



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:22 AM GMT

PDB ID : 2DF4
Title : Structure of tRNA-Dependent Amidotransferase GatCAB complexed with Mn²⁺
Authors : Nakamura, A.; Yao, M.; Tanaka, I.
Deposited on : 2006-02-23
Resolution : 3.20 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>

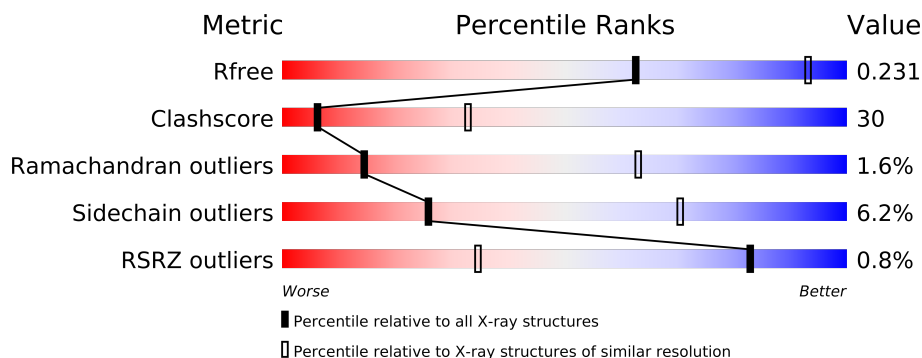
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	485	
2	B	483	
3	C	100	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7766 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3716	2359	605	739	13			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	0	0
			3179	2005	535	627	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	476	LEU	-	EXPRESSION TAG	UNP P64201
B	477	GLU	-	EXPRESSION TAG	UNP P64201
B	478	HIS	-	EXPRESSION TAG	UNP P64201
B	479	HIS	-	EXPRESSION TAG	UNP P64201
B	480	HIS	-	EXPRESSION TAG	UNP P64201
B	481	HIS	-	EXPRESSION TAG	UNP P64201
B	482	HIS	-	EXPRESSION TAG	UNP P64201
B	483	HIS	-	EXPRESSION TAG	UNP P64201

- Molecule 3 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	99	Total	C	N	O	S	0	0	0
			781	480	130	169	2			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Mn 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total 31	O 31	0	0
5	B	44	Total 44	O 44	0	0
5	C	13	Total 13	O 13	0	0

ASN	GLY	LYS	GLY	LYS	ALA	MET	GLY	PHE	LEU	VAL	GLY	GLN	ILE	MET	LYS	ALA	SER	LYS	GLY	GLN	ALA	ASN	PRO	GLN	LEU	VAL	ASN	GLN	LEU	LEU	LYS	GLN	GLU	LEU	ASP	LYS	ARG	LEU	GLU	HIS	HIS	HIS	HIS
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● Molecule 3: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit C

Chain C: 

MET	T2	E8	I12	A13	N14	R17	L18	Q19	T20	S21	P22	E23	E24	T25	L32	E33	S34	I35	L36	D37	F38	A39	K40	T47	V50	E51	P52	L57	D58	L59	Q60	L63	R64	E65	A68	I69	K70	G71	I72	P73	Q74	E75	L76	K82	G87	Q88	Y91
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P92	T93	I94	N95	N96	E97	E98	D99	A100
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.02Å 91.65Å 181.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 41.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.20) 97.3 (41.13-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.277 0.233 , 0.231	Depositor DCC
R_{free} test set	1971 reflections (10.09%)	DCC
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 19623 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7766	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.30	0/3784	0.56	0/5116
2	B	0.45	2/3242 (0.1%)	0.63	3/4379 (0.1%)
3	C	0.38	0/789	0.57	0/1066
All	All	0.38	2/7815 (0.0%)	0.59	3/10561 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	HIS	N-CA	16.03	1.78	1.46
2	B	2	HIS	CA-CB	5.79	1.66	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	ALA	N-CA-C	-6.25	94.11	111.00
2	B	383	SER	N-CA-C	5.40	125.59	111.00
2	B	2	HIS	N-CA-CB	5.09	119.77	110.60

There are no chirality outliers.

There are no planarity outliers.

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	3716	0	3709	149	0
2	B	3179	0	3126	289	0
3	C	781	0	760	52	0
4	B	2	0	0	0	0
5	A	31	0	0	2	0
5	B	44	0	0	5	0
5	C	13	0	0	3	0
All	All	7766	0	7595	464	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 30.

All (464) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2:HIS:CA	2:B:2:HIS:N	1.78	1.47
2:B:2:HIS:CA	5:B:529:HOH:O	1.67	1.28
3:C:70:LYS:HE2	5:C:101:HOH:O	1.36	1.22
2:B:3:PHE:HD2	2:B:3:PHE:O	1.32	1.13
2:B:2:HIS:O	2:B:199:PRO:HA	1.47	1.12
2:B:2:HIS:CB	5:B:529:HOH:O	1.96	1.00
2:B:199:PRO:HG2	2:B:202:GLN:HE22	1.25	0.99
2:B:300:LYS:HG3	2:B:314:ALA:HB1	1.47	0.95
2:B:56:VAL:HG22	2:B:123:MET:HE1	1.50	0.93
2:B:221:ARG:HH21	2:B:222:LYS:HZ1	1.19	0.90
2:B:388:LYS:HE2	2:B:392:GLU:HG2	1.53	0.90
2:B:3:PHE:O	2:B:3:PHE:CD2	2.23	0.90
2:B:7:ILE:HG13	2:B:157:ILE:HG13	1.52	0.89
3:C:96:ASN:ND2	3:C:98:GLU:HB3	1.89	0.88
1:A:338:SER:HA	3:C:94:ILE:HD11	1.56	0.86
2:B:7:ILE:HD11	2:B:157:ILE:HD11	1.56	0.86
2:B:26:PRO:HG3	3:C:68:ALA:HB1	1.58	0.86
2:B:390:PHE:HB3	2:B:391:PRO:HD3	1.59	0.85
2:B:204:LYS:HD2	2:B:205:PHE:H	1.41	0.85
2:B:2:HIS:N	2:B:200:TYR:HD2	1.73	0.84
2:B:5:THR:HG22	2:B:197:LEU:HG	1.60	0.84
2:B:60:MET:HB3	2:B:99:ILE:HD11	1.61	0.83
2:B:343:TRP:O	2:B:348:VAL:HG13	1.80	0.81
3:C:94:ILE:HD13	3:C:94:ILE:H	1.44	0.81
1:A:150:VAL:HG12	1:A:411:LEU:HD23	1.63	0.80
2:B:295:LEU:H	2:B:295:LEU:HD22	1.46	0.80
1:A:1:MET:O	1:A:4:ARG:HG2	1.82	0.79
2:B:33:PRO:HA	2:B:142:ASN:HD21	1.47	0.79
1:A:256:ILE:HG23	1:A:471:GLN:HG3	1.65	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:386:ALA:HA	2:B:389:VAL:HG22	1.63	0.79
2:B:371:GLY:O	2:B:374:LYS:HG2	1.82	0.78
2:B:348:VAL:HG12	2:B:390:PHE:CZ	2.19	0.78
2:B:388:LYS:O	2:B:388:LYS:HD3	1.83	0.78
3:C:20:ILE:HD11	3:C:25:THR:HA	1.67	0.76
1:A:484:LYS:O	1:A:485:LEU:HB2	1.85	0.76
2:B:202:GLN:HG2	2:B:204:LYS:H	1.50	0.76
1:A:174:ASP:HB3	1:A:192:LYS:HG3	1.68	0.75
2:B:338:LYS:HZ2	2:B:338:LYS:HB3	1.52	0.75
1:A:299:LEU:HD11	1:A:392:VAL:HG21	1.68	0.75
3:C:47:THR:O	3:C:50:VAL:HG12	1.86	0.74
2:B:304:VAL:O	2:B:308:GLY:HA2	1.88	0.74
2:B:199:PRO:HG2	2:B:202:GLN:NE2	2.01	0.74
1:A:84:THR:OG1	1:A:121:LYS:HE3	1.89	0.73
2:B:348:VAL:O	2:B:352:LEU:HD13	1.87	0.72
3:C:96:ASN:HB3	3:C:99:ASP:OD1	1.89	0.72
2:B:230:ARG:NH1	2:B:246:ARG:HE	1.87	0.72
2:B:221:ARG:O	2:B:225:GLU:HG2	1.88	0.72
1:A:47:ASP:HB2	1:A:87:LEU:HD11	1.72	0.72
1:A:1:MET:H2	1:A:28:ASP:CG	1.94	0.72
1:A:332:HIS:HB3	3:C:82:LYS:HD3	1.70	0.72
2:B:32:GLU:HG2	2:B:35:SER:HB3	1.72	0.71
1:A:1:MET:H2	1:A:28:ASP:CB	2.04	0.71
2:B:204:LYS:HD2	2:B:205:PHE:N	2.05	0.71
2:B:2:HIS:O	2:B:199:PRO:CA	2.32	0.71
2:B:2:HIS:N	2:B:200:TYR:CD2	2.58	0.71
2:B:288:VAL:HA	2:B:291:THR:HG22	1.71	0.71
2:B:33:PRO:HA	2:B:142:ASN:ND2	2.07	0.70
2:B:313:ASP:HA	2:B:345:MET:SD	2.32	0.69
2:B:386:ALA:HA	2:B:389:VAL:CG2	2.22	0.69
1:A:332:HIS:HB3	3:C:82:LYS:CD	2.22	0.69
3:C:23:GLU:OE2	3:C:24:GLU:HG3	1.93	0.69
2:B:330:THR:HG21	2:B:369:LEU:HD12	1.73	0.69
2:B:53:LYS:HB2	3:C:63:LEU:HB3	1.73	0.69
2:B:221:ARG:HH21	2:B:222:LYS:NZ	1.90	0.69
2:B:94:GLN:HB2	2:B:122:HIS:HB2	1.75	0.68
2:B:351:TYR:CE1	2:B:357:VAL:HG21	2.29	0.68
1:A:77:GLY:C	1:A:78:ILE:HD12	2.15	0.67
2:B:335:ALA:HB1	2:B:373:ILE:HG21	1.76	0.67
2:B:67:ASN:O	2:B:103:GLY:HA2	1.95	0.67
2:B:364:LEU:CD1	2:B:369:LEU:HB2	2.26	0.66
1:A:273:ALA:HB2	1:A:406:THR:HG22	1.75	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:328:GLU:O	2:B:331:ILE:HG22	1.96	0.66
2:B:217:PHE:O	2:B:220:VAL:HG22	1.96	0.65
2:B:225:GLU:O	2:B:229:LYS:HD3	1.95	0.65
1:A:8:VAL:HG22	1:A:168:PRO:HB2	1.78	0.65
2:B:344:LEU:HA	2:B:348:VAL:HG22	1.79	0.65
1:A:280:VAL:O	1:A:284:VAL:HG23	1.96	0.65
2:B:348:VAL:HG12	2:B:390:PHE:HZ	1.59	0.65
2:B:256:ILE:N	2:B:256:ILE:HD12	2.12	0.65
3:C:57:LEU:HD22	3:C:59:LEU:HD13	1.79	0.65
1:A:299:LEU:CD1	1:A:392:VAL:HG21	2.27	0.64
2:B:198:ARG:HG3	2:B:198:ARG:O	1.97	0.64
1:A:175:THR:HG23	1:A:210:LEU:HB2	1.79	0.64
2:B:295:LEU:HD22	2:B:295:LEU:N	2.12	0.64
2:B:300:LYS:HG3	2:B:314:ALA:CB	2.25	0.64
1:A:360:PHE:HB3	3:C:32:LEU:HD21	1.80	0.64
2:B:171:ARG:CZ	2:B:182:VAL:HG23	2.28	0.64
1:A:261:VAL:HB	1:A:294:VAL:HG22	1.80	0.63
1:A:7:SER:HB2	1:A:222:ASP:OD2	1.99	0.63
1:A:402:PRO:HG2	1:A:427:LEU:HD13	1.79	0.63
2:B:109:VAL:O	2:B:111:GLY:N	2.30	0.63
1:A:340:GLU:HB2	3:C:100:ALA:O	1.98	0.63
2:B:169:LYS:HD3	2:B:169:LYS:O	1.99	0.63
2:B:220:VAL:O	2:B:224:LEU:HB2	1.98	0.63
2:B:3:PHE:C	2:B:3:PHE:HD2	2.00	0.63
1:A:179:ILE:HG23	1:A:216:LEU:HD11	1.79	0.63
1:A:4:ARG:HD2	1:A:5:TYR:CE2	2.34	0.63
2:B:364:LEU:HB3	2:B:394:ALA:HA	1.79	0.63
2:B:2:HIS:CE1	2:B:3:PHE:CE2	2.87	0.62
2:B:7:ILE:HG13	2:B:157:ILE:CG1	2.28	0.62
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.65	0.62
2:B:7:ILE:CG1	2:B:157:ILE:HG13	2.27	0.62
2:B:214:LEU:HB3	2:B:220:VAL:HG12	1.81	0.62
2:B:336:ASP:OD2	2:B:339:LEU:HD23	1.99	0.62
3:C:94:ILE:HD13	3:C:94:ILE:N	2.15	0.62
1:A:207:ALA:HB1	1:A:210:LEU:HD23	1.81	0.61
2:B:336:ASP:HB3	2:B:339:LEU:HD23	1.81	0.61
2:B:129:LYS:HE2	2:B:143:ARG:HH21	1.65	0.61
1:A:364:PHE:HD2	3:C:12:ILE:HD11	1.65	0.61
2:B:338:LYS:HZ2	2:B:338:LYS:CB	2.13	0.61
2:B:105:ILE:HD11	2:B:166:TYR:CE1	2.35	0.61
2:B:2:HIS:CE1	2:B:3:PHE:CD2	2.89	0.61
2:B:351:TYR:HE1	2:B:357:VAL:HG21	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:295:LEU:H	2:B:295:LEU:CD2	2.13	0.61
2:B:243:GLN:HG3	2:B:261:LYS:HG3	1.82	0.60
2:B:75:LYS:HG3	2:B:97:GLN:OE1	2.00	0.60
1:A:1:MET:N	1:A:28:ASP:HA	2.15	0.60
2:B:366:PRO:HD2	2:B:367:GLU:OE2	2.02	0.60
1:A:429:THR:OG1	1:A:430:PRO:HD3	2.01	0.60
2:B:7:ILE:HG22	2:B:195:ILE:CB	2.32	0.60
2:B:288:VAL:HA	2:B:291:THR:CG2	2.32	0.60
1:A:93:SER:HB2	1:A:126:GLU:HG3	1.82	0.60
1:A:11:LEU:O	1:A:15:ILE:HG13	2.02	0.60
2:B:310:PRO:HB2	2:B:313:ASP:OD1	2.02	0.59
1:A:22:PRO:HD2	1:A:59:ASP:OD1	2.02	0.59
2:B:230:ARG:CZ	2:B:246:ARG:HE	2.15	0.59
1:A:25:VAL:O	1:A:29:ILE:HG12	2.02	0.59
2:B:183:LYS:HD2	2:B:186:GLU:OE2	2.03	0.59
1:A:1:MET:HG3	1:A:4:ARG:HE	1.67	0.59
2:B:241:ILE:C	2:B:241:ILE:HD13	2.23	0.59
1:A:1:MET:H2	1:A:28:ASP:CA	2.16	0.59
3:C:21:SER:OG	3:C:23:GLU:HG3	2.03	0.59
1:A:108:MET:CE	1:A:111:LEU:HD12	2.33	0.59
2:B:157:ILE:HD12	2:B:159:SER:H	1.68	0.58
2:B:344:LEU:HA	2:B:348:VAL:CG2	2.32	0.58
2:B:388:LYS:HE2	2:B:392:GLU:CG	2.31	0.58
1:A:8:VAL:O	1:A:12:LEU:HB2	2.02	0.58
2:B:171:ARG:NE	2:B:182:VAL:HG23	2.18	0.58
2:B:138:LEU:HB3	3:C:88:GLN:OE1	2.04	0.58
3:C:60:GLN:NE2	5:C:112:HOH:O	2.37	0.58
1:A:255:ASP:OD1	1:A:257:LYS:HG2	2.04	0.58
2:B:197:LEU:HD13	2:B:231:GLN:OE1	2.04	0.57
2:B:98:PRO:HB3	2:B:120:ARG:HH21	1.69	0.57
1:A:40:ILE:HA	1:A:142:VAL:HG22	1.86	0.57
1:A:80:ASP:OD2	1:A:90:THR:N	2.31	0.57
2:B:295:LEU:O	2:B:299:ARG:HB2	2.05	0.56
2:B:176:TYR:HE2	2:B:299:ARG:HD2	1.69	0.56
2:B:140:ASP:HB2	3:C:88:GLN:HE21	1.69	0.56
2:B:290:GLN:NE2	2:B:291:THR:N	2.54	0.56
2:B:60:MET:HB3	2:B:99:ILE:CD1	2.34	0.56
2:B:202:GLN:HG2	2:B:203:GLU:N	2.19	0.56
2:B:371:GLY:HA2	2:B:374:LYS:HE2	1.87	0.56
1:A:181:GLN:HB3	1:A:182:PRO:HD3	1.88	0.56
2:B:204:LYS:HE3	2:B:205:PHE:O	2.06	0.56
1:A:429:THR:O	1:A:433:LEU:HD22	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:399:VAL:HB	1:A:456:ILE:HB	1.87	0.55
2:B:177:THR:OG1	2:B:179:VAL:HG22	2.06	0.55
2:B:60:MET:HE3	2:B:70:ILE:HG21	1.89	0.55
2:B:3:PHE:C	2:B:3:PHE:CD2	2.74	0.55
2:B:351:TYR:HD1	2:B:352:LEU:HD12	1.71	0.55
2:B:344:LEU:HD12	2:B:348:VAL:HG21	1.89	0.55
1:A:78:ILE:HG12	1:A:108:MET:SD	2.46	0.55
1:A:133:THR:HG22	1:A:133:THR:O	2.07	0.55
2:B:157:ILE:CD1	2:B:162:GLU:HB2	2.38	0.54
3:C:96:ASN:O	3:C:98:GLU:N	2.36	0.54
3:C:57:LEU:HD22	3:C:59:LEU:CD1	2.37	0.54
2:B:219:TYR:CD1	2:B:248:PHE:HE2	2.25	0.54
2:B:171:ARG:NH1	2:B:175:GLN:HG3	2.22	0.54
2:B:98:PRO:HB3	2:B:120:ARG:NH2	2.21	0.54
2:B:20:LYS:HD2	2:B:25:SER:HB2	1.89	0.54
1:A:87:LEU:HD12	1:A:118:LEU:HD21	1.89	0.54
1:A:228:GLU:OE2	1:A:247:ASP:HA	2.08	0.54
2:B:202:GLN:HG2	2:B:204:LYS:N	2.21	0.54
1:A:276:VAL:HG21	1:A:406:THR:HA	1.90	0.54
1:A:169:LEU:C	1:A:169:LEU:HD22	2.28	0.54
1:A:436:LEU:CD2	1:A:459:PRO:HD3	2.38	0.54
2:B:276:VAL:HG21	3:C:59:LEU:CB	2.37	0.54
2:B:227:GLU:OE2	2:B:230:ARG:HD3	2.08	0.53
2:B:60:MET:O	2:B:64:MET:HG3	2.09	0.53
2:B:211:LEU:HD12	2:B:224:LEU:HD12	1.90	0.53
2:B:22:PHE:CE2	2:B:92:ILE:HB	2.44	0.53
2:B:93:SER:OG	2:B:124:GLU:HG2	2.07	0.53
2:B:2:HIS:CG	5:B:529:HOH:O	2.46	0.53
2:B:122:HIS:CE1	2:B:150:GLU:HB3	2.44	0.53
2:B:362:THR:HB	5:B:508:HOH:O	2.08	0.53
1:A:154:SER:OG	1:A:178:SER:HB3	2.09	0.53
2:B:288:VAL:CA	2:B:291:THR:HG22	2.38	0.53
2:B:133:LYS:HB2	2:B:138:LEU:HD23	1.90	0.53
1:A:262:ALA:HB1	1:A:297:VAL:HG21	1.90	0.53
2:B:307:LEU:O	2:B:307:LEU:HD23	2.09	0.53
1:A:338:SER:OG	1:A:341:GLU:HG3	2.09	0.53
2:B:330:THR:HG21	2:B:369:LEU:CD1	2.39	0.53
2:B:364:LEU:HD13	2:B:369:LEU:HB2	1.90	0.53
2:B:38:ASN:O	2:B:42:LEU:HG	2.09	0.53
2:B:56:VAL:CG2	2:B:123:MET:HE1	2.33	0.52
2:B:7:ILE:HA	2:B:194:ASN:O	2.09	0.52
3:C:94:ILE:H	3:C:94:ILE:CD1	2.17	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:470:TYR:O	1:A:474:THR:HG23	2.10	0.52
1:A:1:MET:H2	1:A:28:ASP:HA	1.73	0.52
1:A:247:ASP:OD2	1:A:250:SER:HB3	2.09	0.52
3:C:35:ILE:O	3:C:38:PHE:HB3	2.10	0.52
3:C:72:ILE:HD12	3:C:76:LEU:HB3	1.90	0.52
1:A:37:ASP:O	1:A:41:LYS:N	2.39	0.52
2:B:352:LEU:HA	2:B:357:VAL:CG2	2.40	0.52
2:B:121:LEU:HA	2:B:150:GLU:O	2.09	0.52
1:A:387:ASN:HD22	1:A:387:ASN:N	2.07	0.52
1:A:355:VAL:HG23	5:A:490:HOH:O	2.09	0.52
2:B:344:LEU:CD1	2:B:348:VAL:HG21	2.40	0.52
2:B:348:VAL:CG2	2:B:349:ASN:N	2.73	0.52
2:B:230:ARG:NH1	2:B:246:ARG:NE	2.58	0.52
1:A:77:GLY:HA3	1:A:122:LEU:HD21	1.92	0.52
1:A:306:ILE:N	1:A:307:PRO:HD2	2.24	0.52
2:B:343:TRP:HA	2:B:343:TRP:CE3	2.45	0.51
1:A:204:VAL:HG22	2:B:45:PRO:HB2	1.92	0.51
1:A:206:PHE:C	1:A:206:PHE:CD1	2.84	0.51
2:B:199:PRO:HD3	2:B:235:LEU:HD21	1.91	0.51
2:B:44:TYR:O	2:B:47:VAL:HG22	2.10	0.51
2:B:359:LEU:O	2:B:361:ASP:N	2.44	0.51
1:A:76:MET:HG2	1:A:117:VAL:O	2.10	0.51
2:B:313:ASP:HA	2:B:345:MET:CE	2.40	0.51
1:A:15:ILE:HG22	1:A:67:MET:CE	2.40	0.51
3:C:73:PRO:HA	5:C:109:HOH:O	2.10	0.51
2:B:7:ILE:HG22	2:B:195:ILE:HB	1.92	0.51
2:B:285:LYS:O	2:B:289:ARG:HB2	2.10	0.51
2:B:276:VAL:HG21	3:C:59:LEU:HB3	1.91	0.51
2:B:368:ASN:N	2:B:368:ASN:HD22	2.09	0.51
3:C:96:ASN:HD22	3:C:98:GLU:HB3	1.71	0.51
2:B:385:ILE:O	2:B:389:VAL:HG13	2.11	0.51
1:A:131:GLY:HA2	1:A:153:GLY:HA3	1.93	0.51
2:B:121:LEU:C	2:B:121:LEU:HD23	2.31	0.51
2:B:348:VAL:HG23	2:B:349:ASN:N	2.26	0.51
2:B:160:PRO:HG3	2:B:225:GLU:HB3	1.93	0.50
1:A:364:PHE:HB2	3:C:12:ILE:HD13	1.92	0.50
2:B:88:LYS:O	2:B:89:ALA:HB3	2.11	0.50
1:A:81:ASN:HB3	1:A:124:MET:SD	2.50	0.50
2:B:199:PRO:O	2:B:202:GLN:NE2	2.44	0.50
2:B:61:ARG:CD	2:B:291:THR:HG23	2.42	0.50
1:A:280:VAL:O	1:A:283:ALA:HB3	2.12	0.50
2:B:170:LEU:O	2:B:174:ILE:HD13	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:40:ILE:HA	1:A:142:VAL:CG2	2.41	0.50
2:B:64:MET:HE1	2:B:288:VAL:HG23	1.94	0.50
2:B:161:LYS:HG2	5:B:545:HOH:O	2.12	0.50
1:A:29:ILE:HG21	1:A:119:ILE:HG12	1.94	0.50
2:B:218:ASN:O	2:B:222:LYS:HG2	2.12	0.50
2:B:64:MET:SD	2:B:289:ARG:HD2	2.52	0.50
1:A:443:CYS:HB2	1:A:472:TYR:OH	2.12	0.50
1:A:402:PRO:HG2	1:A:427:LEU:CD1	2.41	0.50
2:B:7:ILE:HD11	2:B:157:ILE:CD1	2.35	0.49
1:A:108:MET:HE1	1:A:111:LEU:HD12	1.94	0.49
2:B:75:LYS:NZ	2:B:271:PRO:HG3	2.28	0.49
2:B:183:LYS:HE2	2:B:358:GLU:OE1	2.12	0.49
2:B:138:LEU:N	2:B:138:LEU:HD22	2.27	0.49
1:A:1:MET:N	1:A:28:ASP:CG	2.65	0.49
2:B:20:LYS:HG3	2:B:25:SER:O	2.11	0.49
1:A:83:ILE:HD12	1:A:103:TYR:OH	2.12	0.49
1:A:108:MET:HE2	1:A:111:LEU:HD12	1.94	0.49
2:B:257:LEU:C	2:B:257:LEU:HD13	2.33	0.49
1:A:412:GLY:HA2	1:A:415:ILE:CG2	2.41	0.49
2:B:374:LYS:HA	2:B:377:GLU:HB3	1.93	0.49
1:A:388:ASP:O	1:A:392:VAL:HG23	2.13	0.49
1:A:262:ALA:O	1:A:264:PRO:HD3	2.12	0.49
1:A:307:PRO:HG2	1:A:308:SER:H	1.78	0.49
1:A:15:ILE:HG22	1:A:67:MET:HE2	1.94	0.48
1:A:262:ALA:HB2	1:A:396:TYR:CG	2.48	0.48
2:B:2:HIS:ND1	2:B:3:PHE:N	2.61	0.48
2:B:309:LEU:HG	2:B:310:PRO:HD2	1.95	0.48
2:B:344:LEU:O	2:B:345:MET:C	2.51	0.48
2:B:157:ILE:HD13	2:B:163:ALA:N	2.28	0.48
2:B:74:SER:O	2:B:278:LEU:HB2	2.12	0.48
2:B:196:SER:HB2	2:B:208:LYS:HG3	1.96	0.48
1:A:20:ILE:HD13	1:A:25:VAL:HG22	1.95	0.48
1:A:8:VAL:CG2	1:A:168:PRO:HB2	2.43	0.48
2:B:64:MET:HG2	2:B:70:ILE:HD11	1.96	0.48
2:B:241:ILE:HD13	2:B:242:GLY:N	2.29	0.48
2:B:356:GLN:HA	2:B:356:GLN:NE2	2.29	0.47
2:B:63:ALA:HA	2:B:121:LEU:HD13	1.94	0.47
1:A:53:LYS:O	1:A:57:GLU:HG3	2.15	0.47
2:B:362:THR:HG23	2:B:363:LYS:HD2	1.95	0.47
2:B:298:GLU:H	2:B:298:GLU:CD	2.18	0.47
2:B:395:ALA:O	2:B:396:LYS:HG2	2.14	0.47
1:A:344:LYS:HA	3:C:17:ARG:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:84:THR:HG23	1:A:121:LYS:HE2	1.96	0.47
1:A:284:VAL:O	1:A:288:LYS:HG3	2.14	0.47
2:B:72:THR:HG22	2:B:279:TYR:CE1	2.50	0.47
1:A:129:MET:SD	1:A:358:ARG:HG3	2.55	0.47
2:B:157:ILE:HD12	2:B:162:GLU:HB2	1.95	0.47
2:B:98:PRO:HG2	2:B:101:GLU:HG3	1.97	0.47
2:B:359:LEU:C	2:B:361:ASP:H	2.18	0.47
1:A:234:ASP:OD2	1:A:236:ASN:HB2	2.15	0.47
2:B:13:VAL:HG22	2:B:189:LEU:HD23	1.96	0.47
2:B:312:TYR:O	2:B:316:VAL:HG12	2.15	0.47
1:A:20:ILE:CD1	1:A:25:VAL:HG22	2.44	0.47
1:A:391:LYS:O	1:A:394:GLU:HB2	2.15	0.47
1:A:372:ASP:HA	1:A:376:LYS:HB3	1.97	0.47
2:B:300:LYS:O	2:B:304:VAL:HG23	2.14	0.47
2:B:338:LYS:NZ	2:B:338:LYS:HB3	2.25	0.47
2:B:169:LYS:O	2:B:173:ILE:HG13	2.13	0.47
1:A:3:ILE:C	1:A:3:ILE:HD12	2.35	0.47
2:B:7:ILE:CD1	2:B:157:ILE:HD11	2.36	0.46
1:A:192:LYS:HD2	1:A:432:ASN:ND2	2.31	0.46
1:A:105:SER:CB	1:A:202:GLY:HA3	2.45	0.46
3:C:36:LEU:O	3:C:40:LYS:HG2	2.16	0.46
2:B:116:ILE:HG23	2:B:156:ASP:HB2	1.97	0.46
2:B:247:ARG:CZ	2:B:258:MET:HB3	2.46	0.46
2:B:388:LYS:O	2:B:391:PRO:HD2	2.14	0.46
2:B:204:LYS:HD2	2:B:204:LYS:HA	1.69	0.46
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.30	0.46
1:A:400:VAL:HG22	1:A:401:GLY:N	2.30	0.46
2:B:369:LEU:O	2:B:373:ILE:HG12	2.15	0.46
1:A:58:LEU:HD22	1:A:72:PHE:CZ	2.51	0.46
1:A:28:ASP:O	1:A:31:ASP:HB2	2.16	0.46
1:A:332:HIS:HB3	3:C:82:LYS:HD2	1.95	0.46
1:A:103:TYR:HB3	2:B:39:VAL:HG11	1.97	0.46
2:B:176:TYR:HE2	2:B:299:ARG:CD	2.29	0.46
2:B:393:LEU:O	2:B:393:LEU:HD22	2.16	0.46
2:B:390:PHE:HB3	2:B:391:PRO:CD	2.40	0.46
2:B:176:TYR:CZ	2:B:296:PRO:HG3	2.51	0.46
2:B:33:PRO:CA	2:B:142:ASN:HD21	2.25	0.46
2:B:315:HIS:C	2:B:315:HIS:CD2	2.90	0.45
1:A:484:LYS:O	1:A:485:LEU:CB	2.58	0.45
2:B:133:LYS:HB2	2:B:138:LEU:CD2	2.47	0.45
3:C:74:GLN:NE2	3:C:87:GLY:HA3	2.31	0.45
1:A:1:MET:HG2	1:A:1:MET:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:241:ALA:HB2	3:C:57:LEU:HD11	1.98	0.45
3:C:59:LEU:O	3:C:60:GLN:HG3	2.16	0.45
2:B:294:GLU:HB2	2:B:299:ARG:NH1	2.32	0.45
2:B:272:GLU:OE1	2:B:273:PRO:HD2	2.17	0.45
2:B:352:LEU:O	2:B:356:GLN:N	2.49	0.45
2:B:281:ASP:O	2:B:285:LYS:HG3	2.17	0.45
1:A:425:ASP:HB3	1:A:429:THR:HG23	1.98	0.45
2:B:316:VAL:HG13	2:B:345:MET:HE1	1.97	0.45
2:B:326:PHE:CE1	2:B:366:PRO:HD3	2.51	0.45
1:A:83:ILE:HD11	2:B:45:PRO:O	2.17	0.45
2:B:2:HIS:C	2:B:2:HIS:N	2.60	0.45
2:B:7:ILE:HG22	2:B:195:ILE:HA	1.98	0.45
2:B:198:ARG:CG	2:B:198:ARG:O	2.63	0.45
1:A:380:LYS:HB3	3:C:50:VAL:CG1	2.47	0.45
2:B:245:THR:OG1	2:B:261:LYS:HE2	2.16	0.45
1:A:132:SER:C	1:A:134:GLU:H	2.20	0.45
2:B:136:TYR:N	2:B:136:TYR:CD1	2.84	0.45
2:B:290:GLN:C	2:B:292:ILE:H	2.20	0.45
2:B:367:GLU:H	2:B:367:GLU:CD	2.20	0.45
1:A:29:ILE:O	1:A:32:ALA:HB3	2.17	0.45
2:B:198:ARG:HH11	2:B:198:ARG:HG3	1.82	0.44
1:A:256:ILE:HG21	1:A:468:VAL:HA	1.99	0.44
1:A:307:PRO:O	1:A:311:VAL:HG23	2.16	0.44
1:A:64:LYS:O	1:A:66:GLN:HG3	2.17	0.44
2:B:356:GLN:CA	2:B:356:GLN:HE21	2.31	0.44
2:B:270:PHE:HA	2:B:271:PRO:HD3	1.88	0.44
1:A:93:SER:HB2	1:A:126:GLU:CG	2.47	0.44
2:B:137:SER:HB2	3:C:91:VAL:HG23	1.99	0.44
2:B:226:TYR:CZ	2:B:254:LYS:HB3	2.52	0.44
2:B:292:ILE:HA	2:B:293:PRO:HD3	1.84	0.44
1:A:2:SER:N	1:A:28:ASP:OD2	2.50	0.44
2:B:330:THR:HG22	2:B:330:THR:O	2.17	0.44
2:B:159:SER:HB2	2:B:160:PRO:HD2	2.00	0.44
2:B:135:GLU:HA	2:B:135:GLU:OE1	2.17	0.44
1:A:425:ASP:O	1:A:429:THR:HG23	2.17	0.44
1:A:215:PRO:C	1:A:216:LEU:HD12	2.38	0.44
2:B:360:LEU:HG	2:B:360:LEU:O	2.17	0.44
2:B:313:ASP:HA	2:B:345:MET:HE1	1.99	0.43
2:B:176:TYR:CE1	2:B:296:PRO:HG3	2.53	0.43
2:B:15:LEU:HD11	2:B:149:ILE:HG23	1.99	0.43
2:B:316:VAL:HG13	2:B:345:MET:CE	2.48	0.43
1:A:84:THR:CG2	1:A:121:LYS:HE2	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:249:ASP:HB2	2:B:256:ILE:HD11	1.99	0.43
2:B:336:ASP:O	2:B:337:VAL:C	2.56	0.43
2:B:134:GLY:HA3	2:B:136:TYR:CE1	2.53	0.43
2:B:287:ARG:NH1	2:B:287:ARG:HB2	2.33	0.43
2:B:185:GLU:CD	2:B:185:GLU:H	2.20	0.43
1:A:185:TYR:O	1:A:450:PRO:HG2	2.18	0.43
2:B:169:LYS:C	2:B:169:LYS:HD3	2.39	0.43
2:B:14:GLU:HG2	2:B:148:LEU:HD21	2.00	0.43
2:B:138:LEU:CD2	2:B:138:LEU:N	2.82	0.43
2:B:363:LYS:NZ	2:B:363:LYS:HB3	2.33	0.43
2:B:368:ASN:N	2:B:368:ASN:ND2	2.65	0.43
1:A:345:MET:HG2	3:C:19:GLN:OE1	2.18	0.43
2:B:66:LEU:HA	2:B:66:LEU:HD12	1.84	0.43
1:A:407:THR:HG21	1:A:446:SER:HB3	2.00	0.43
2:B:159:SER:OG	2:B:162:GLU:HG3	2.18	0.43
2:B:340:THR:HA	2:B:343:TRP:HB2	1.99	0.43
2:B:288:VAL:C	2:B:291:THR:HG22	2.38	0.43
1:A:131:GLY:CA	1:A:153:GLY:HA3	2.49	0.43
1:A:275:ASP:N	1:A:275:ASP:OD1	2.51	0.43
3:C:20:ILE:HD11	3:C:25:THR:CA	2.43	0.43
1:A:78:ILE:HG12	1:A:108:MET:CE	2.49	0.43
2:B:56:VAL:HA	2:B:123:MET:CE	2.49	0.43
2:B:7:ILE:CG2	2:B:195:ILE:HG13	2.48	0.43
1:A:439:ILE:CG2	1:A:455:PHE:HB2	2.48	0.43
2:B:17:THR:O	2:B:27:ALA:HB3	2.17	0.43
1:A:206:PHE:CD1	1:A:206:PHE:O	2.72	0.43
1:A:338:SER:CB	3:C:99:ASP:HB2	2.49	0.42
2:B:9:LEU:HD12	2:B:166:TYR:CD2	2.54	0.42
2:B:307:LEU:O	2:B:309:LEU:N	2.52	0.42
3:C:47:THR:HB	3:C:50:VAL:CG1	2.48	0.42
1:A:210:LEU:HD13	1:A:382:ARG:NH2	2.34	0.42
2:B:365:THR:HB	2:B:366:PRO:CD	2.49	0.42
1:A:410:ASN:HB2	1:A:413:GLU:HB2	2.01	0.42
2:B:144:GLN:CD	2:B:145:GLY:N	2.72	0.42
2:B:352:LEU:HA	2:B:357:VAL:HG23	2.01	0.42
3:C:65:GLU:OE1	3:C:65:GLU:HA	2.18	0.42
1:A:309:TYR:HD2	1:A:310:TYR:CD1	2.37	0.42
1:A:337:HIS:HD2	5:A:513:HOH:O	2.00	0.42
2:B:284:TRP:O	2:B:288:VAL:HG22	2.20	0.42
2:B:156:ASP:O	2:B:158:ARG:HG2	2.19	0.42
1:A:193:PRO:HB2	1:A:197:ARG:HB3	2.01	0.42
1:A:110:LYS:O	1:A:114:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:344:LEU:O	2:B:348:VAL:HG22	2.19	0.42
2:B:388:LYS:C	2:B:391:PRO:HD2	2.40	0.42
1:A:439:ILE:HG22	1:A:455:PHE:HB2	2.01	0.42
2:B:4:GLU:HB3	2:B:200:TYR:CE1	2.54	0.42
2:B:356:GLN:HA	2:B:356:GLN:HE21	1.85	0.42
2:B:140:ASP:HB2	3:C:88:GLN:NE2	2.34	0.42
1:A:104:GLU:HB3	1:A:109:GLU:OE1	2.20	0.42
1:A:26:VAL:HG21	1:A:55:ALA:HB2	2.02	0.42
2:B:109:VAL:HG21	2:B:114:LYS:NZ	2.34	0.42
2:B:386:ALA:CA	2:B:389:VAL:HG22	2.43	0.42
2:B:256:ILE:N	2:B:256:ILE:CD1	2.81	0.42
1:A:125:ASP:CG	1:A:133:THR:HA	2.41	0.42
1:A:105:SER:HB2	1:A:202:GLY:HA3	2.02	0.42
3:C:2:THR:N	3:C:33:GLU:HG3	2.35	0.42
3:C:2:THR:HA	3:C:33:GLU:OE2	2.20	0.42
2:B:359:LEU:O	2:B:363:LYS:HG2	2.20	0.42
2:B:287:ARG:HB2	2:B:287:ARG:HH11	1.85	0.42
2:B:64:MET:HE1	2:B:288:VAL:C	2.41	0.41
1:A:36:THR:HB	1:A:166:LEU:HD21	2.02	0.41
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.91	0.41
2:B:300:LYS:HE2	2:B:314:ALA:C	2.39	0.41
2:B:336:ASP:O	2:B:339:LEU:HB2	2.20	0.41
2:B:61:ARG:HD3	2:B:291:THR:HG23	2.02	0.41
1:A:141:THR:HB	1:A:151:PRO:HG2	2.01	0.41
2:B:340:THR:O	2:B:344:LEU:HD22	2.20	0.41
1:A:37:ASP:N	1:A:38:PRO:CD	2.83	0.41
2:B:315:HIS:CD2	2:B:316:VAL:N	2.89	0.41
1:A:134:GLU:HB2	1:A:415:ILE:HD13	2.03	0.41
1:A:60:GLU:HB3	1:A:64:LYS:NZ	2.35	0.41
2:B:202:GLN:OE1	2:B:204:LYS:O	2.39	0.41
2:B:288:VAL:O	2:B:291:THR:HG22	2.20	0.41
2:B:371:GLY:HA2	2:B:374:LYS:CE	2.50	0.41
1:A:391:LYS:HE2	1:A:391:LYS:HB3	1.90	0.41
2:B:234:GLU:O	2:B:239:GLY:N	2.54	0.41
2:B:114:LYS:HE2	2:B:162:GLU:OE1	2.20	0.41
3:C:63:LEU:N	3:C:63:LEU:HD22	2.36	0.41
1:A:78:ILE:HD12	1:A:78:ILE:N	2.36	0.41
2:B:331:ILE:CG2	2:B:332:GLU:N	2.84	0.41
2:B:168:GLU:HA	2:B:217:PHE:CE2	2.56	0.41
2:B:365:THR:HB	2:B:366:PRO:HD2	2.03	0.41
2:B:50:VAL:HG12	3:C:64:ARG:HB2	2.03	0.41
3:C:51:GLU:HA	3:C:52:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:197:LEU:CD1	2:B:197:LEU:N	2.84	0.40
2:B:105:ILE:HD11	2:B:166:TYR:CD1	2.55	0.40
2:B:138:LEU:HB3	3:C:88:GLN:CD	2.40	0.40
2:B:104:TYR:CE2	2:B:115:ARG:CZ	3.04	0.40
2:B:396:LYS:HB3	2:B:397:GLY:H	1.62	0.40
2:B:247:ARG:HB3	2:B:258:MET:HE1	2.03	0.40
2:B:286:GLU:O	2:B:287:ARG:C	2.59	0.40
2:B:221:ARG:NH1	2:B:225:GLU:OE1	2.55	0.40
3:C:99:ASP:N	3:C:99:ASP:OD1	2.54	0.40
2:B:140:ASP:OD1	2:B:140:ASP:C	2.60	0.40
2:B:359:LEU:C	2:B:361:ASP:N	2.74	0.40
2:B:197:LEU:HD13	2:B:231:GLN:CD	2.42	0.40
1:A:29:ILE:HG23	1:A:166:LEU:O	2.22	0.40
2:B:14:GLU:HA	2:B:148:LEU:HD23	2.04	0.40
1:A:85:ASN:HD22	1:A:86:GLY:N	2.19	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	483/485 (100%)	442 (92%)	39 (8%)	2 (0%)	43 88
2	B	397/483 (82%)	339 (85%)	46 (12%)	12 (3%)	7 42
3	C	97/100 (97%)	83 (86%)	12 (12%)	2 (2%)	11 55
All	All	977/1068 (92%)	864 (88%)	97 (10%)	16 (2%)	14 63

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	110	ASP
2	B	239	GLY
2	B	308	GLY
2	B	310	PRO

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Mol	Chain	Res	Type
2	B	337	VAL
2	B	381	MET
2	B	383	SER
1	A	245	ASP
2	B	291	THR
2	B	360	LEU
2	B	380	THR
2	B	384	LYS
3	C	97	GLU
3	C	93	THR
1	A	269	GLY
2	B	238	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	406/406 (100%)	393 (97%)	13 (3%)	51 87
2	B	346/419 (83%)	316 (91%)	30 (9%)	15 51
3	C	87/88 (99%)	78 (90%)	9 (10%)	10 40
All	All	839/913 (92%)	787 (94%)	52 (6%)	26 70

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	56	GLN
1	A	85	ASN
1	A	87	LEU
1	A	169	LEU
1	A	206	PHE
1	A	263	LEU
1	A	268	LEU
1	A	321	LEU
1	A	361	LEU
1	A	376	LYS

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Mol	Chain	Res	Type
1	A	387	ASN
1	A	433	LEU
2	B	2	HIS
2	B	3	PHE
2	B	57	ASP
2	B	66	LEU
2	B	75	LYS
2	B	119	THR
2	B	132	HIS
2	B	136	TYR
2	B	141	LEU
2	B	157	ILE
2	B	167	LEU
2	B	185	GLU
2	B	192	ASP
2	B	197	LEU
2	B	202	GLN
2	B	204	LYS
2	B	230	ARG
2	B	241	ILE
2	B	254	LYS
2	B	290	GLN
2	B	313	ASP
2	B	322	GLU
2	B	340	THR
2	B	345	MET
2	B	355	ASN
2	B	363	LYS
2	B	364	LEU
2	B	378	ASP
2	B	393	LEU
2	B	396	LYS
3	C	8	GLU
3	C	14	ASN
3	C	23	GLU
3	C	32	LEU
3	C	57	LEU
3	C	65	GLU
3	C	76	LEU
3	C	94	ILE
3	C	99	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	212	GLN
1	A	281	GLN
1	A	387	ASN
2	B	202	GLN
2	B	290	GLN
2	B	315	HIS
2	B	342	ASN
2	B	356	GLN
2	B	368	ASN
3	C	60	GLN
3	C	74	GLN
3	C	88	GLN
3	C	96	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 ⓘ

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	485/485 (100%)	-0.15	1 (0%) 93 66	34, 55, 81, 95	0
2	B	399/483 (82%)	0.04	6 (1%) 70 21	31, 76, 95, 95	0
3	C	99/100 (99%)	0.09	1 (1%) 79 29	52, 77, 95, 95	0
All	All	983/1068 (92%)	-0.05	8 (0%) 83 35	31, 63, 95, 95	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	381	MET	3.4
2	B	369	LEU	2.4
1	A	1	MET	2.4
2	B	393	LEU	2.3
2	B	382	SER	2.3
3	C	96	ASN	2.1
2	B	395	ALA	2.0
2	B	394	ALA	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MN	B	502	1/1	0.22	0.70	86,86,86,86	0
4	MN	B	501	1/1	0.19	-0.16	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.