1:C:291:ARG:HH21	1.71	0.53
1:C:13:ALA:O	1:C:15:PHE:N	2.42	0.53
1:A:139:ASN:OD1	1:A:139:ASN:N	2.41	0.53
1:A:287:GLU:CG	1:A:291:ARG:NH2	2.68	0.53
1:A:65:GLN:HE22	1:A:157:PRO:HG3	1.73	0.53
1:C:121:ILE:N	1:C:121:ILE:HD12	2.23	0.53
1:A:13:ALA:O	1:A:15:PHE:N	2.42	0.53
1:C:139:ASN:OD1	1:C:139:ASN:N	2.41	0.53
1:C:102:SER:HB3	1:C:141:HIS:HA	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:100:ASP:OD1	1:C:102:SER:N	2.34	0.53
1:B:186:GLU:O	1:B:190:ILE:HG12	2.08	0.53
1:A:186:GLU:O	1:A:190:ILE:HG12	2.08	0.53
1:B:102:SER:HB3	1:B:141:HIS:HA	1.91	0.53
1:C:162:PHE:CD1	1:C:162:PHE:N	2.77	0.53
1:B:139:ASN:N	1:B:139:ASN:OD1	2.41	0.52
1:B:175:VAL:HG11	1:B:215:THR:CG2	2.39	0.52
1:B:180:ARG:NH2	1:B:251:GLY:HA3	2.23	0.52
1:C:105:ILE:HA	1:C:148:LEU:HD21	1.90	0.52
1:B:162:PHE:CD1	1:B:162:PHE:N	2.77	0.52
1:C:63:PRO:O	1:C:65:GLN:N	2.43	0.52
1:A:63:PRO:O	1:A:65:GLN:N	2.43	0.52
1:B:16:SER:HB3	1:B:24:VAL:HG23	1.92	0.52
1:A:287:GLU:HG3	1:A:291:ARG:NH2	2.25	0.52
1:A:130:ASN:O	1:A:143:GLN:HG2	2.09	0.52
1:C:23:GLY:HA3	1:C:279:ASN:OD1	2.10	0.52
1:B:13:ALA:O	1:B:15:PHE:N	2.42	0.52
1:B:86:GLU:O	1:B:90:ASN:ND2	2.43	0.52
1:A:86:GLU:O	1:A:90:ASN:ND2	2.43	0.52
1:C:98:GLY:HA3	1:C:276:MET:CE	2.40	0.52
1:C:130:ASN:O	1:C:143:GLN:HG2	2.09	0.51
1:C:16:SER:HB3	1:C:24:VAL:HG23	1.92	0.51
1:B:130:ASN:O	1:B:143:GLN:HG2	2.09	0.51
1:C:175:VAL:HG11	1:C:215:THR:CG2	2.39	0.51
1:B:198:PHE:CE1	1:B:215:THR:HG23	2.46	0.51
1:A:162:PHE:N	1:A:162:PHE:CD1	2.77	0.51
1:A:102:SER:HB3	1:A:141:HIS:HA	1.91	0.51
1:B:287:GLU:HG3	1:B:291:ARG:HH21	1.71	0.51
1:A:175:VAL:HG11	1:A:215:THR:CG2	2.39	0.51
1:B:39:LYS:O	1:B:42:GLU:HB2	2.10	0.51
1:B:193:LEU:N	1:B:193:LEU:HD12	2.26	0.51
1:C:287:GLU:HG3	1:C:291:ARG:NH2	2.25	0.51
1:A:23:GLY:HA3	1:A:279:ASN:OD1	2.10	0.51
1:C:86:GLU:O	1:C:90:ASN:ND2	2.43	0.51
1:A:152:LEU:O	1:A:155:LYS:HB2	2.11	0.51
1:C:131:THR:N	1:C:134:THR:OG1	2.42	0.51
1:B:63:PRO:O	1:B:65:GLN:N	2.43	0.51
1:C:193:LEU:HD12	1:C:193:LEU:N	2.26	0.51
1:A:193:LEU:HD12	1:A:193:LEU:N	2.26	0.51
1:C:227:ILE:HD13	1:C:269:LEU:HB2	1.93	0.51
1:A:98:GLY:HA3	1:A:276:MET:CE	2.40	0.51
1:A:16:SER:HB3	1:A:24:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:23:GLY:HA3	1:B:279:ASN:OD1	2.10	0.51
1:A:39:LYS:O	1:A:42:GLU:HB2	2.10	0.51
1:C:171:ALA:HB1	1:C:195:ILE:HG12	1.93	0.51
1:C:93:ILE:HD12	1:C:271:SER:HA	1.93	0.51
1:C:118:LEU:C	1:C:118:LEU:HD12	2.31	0.51
1:C:198:PHE:CE1	1:C:215:THR:HG23	2.46	0.51
1:C:152:LEU:O	1:C:155:LYS:HB2	2.11	0.50
1:A:287:GLU:HG3	1:A:288:GLU:N	2.26	0.50
1:B:98:GLY:HA3	1:B:276:MET:CE	2.40	0.50
1:A:131:THR:N	1:A:134:THR:OG1	2.42	0.50
1:A:37:VAL:HG12	1:A:41:LYS:HE3	1.93	0.50
1:C:105:ILE:HG22	1:C:148:LEU:CD2	2.42	0.50
1:A:171:ALA:HB1	1:A:195:ILE:HG12	1.93	0.50
1:C:37:VAL:HG12	1:C:41:LYS:HE3	1.93	0.50
1:A:20:PRO:HD3	1:A:139:ASN:ND2	2.27	0.50
1:B:118:LEU:C	1:B:118:LEU:HD12	2.31	0.50
1:A:227:ILE:HD13	1:A:269:LEU:HB2	1.93	0.50
1:B:37:VAL:HG12	1:B:41:LYS:HE3	1.93	0.50
1:B:152:LEU:O	1:B:155:LYS:HB2	2.11	0.50
1:C:287:GLU:HG3	1:C:288:GLU:N	2.26	0.50
1:B:287:GLU:HG3	1:B:291:ARG:NH2	2.25	0.50
1:B:227:ILE:HD13	1:B:269:LEU:HB2	1.93	0.50
1:B:8:ILE:HG12	1:B:45:TYR:HB3	1.94	0.50
1:C:279:ASN:C	1:C:281:THR:H	2.15	0.50
1:A:279:ASN:C	1:A:281:THR:H	2.15	0.50
1:C:8:ILE:HG12	1:C:45:TYR:HB3	1.94	0.50
1:B:131:THR:N	1:B:134:THR:OG1	2.42	0.50
1:B:93:ILE:HD12	1:B:271:SER:HA	1.93	0.50
1:C:20:PRO:HD3	1:C:139:ASN:ND2	2.27	0.50
1:C:125:ALA:O	1:C:179:LEU:HA	2.12	0.50
1:B:125:ALA:O	1:B:179:LEU:HA	2.12	0.50
1:A:151:GLU:OE1	1:A:170:SER:HA	2.12	0.50
1:A:308:ARG:HB2	1:B:201:THR:HG22	1.93	0.50
1:B:199:SER:O	1:B:202:GLU:N	2.41	0.50
1:C:39:LYS:O	1:C:42:GLU:HB2	2.11	0.50
1:A:105:ILE:HG22	1:A:148:LEU:CD2	2.42	0.49
1:C:98:GLY:HA3	1:C:276:MET:HE3	1.94	0.49
1:C:151:GLU:OE1	1:C:170:SER:HA	2.12	0.49
1:A:243:ALA:HA	1:A:282:LEU:O	2.12	0.49
1:C:243:ALA:HA	1:C:282:LEU:O	2.12	0.49
1:A:198:PHE:CE1	1:A:215:THR:HG23	2.46	0.49
1:A:149:LEU:O	1:A:167:PRO:HB3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:212:MET:SD	1:B:260:ILE:HG12	2.52	0.49
1:B:287:GLU:HG3	1:B:288:GLU:N	2.26	0.49
1:C:232:ASP:OD2	3:C:908:HAR:OH1	2.31	0.49
1:B:232:ASP:OD2	3:B:907:HAR:OH1	2.31	0.49
1:C:212:MET:SD	1:C:260:ILE:HG12	2.52	0.49
1:A:93:ILE:HD12	1:A:271:SER:HA	1.93	0.49
1:A:118:LEU:C	1:A:118:LEU:HD12	2.31	0.49
1:A:102:SER:HA	1:A:144:PRO:HG3	1.95	0.49
1:A:104:ALA:O	1:A:108:ILE:HG13	2.13	0.49
1:B:104:ALA:O	1:B:108:ILE:HG13	2.13	0.49
1:B:108:ILE:HD12	1:B:148:LEU:CD1	2.43	0.49
1:B:105:ILE:HG22	1:B:148:LEU:CD2	2.42	0.49
1:A:188:TYR:CZ	1:C:317:ASP:HA	2.47	0.49
1:C:102:SER:HA	1:C:144:PRO:HG3	1.95	0.49
1:C:183:ASP:HB2	1:C:186:GLU:OE1	2.13	0.49
1:B:20:PRO:HD3	1:B:139:ASN:ND2	2.27	0.49
1:A:8:ILE:HD13	1:A:93:ILE:HB	1.95	0.49
1:B:279:ASN:C	1:B:281:THR:H	2.15	0.49
1:B:243:ALA:HA	1:B:282:LEU:O	2.12	0.49
1:B:183:ASP:HB2	1:B:186:GLU:OE1	2.13	0.49
1:B:123:VAL:HA	1:B:177:ILE:O	2.13	0.49
1:C:123:VAL:HA	1:C:177:ILE:O	2.13	0.49
1:C:108:ILE:HD12	1:C:148:LEU:CD1	2.43	0.49
1:C:149:LEU:O	1:C:167:PRO:HB3	2.12	0.49
1:A:212:MET:SD	1:A:260:ILE:HG12	2.52	0.49
1:B:61:ASP:OD1	1:B:70:PRO:HD2	2.13	0.49
1:C:61:ASP:OD1	1:C:70:PRO:HD2	2.13	0.49
1:B:8:ILE:HD13	1:B:93:ILE:HB	1.95	0.48
1:C:8:ILE:HD13	1:C:93:ILE:HB	1.95	0.48
1:A:125:ALA:O	1:A:179:LEU:HA	2.12	0.48
1:B:102:SER:HA	1:B:144:PRO:HG3	1.95	0.48
1:C:198:PHE:CE1	1:C:215:THR:CG2	2.97	0.48
1:A:98:GLY:HA3	1:A:276:MET:HE3	1.94	0.48
1:B:151:GLU:OE1	1:B:170:SER:HA	2.12	0.48
1:C:104:ALA:O	1:C:108:ILE:HG13	2.13	0.48
1:B:171:ALA:HB1	1:B:195:ILE:HG12	1.93	0.48
1:A:123:VAL:HA	1:A:177:ILE:O	2.13	0.48
1:C:87:THR:CG2	1:C:92:THR:OG1	2.61	0.48
1:A:100:ASP:OD1	1:A:102:SER:N	2.34	0.48
1:A:108:ILE:HD12	1:A:148:LEU:CD1	2.43	0.48
1:B:129:ILE:HG22	1:B:186:GLU:HG2	1.95	0.48
1:A:232:ASP:OD2	3:A:906:HAR:OH1	2.31	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:ILE:HG12	1:A:45:TYR:HB3	1.94	0.48
1:A:183:ASP:HB2	1:A:186:GLU:OE1	2.13	0.48
1:B:108:ILE:HG12	1:B:228:HIS:CD2	2.49	0.48
1:A:61:ASP:OD1	1:A:70:PRO:HD2	2.13	0.48
1:C:149:LEU:HD23	1:C:169:ILE:O	2.14	0.48
1:B:190:ILE:HA	1:B:195:ILE:HD12	1.95	0.48
1:C:108:ILE:HG12	1:C:228:HIS:CD2	2.49	0.48
1:B:149:LEU:O	1:B:167:PRO:HB3	2.13	0.48
1:C:127:THR:HA	1:C:176:TYR:CE1	2.50	0.47
1:A:190:ILE:HA	1:A:195:ILE:HD12	1.95	0.47
1:B:180:ARG:HG3	1:B:248:VAL:CG1	2.44	0.47
1:A:87:THR:CG2	1:A:92:THR:OG1	2.61	0.47
1:A:108:ILE:HG12	1:A:228:HIS:CD2	2.49	0.47
1:A:149:LEU:HD23	1:A:169:ILE:O	2.13	0.47
1:B:19:GLN:HB3	1:B:141:HIS:CE1	2.49	0.47
1:B:149:LEU:HD23	1:B:169:ILE:O	2.13	0.47
1:A:180:ARG:HG3	1:A:248:VAL:CG1	2.44	0.47
1:C:180:ARG:HG3	1:C:248:VAL:CG1	2.44	0.47
1:C:190:ILE:HA	1:C:195:ILE:HD12	1.95	0.47
1:B:127:THR:HA	1:B:176:TYR:CE1	2.50	0.47
1:B:131:THR:H	1:B:134:THR:HG1	1.61	0.47
1:A:129:ILE:HG22	1:A:186:GLU:HG2	1.95	0.47
1:C:214:GLU:O	1:C:216:PHE:N	2.48	0.47
1:B:198:PHE:CE1	1:B:215:THR:CG2	2.97	0.47
1:A:127:THR:HA	1:A:176:TYR:CE1	2.49	0.47
1:A:198:PHE:CE1	1:A:215:THR:CG2	2.97	0.47
1:B:152:LEU:HA	1:B:155:LYS:HG3	1.97	0.47
1:B:214:GLU:O	1:B:216:PHE:N	2.48	0.47
1:B:277:GLU:OE2	3:B:907:HAR:NH2	2.48	0.47
1:A:152:LEU:HA	1:A:155:LYS:HG3	1.97	0.47
1:A:189:ILE:O	1:A:193:LEU:HD13	2.15	0.47
1:B:9:GLU:HA	1:B:48:ARG:O	2.15	0.47
1:B:291:ARG:O	1:B:295:THR:HG22	2.15	0.47
1:A:214:GLU:O	1:A:216:PHE:N	2.48	0.47
1:B:87:THR:CG2	1:B:92:THR:OG1	2.61	0.47
1:A:19:GLN:HB3	1:A:141:HIS:CE1	2.49	0.47
1:B:180:ARG:HG3	1:B:248:VAL:HG11	1.97	0.47
1:A:180:ARG:HG3	1:A:248:VAL:HG11	1.97	0.47
1:C:150:LYS:C	1:C:152:LEU:H	2.18	0.47
1:C:152:LEU:HA	1:C:155:LYS:HG3	1.97	0.47
1:C:189:ILE:O	1:C:193:LEU:HD13	2.15	0.47
1:B:189:ILE:O	1:B:193:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:ILE:N	1:A:121:ILE:CD1	2.78	0.47
1:C:131:THR:H	1:C:134:THR:HG1	1.59	0.47
1:C:180:ARG:HG3	1:C:248:VAL:HG11	1.97	0.46
1:B:150:LYS:C	1:B:152:LEU:H	2.18	0.46
1:A:277:GLU:OE2	3:A:906:HAR:NH2	2.48	0.46
1:A:188:TYR:HE2	1:C:319:LEU:HG	1.79	0.46
1:A:8:ILE:HD12	1:A:304:PHE:CE1	2.50	0.46
1:B:8:ILE:HD12	1:B:304:PHE:CE1	2.50	0.46
1:C:8:ILE:HD12	1:C:304:PHE:CE1	2.50	0.46
1:A:291:ARG:O	1:A:295:THR:HG22	2.15	0.46
1:C:277:GLU:OE2	3:C:908:HAR:NH2	2.48	0.46
1:B:98:GLY:HA3	1:B:276:MET:HE3	1.97	0.46
1:A:273:LEU:HD13	1:A:275:ILE:CD1	2.45	0.46
1:C:121:ILE:CD1	1:C:121:ILE:N	2.79	0.46
1:C:291:ARG:O	1:C:295:THR:HG22	2.15	0.46
1:C:293:VAL:O	1:C:297:VAL:HG23	2.16	0.46
1:C:9:GLU:HA	1:C:48:ARG:O	2.15	0.46
1:B:95:VAL:HG13	1:B:273:LEU:HB3	1.98	0.46
1:C:95:VAL:HG13	1:C:273:LEU:HB3	1.98	0.46
1:A:197:TYR:C	1:A:197:TYR:CD1	2.89	0.46
1:A:9:GLU:HA	1:A:48:ARG:O	2.15	0.46
1:B:62:SER:HA	1:B:63:PRO:HD3	1.78	0.46
1:A:293:VAL:O	1:A:297:VAL:HG23	2.16	0.46
1:C:141:HIS:C	1:C:141:HIS:CD2	2.89	0.46
1:C:19:GLN:HB3	1:C:141:HIS:CE1	2.49	0.46
1:A:188:TYR:CD1	1:C:318:TYR:HD2	2.34	0.46
1:A:118:LEU:O	1:A:118:LEU:HD12	2.16	0.46
1:B:141:HIS:CD2	1:B:141:HIS:C	2.89	0.46
1:C:124:ASP:OD2	1:C:232:ASP:OD2	2.33	0.45
1:A:150:LYS:C	1:A:152:LEU:H	2.18	0.45
1:A:95:VAL:HG13	1:A:273:LEU:HB3	1.98	0.45
1:A:124:ASP:OD2	1:A:232:ASP:OD2	2.34	0.45
1:C:159:VAL:HA	1:C:160:PRO:HD3	1.76	0.45
1:B:132:PRO:HD2	1:B:156:PHE:CD2	2.52	0.45
1:B:124:ASP:OD2	1:B:232:ASP:OD2	2.34	0.45
1:B:121:ILE:CD1	1:B:121:ILE:N	2.78	0.45
1:C:197:TYR:CD1	1:C:197:TYR:C	2.89	0.45
1:B:197:TYR:C	1:B:197:TYR:CD1	2.89	0.45
1:C:7:PRO:HG2	1:C:92:THR:CB	2.46	0.45
1:B:293:VAL:O	1:B:297:VAL:HG23	2.16	0.45
1:A:232:ASP:OD2	1:A:234:ASP:OD2	2.34	0.45
1:B:310:GLY:C	1:C:187:HIS:ND1	2.69	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:118:LEU:O	1:C:118:LEU:HD12	2.16	0.45
1:A:132:PRO:HD2	1:A:156:PHE:CD2	2.52	0.45
1:B:273:LEU:HD13	1:B:275:ILE:CD1	2.45	0.45
1:B:7:PRO:HG2	1:B:92:THR:CB	2.46	0.45
1:C:312:HIS:HB2	1:C:318:TYR:HE2	1.82	0.45
1:B:118:LEU:O	1:B:118:LEU:HD12	2.16	0.45
1:C:132:PRO:HD2	1:C:156:PHE:CD2	2.52	0.45
1:C:144:PRO:O	1:C:148:LEU:HG	2.17	0.45
1:A:169:ILE:CD1	1:A:169:ILE:N	2.79	0.45
1:C:273:LEU:HD13	1:C:275:ILE:CD1	2.45	0.45
1:C:129:ILE:HG22	1:C:186:GLU:HG2	1.96	0.45
1:B:144:PRO:O	1:B:148:LEU:HG	2.17	0.45
1:A:7:PRO:HG2	1:A:92:THR:CB	2.46	0.44
1:A:144:PRO:O	1:A:148:LEU:HG	2.17	0.44
1:B:58:VAL:HG11	1:B:71:ARG:HB2	1.99	0.44
1:C:58:VAL:HG11	1:C:71:ARG:HB2	1.99	0.44
1:A:208:ILE:HG23	1:A:259:TYR:CD2	2.52	0.44
1:A:19:GLN:HB3	1:A:141:HIS:ND1	2.33	0.44
1:C:216:PHE:O	1:C:217:SER:C	2.56	0.44
1:B:133:LEU:HD21	1:B:157:PRO:CD	2.48	0.44
1:C:169:ILE:CD1	1:C:169:ILE:N	2.79	0.44
1:C:62:SER:HA	1:C:63:PRO:HD3	1.78	0.44
1:A:58:VAL:HG11	1:A:71:ARG:CB	2.48	0.44
1:C:19:GLN:HB3	1:C:141:HIS:ND1	2.33	0.44
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.76	0.44
1:A:141:HIS:CD2	1:A:141:HIS:C	2.89	0.44
1:A:187:HIS:ND1	1:C:311:ASN:N	2.66	0.44
1:A:187:HIS:ND1	1:C:310:GLY:C	2.70	0.44
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.74	0.43
1:C:307:LYS:H	1:C:311:ASN:HD21	1.66	0.43
1:A:133:LEU:HD21	1:A:157:PRO:CD	2.47	0.43
1:C:70:PRO:HG2	1:C:71:ARG:H	1.83	0.43
1:A:58:VAL:HG11	1:A:71:ARG:HB2	2.00	0.43
1:A:9:GLU:OE1	1:A:50:HIS:CD2	2.72	0.43
1:B:70:PRO:HG2	1:B:71:ARG:H	1.83	0.43
1:B:208:ILE:HG23	1:B:259:TYR:CD2	2.53	0.43
1:B:129:ILE:HD13	1:B:145:VAL:CB	2.48	0.43
1:A:233:VAL:HG12	1:A:277:GLU:HB2	2.00	0.43
1:A:216:PHE:O	1:A:217:SER:C	2.56	0.43
1:A:11:ILE:HD13	1:A:50:HIS:CB	2.48	0.43
1:B:307:LYS:H	1:B:311:ASN:HD21	1.66	0.43
1:B:19:GLN:HB3	1:B:141:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:ILE:HD12	1:A:175:VAL:H	1.84	0.43
1:B:9:GLU:OE1	1:B:50:HIS:CD2	2.72	0.43
1:C:58:VAL:HG11	1:C:71:ARG:CB	2.48	0.43
1:C:208:ILE:HG23	1:C:259:TYR:CD2	2.52	0.43
1:C:129:ILE:HD13	1:C:145:VAL:CB	2.48	0.43
1:B:174:ILE:HD12	1:B:175:VAL:H	1.84	0.43
1:B:312:HIS:HB2	1:B:318:TYR:HE2	1.82	0.43
1:A:235:GLY:O	1:A:252:LEU:HD12	2.19	0.43
1:B:233:VAL:HG12	1:B:277:GLU:HB2	2.00	0.43
1:A:101:HIS:CE1	1:A:232:ASP:HB2	2.54	0.43
1:B:216:PHE:O	1:B:217:SER:C	2.56	0.43
1:C:93:ILE:HG23	1:C:271:SER:O	2.19	0.43
1:C:80:LEU:O	1:C:81:ALA:C	2.57	0.43
1:A:129:ILE:HD13	1:A:145:VAL:CB	2.48	0.43
1:B:169:ILE:CD1	1:B:169:ILE:N	2.79	0.43
1:A:273:LEU:CD1	1:A:275:ILE:HD11	2.49	0.43
1:B:6:LYS:NZ	1:B:91:GLY:O	2.49	0.43
1:B:200:MET:SD	1:B:251:GLY:HA2	2.59	0.43
1:C:9:GLU:OE1	1:C:50:HIS:CD2	2.72	0.43
1:B:21:ARG:HD3	1:B:245:GLY:HA2	2.01	0.43
1:C:174:ILE:HD12	1:C:175:VAL:H	1.84	0.43
1:B:11:ILE:HD13	1:B:50:HIS:CB	2.48	0.43
1:B:58:VAL:HG11	1:B:71:ARG:CB	2.48	0.43
1:C:233:VAL:HG12	1:C:277:GLU:HB2	2.00	0.42
1:B:77:ASN:OD1	1:B:103:MET:HA	2.19	0.42
1:C:152:LEU:HD12	1:C:152:LEU:HA	1.86	0.42
1:A:124:ASP:HA	1:A:232:ASP:HB3	2.02	0.42
1:B:124:ASP:HA	1:B:232:ASP:HB3	2.02	0.42
1:C:235:GLY:O	1:C:252:LEU:HD12	2.19	0.42
1:C:77:ASN:OD1	1:C:103:MET:HA	2.19	0.42
1:C:225:ARG:HB2	1:C:226:PRO:CD	2.49	0.42
1:B:305:GLY:O	1:B:306:THR:C	2.58	0.42
1:C:124:ASP:HA	1:C:232:ASP:HB3	2.02	0.42
1:B:101:HIS:CE1	1:B:232:ASP:HB2	2.54	0.42
1:A:200:MET:HE2	1:A:250:GLY:O	2.20	0.42
1:C:81:ALA:O	1:C:110:GLY:HA3	2.20	0.42
1:A:305:GLY:O	1:A:306:THR:C	2.58	0.42
1:C:127:THR:OG1	1:C:182:VAL:HG22	2.19	0.42
1:A:127:THR:OG1	1:A:182:VAL:HG22	2.19	0.42
1:A:200:MET:SD	1:A:251:GLY:HA2	2.59	0.42
1:A:157:PRO:O	1:A:158:ASP:C	2.57	0.42
1:B:80:LEU:O	1:B:81:ALA:C	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:200:MET:SD	1:C:251:GLY:HA2	2.59	0.42
1:B:129:ILE:HD11	1:B:149:LEU:HD12	2.02	0.42
1:B:81:ALA:O	1:B:110:GLY:HA3	2.20	0.42
1:A:56:VAL:HG23	1:A:56:VAL:O	2.19	0.42
1:A:21:ARG:HD3	1:A:245:GLY:HA2	2.01	0.42
1:A:93:ILE:HG23	1:A:271:SER:O	2.19	0.42
1:B:93:ILE:HG23	1:B:271:SER:O	2.19	0.42
1:C:219:LEU:O	1:C:225:ARG:NE	2.53	0.42
1:C:289:VAL:O	1:C:290:THR:C	2.58	0.42
1:A:225:ARG:HB2	1:A:226:PRO:CD	2.49	0.42
1:B:225:ARG:HB2	1:B:226:PRO:CD	2.49	0.42
1:C:129:ILE:HD11	1:C:149:LEU:HD12	2.02	0.42
1:A:19:GLN:CB	1:A:20:PRO:HD2	2.43	0.42
1:C:305:GLY:O	1:C:306:THR:C	2.58	0.42
1:A:58:VAL:HA	1:A:59:PRO:HD2	1.94	0.42
1:C:156:PHE:CD1	1:C:156:PHE:N	2.88	0.42
1:B:86:GLU:HA	1:B:86:GLU:OE1	2.20	0.42
1:C:200:MET:HE2	1:C:250:GLY:O	2.20	0.42
1:A:307:LYS:H	1:A:311:ASN:HD21	1.66	0.42
1:C:11:ILE:HD13	1:C:50:HIS:CB	2.48	0.42
1:A:77:ASN:OD1	1:A:103:MET:HA	2.19	0.42
1:B:289:VAL:O	1:B:290:THR:C	2.58	0.42
1:C:56:VAL:O	1:C:56:VAL:HG23	2.19	0.42
1:A:80:LEU:O	1:A:81:ALA:C	2.57	0.42
1:B:300:THR:C	1:B:302:SER:N	2.73	0.42
1:C:300:THR:C	1:C:302:SER:N	2.73	0.42
1:C:130:ASN:OD1	1:C:186:GLU:HG3	2.20	0.42
1:A:129:ILE:HD11	1:A:149:LEU:HD12	2.02	0.42
1:A:130:ASN:OD1	1:A:186:GLU:HG3	2.20	0.42
1:C:133:LEU:HD21	1:C:157:PRO:CD	2.48	0.42
1:B:235:GLY:O	1:B:252:LEU:HD12	2.19	0.42
1:B:156:PHE:CD1	1:B:156:PHE:N	2.88	0.42
1:B:219:LEU:O	1:B:225:ARG:NE	2.53	0.42
1:B:56:VAL:O	1:B:56:VAL:HG23	2.19	0.42
1:B:127:THR:OG1	1:B:182:VAL:HG22	2.19	0.41
1:B:157:PRO:O	1:B:158:ASP:C	2.58	0.41
1:A:70:PRO:HG2	1:A:71:ARG:H	1.83	0.41
1:A:219:LEU:O	1:A:225:ARG:NE	2.53	0.41
1:A:81:ALA:O	1:A:110:GLY:HA3	2.20	0.41
1:C:258:LEU:HA	1:C:258:LEU:HD23	1.74	0.41
1:B:130:ASN:OD1	1:B:186:GLU:HG3	2.20	0.41
1:B:200:MET:HE2	1:B:250:GLY:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:273:LEU:CD1	1:B:275:ILE:HD11	2.49	0.41
1:A:231:PHE:CE2	1:A:299:LEU:HD13	2.55	0.41
1:C:192:THR:HG22	1:C:193:LEU:HD12	2.03	0.41
1:C:101:HIS:CE1	1:C:232:ASP:HB2	2.54	0.41
1:C:157:PRO:O	1:C:158:ASP:C	2.58	0.41
1:A:300:THR:C	1:A:302:SER:N	2.73	0.41
1:C:21:ARG:HD3	1:C:245:GLY:HA2	2.01	0.41
1:A:227:ILE:HD13	1:A:269:LEU:CB	2.51	0.41
1:C:220:LEU:HD13	1:C:269:LEU:CD1	2.47	0.41
1:A:289:VAL:O	1:A:290:THR:C	2.58	0.41
1:B:258:LEU:HD23	1:B:258:LEU:HA	1.74	0.41
1:B:192:THR:HG22	1:B:193:LEU:HD12	2.02	0.41
1:A:156:PHE:CD1	1:A:156:PHE:N	2.88	0.41
1:C:127:THR:HG23	1:C:179:LEU:HD13	2.03	0.41
1:C:224:LYS:N	1:C:224:LYS:HD2	2.36	0.41
1:B:231:PHE:CE2	1:B:299:LEU:HD13	2.55	0.41
1:B:19:GLN:CB	1:B:20:PRO:HD2	2.43	0.41
1:C:273:LEU:CD1	1:C:275:ILE:HD11	2.49	0.41
1:C:300:THR:C	1:C:302:SER:H	2.24	0.41
1:C:239:VAL:HG12	1:C:240:PHE:CD2	2.56	0.41
1:C:231:PHE:CE2	1:C:299:LEU:HD13	2.55	0.41
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.86	0.41
1:A:224:LYS:N	1:A:224:LYS:HD2	2.36	0.41
1:B:10:ILE:HD11	1:B:40:LEU:CD1	2.51	0.41
1:C:149:LEU:HD12	1:C:152:LEU:HD22	2.03	0.41
1:B:143:GLN:N	1:B:144:PRO:HD2	2.35	0.41
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.86	0.41
1:A:220:LEU:HD13	1:A:269:LEU:CD1	2.47	0.41
1:C:8:ILE:N	1:C:46:ASN:O	2.47	0.41
1:B:275:ILE:HG22	1:B:275:ILE:O	2.21	0.41
1:A:312:HIS:HB2	1:A:318:TYR:HE2	1.82	0.41
1:C:71:ARG:HG3	1:C:71:ARG:HH11	1.86	0.41
1:A:239:VAL:HG12	1:A:240:PHE:CD2	2.56	0.41
1:C:10:ILE:HD11	1:C:40:LEU:CD1	2.51	0.41
1:B:127:THR:HG23	1:B:179:LEU:HD13	2.03	0.41
1:B:149:LEU:HD12	1:B:152:LEU:HD22	2.03	0.40
1:A:278:VAL:O	1:A:280:PRO:HD3	2.21	0.40
1:B:308:ARG:HH11	1:C:200:MET:HB3	1.86	0.40
1:C:227:ILE:HD13	1:C:269:LEU:CB	2.51	0.40
1:C:275:ILE:HG22	1:C:275:ILE:O	2.21	0.40
1:B:87:THR:HA	1:B:90:ASN:HD22	1.86	0.40
1:B:278:VAL:O	1:B:280:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:278:VAL:O	1:C:280:PRO:HD3	2.21	0.40
1:A:62:SER:HA	1:A:63:PRO:HD3	1.78	0.40
1:B:300:THR:C	1:B:302:SER:H	2.24	0.40
1:B:220:LEU:HD13	1:B:269:LEU:CD1	2.47	0.40
1:A:127:THR:HG23	1:A:179:LEU:HD13	2.03	0.40
1:A:15:PHE:CD2	1:A:103:MET:SD	3.15	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	312/323 (97%)	240 (77%)	57 (18%)	15 (5%)	4	12
1	B	312/323 (97%)	240 (77%)	57 (18%)	15 (5%)	4	12
1	C	312/323 (97%)	240 (77%)	57 (18%)	15 (5%)	4	12
All	All	936/969 (97%)	720 (77%)	171 (18%)	45 (5%)	4	12

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PHE
1	A	233	VAL
1	B	64	PHE
1	B	233	VAL
1	C	64	PHE
1	C	233	VAL
1	A	143	GLN
1	A	215	THR
1	A	280	PRO
1	B	143	GLN
1	B	215	THR
1	B	280	PRO
1	C	143	GLN

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Mol	Chain	Res	Type
1	C	215	THR
1	C	280	PRO
1	A	14	PRO
1	A	266	LYS
1	B	14	PRO
1	B	266	LYS
1	C	14	PRO
1	C	266	LYS
1	A	16	SER
1	A	65	GLN
1	B	16	SER
1	B	65	GLN
1	C	16	SER
1	C	65	GLN
1	A	144	PRO
1	A	184	PRO
1	B	144	PRO
1	B	184	PRO
1	C	144	PRO
1	C	184	PRO
1	A	7	PRO
1	A	160	PRO
1	A	208	ILE
1	B	7	PRO
1	B	160	PRO
1	B	208	ILE
1	C	7	PRO
1	C	160	PRO
1	C	208	ILE
1	A	194	GLY
1	B	194	GLY
1	C	194	GLY

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	264/273 (97%)	240 (91%)	24 (9%)	14 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	264/273 (97%)	240 (91%)	24 (9%)	14	38
1	C	264/273 (97%)	240 (91%)	24 (9%)	14	38
All	All	792/819 (97%)	720 (91%)	72 (9%)	14	38

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	17	LYS
1	A	24	VAL
1	A	66	ILE
1	A	92	THR
1	A	100	ASP
1	A	105	ILE
1	A	139	ASN
1	A	141	HIS
1	A	152	LEU
1	A	156	PHE
1	A	169	ILE
1	A	197	TYR
1	A	201	THR
1	A	208	ILE
1	A	225	ARG
1	A	231	PHE
1	A	236	LEU
1	A	239	VAL
1	A	246	THR
1	A	271	SER
1	A	273	LEU
1	A	284	LYS
1	A	287	GLU
1	B	7	PRO
1	B	17	LYS
1	B	24	VAL
1	B	66	ILE
1	B	92	THR
1	B	100	ASP
1	B	105	ILE
1	B	139	ASN
1	B	141	HIS
1	B	152	LEU

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Mol	Chain	Res	Type
1	B	156	PHE
1	B	169	ILE
1	B	197	TYR
1	B	201	THR
1	B	208	ILE
1	B	225	ARG
1	B	231	PHE
1	B	236	LEU
1	B	239	VAL
1	B	246	THR
1	B	271	SER
1	B	273	LEU
1	B	284	LYS
1	B	287	GLU
1	C	7	PRO
1	C	17	LYS
1	C	24	VAL
1	C	66	ILE
1	C	92	THR
1	C	100	ASP
1	C	105	ILE
1	C	139	ASN
1	C	141	HIS
1	C	152	LEU
1	C	156	PHE
1	C	169	ILE
1	C	197	TYR
1	C	201	THR
1	C	208	ILE
1	C	225	ARG
1	C	231	PHE
1	C	236	LEU
1	C	239	VAL
1	C	246	THR
1	C	271	SER
1	C	273	LEU
1	C	284	LYS
1	C	287	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	79	GLN
1	A	90	ASN
1	A	294	ASN
1	A	311	ASN
1	B	65	GLN
1	B	79	GLN
1	B	90	ASN
1	B	294	ASN
1	B	311	ASN
1	B	312	HIS
1	C	65	GLN
1	C	79	GLN
1	C	90	ASN
1	C	294	ASN
1	C	311	ASN

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 ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HAR	A	906	2	12,12,12	1.44	3 (25%)	14,14,14	0.77	0
3	HAR	B	907	2	12,12,12	1.44	3 (25%)	14,14,14	0.76	0
3	HAR	C	908	2	12,12,12	1.44	3 (25%)	14,14,14	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HAR	A	906	2	-	0/12/13/13	0/0/0/0
3	HAR	B	907	2	-	0/12/13/13	0/0/0/0
3	HAR	C	908	2	-	0/12/13/13	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	907	HAR	O-C	2.91	1.32	1.22
3	A	906	HAR	O-C	2.91	1.32	1.22
3	C	908	HAR	O-C	2.90	1.32	1.22
3	A	906	HAR	CA-C	2.78	1.63	1.53
3	B	907	HAR	CA-C	2.78	1.63	1.53
3	C	908	HAR	CA-C	2.78	1.63	1.53
3	B	907	HAR	OH1-NH1	-2.64	1.35	1.39
3	A	906	HAR	OH1-NH1	-2.64	1.35	1.39
3	C	908	HAR	OH1-NH1	-2.62	1.35	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.