



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:48 PM GMT

PDB ID : 2PJQ
Title : Crystal structure of Q88U62_LACPL from Lactobacillus plantarum. Northeast Structural Genomics target LpR71
Authors : Benach, J.; Su, M.; Seetharaman, J.; Forouhar, F.; Chen, C.X.; Cunningham, K.; Ma, L-C.; Owens, L.; Baran, M.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2007-04-16
Resolution : 2.80 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>

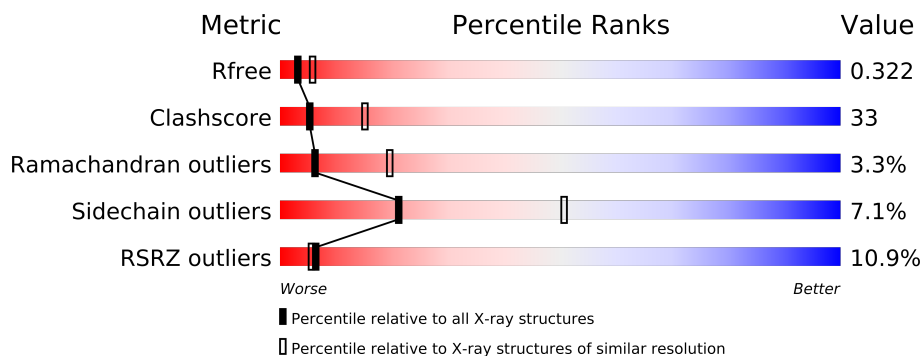
The following versions of software and data (see [references](#)) were used in the production of this report:

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

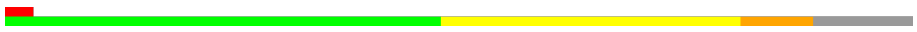

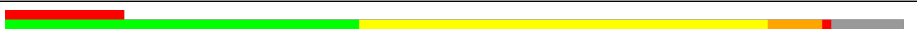
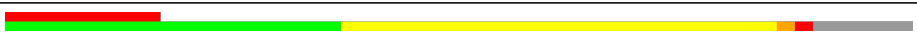
The reported resolution of this entry is 2.80 Å.

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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	231	
1	B	231	
1	C	231	
1	D	231	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6575 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 Uncharacterized protein lp_2664.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	Se	0	0	0
			1625	1019	298	303	5			
1	B	212	Total	C	N	O	Se	0	0	0
			1667	1047	306	308	6			
1	C	212	Total	C	N	O	Se	0	0	0
			1667	1045	306	310	6			
1	D	203	Total	C	N	O	Se	0	0	0
			1604	1008	295	296	5			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MSE	-	CLONING ARTIFACT	UNP Q88U62
A	-3	ALA	-	CLONING ARTIFACT	UNP Q88U62
A	-2	GLY	-	CLONING ARTIFACT	UNP Q88U62
A	-1	ASP	-	CLONING ARTIFACT	UNP Q88U62
A	0	PRO	-	CLONING ARTIFACT	UNP Q88U62
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
A	66	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
A	100	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
A	158	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
A	185	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
A	201	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
A	219	LEU	-	CLONING ARTIFACT	UNP Q88U62
A	220	GLU	-	CLONING ARTIFACT	UNP Q88U62
A	221	HIS	-	CLONING ARTIFACT	UNP Q88U62
A	222	HIS	-	CLONING ARTIFACT	UNP Q88U62
A	223	HIS	-	CLONING ARTIFACT	UNP Q88U62
A	224	HIS	-	CLONING ARTIFACT	UNP Q88U62
A	225	HIS	-	CLONING ARTIFACT	UNP Q88U62
A	226	HIS	-	CLONING ARTIFACT	UNP Q88U62
B	-4	MSE	-	CLONING ARTIFACT	UNP Q88U62
B	-3	ALA	-	CLONING ARTIFACT	UNP Q88U62

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	CLONING ARTIFACT	UNP Q88U62
B	-1	ASP	-	CLONING ARTIFACT	UNP Q88U62
B	0	PRO	-	CLONING ARTIFACT	UNP Q88U62
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
B	66	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
B	100	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
B	158	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
B	185	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
B	201	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
B	219	LEU	-	CLONING ARTIFACT	UNP Q88U62
B	220	GLU	-	CLONING ARTIFACT	UNP Q88U62
B	221	HIS	-	CLONING ARTIFACT	UNP Q88U62
B	222	HIS	-	CLONING ARTIFACT	UNP Q88U62
B	223	HIS	-	CLONING ARTIFACT	UNP Q88U62
B	224	HIS	-	CLONING ARTIFACT	UNP Q88U62
B	225	HIS	-	CLONING ARTIFACT	UNP Q88U62
B	226	HIS	-	CLONING ARTIFACT	UNP Q88U62
C	-4	MSE	-	CLONING ARTIFACT	UNP Q88U62
C	-3	ALA	-	CLONING ARTIFACT	UNP Q88U62
C	-2	GLY	-	CLONING ARTIFACT	UNP Q88U62
C	-1	ASP	-	CLONING ARTIFACT	UNP Q88U62
C	0	PRO	-	CLONING ARTIFACT	UNP Q88U62
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
C	66	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
C	100	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
C	158	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
C	185	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
C	201	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
C	219	LEU	-	CLONING ARTIFACT	UNP Q88U62
C	220	GLU	-	CLONING ARTIFACT	UNP Q88U62
C	221	HIS	-	CLONING ARTIFACT	UNP Q88U62
C	222	HIS	-	CLONING ARTIFACT	UNP Q88U62
C	223	HIS	-	CLONING ARTIFACT	UNP Q88U62
C	224	HIS	-	CLONING ARTIFACT	UNP Q88U62
C	225	HIS	-	CLONING ARTIFACT	UNP Q88U62
C	226	HIS	-	CLONING ARTIFACT	UNP Q88U62
D	-4	MSE	-	CLONING ARTIFACT	UNP Q88U62
D	-3	ALA	-	CLONING ARTIFACT	UNP Q88U62
D	-2	GLY	-	CLONING ARTIFACT	UNP Q88U62
D	-1	ASP	-	CLONING ARTIFACT	UNP Q88U62
D	0	PRO	-	CLONING ARTIFACT	UNP Q88U62
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q88U62

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Chain	Residue	Modelled	Actual	Comment	Reference
D	66	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
D	100	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
D	158	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
D	185	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
D	201	MSE	MET	MODIFIED RESIDUE	UNP Q88U62
D	219	LEU	-	CLONING ARTIFACT	UNP Q88U62
D	220	GLU	-	CLONING ARTIFACT	UNP Q88U62
D	221	HIS	-	CLONING ARTIFACT	UNP Q88U62
D	222	HIS	-	CLONING ARTIFACT	UNP Q88U62
D	223	HIS	-	CLONING ARTIFACT	UNP Q88U62
D	224	HIS	-	CLONING ARTIFACT	UNP Q88U62
D	225	HIS	-	CLONING ARTIFACT	UNP Q88U62
D	226	HIS	-	CLONING ARTIFACT	UNP Q88U62

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	6	Total O 6 6	0	0
2	C	3	Total O 3 3	0	0
2	D	1	Total O 1 1	0	0



● Molecule 1: Uncharacterized protein lp_2664

Chain D: A horizontal bar chart representing the sequence of Chain D. The bar is divided into segments of different colors (green, yellow, red, grey) corresponding to the quality of the data for each residue. The residues are labeled from M5E to A127.



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.93Å 167.44Å 63.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 47.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.1 (20.00-2.80) 96.4 (47.78-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.307 0.251 , 0.322	Depositor DCC
R_{free} test set	2060 reflections (9.82%)	DCC
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 7.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 40517 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.43	0/1653	0.69	0/2232
1	B	0.50	0/1695	0.74	6/2287 (0.3%)
1	C	0.70	5/1696 (0.3%)	0.78	5/2290 (0.2%)
1	D	0.62	5/1631 (0.3%)	0.86	11/2200 (0.5%)
All	All	0.57	10/6675 (0.1%)	0.77	22/9009 (0.2%)

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	D	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	VAL	CA-CB	-12.41	1.28	1.54
1	C	60	VAL	CB-CG1	-10.32	1.31	1.52
1	D	84	ASN	CA-C	-9.27	1.28	1.52
1	C	60	VAL	CB-CG2	-8.10	1.35	1.52
1	D	82	ALA	CA-CB	-7.50	1.36	1.52
1	D	92	ALA	CA-CB	-7.26	1.37	1.52
1	C	61	ILE	CB-CG2	-5.71	1.35	1.52
1	D	84	ASN	CB-CG	5.20	1.63	1.51
1	D	84	ASN	CA-CB	5.18	1.66	1.53
1	C	60	VAL	C-O	5.02	1.32	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	83	GLN	CA-C-N	-9.64	95.99	117.20
1	C	61	ILE	CA-C-N	8.79	136.54	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	MSE	CG-SE-CE	-8.73	79.68	98.90
1	D	84	ASN	CA-C-N	-8.42	98.67	117.20
1	D	85	VAL	CA-CB-CG1	-8.40	98.31	110.90
1	D	85	VAL	CB-CA-C	-8.28	95.66	111.40
1	C	61	ILE	CA-C-O	-7.74	103.84	120.10
1	D	83	GLN	O-C-N	7.71	135.04	122.70
1	D	85	VAL	CA-C-N	-7.30	101.15	117.20
1	B	61	ILE	CB-CA-C	-6.55	98.50	111.60
1	C	61	ILE	C-N-CA	-6.45	105.56	121.70
1	B	61	ILE	CB-CG1-CD1	6.38	131.76	113.90
1	D	86	THR	CA-CB-CG2	-6.16	103.78	112.40
1	D	85	VAL	CG1-CB-CG2	-5.99	101.31	110.90
1	C	59	ASP	N-CA-CB	-5.87	100.04	110.60
1	B	65	LEU	CB-CA-C	-5.59	99.58	110.20
1	D	86	THR	N-CA-CB	-5.50	99.86	110.30
1	B	61	ILE	CA-CB-CG1	5.46	121.38	111.00
1	D	83	GLN	N-CA-CB	-5.19	101.26	110.60
1	B	61	ILE	CA-CB-CG2	5.07	121.03	110.90
1	D	83	GLN	CB-CA-C	5.07	120.53	110.40
1	B	66	MSE	CB-CG-SE	5.06	127.87	112.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	83	GLN	Mainchain,Peptide
1	D	84	ASN	Mainchain
1	D	85	VAL	Mainchain

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	1625	0	1590	90	0
1	B	1667	0	1642	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1667	0	1635	136	0
1	D	1604	0	1576	121	0
2	A	2	0	0	1	0
2	B	6	0	0	1	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
All	All	6575	0	6443	427	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 33.

All (427) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:60:VAL:O	1:C:61:ILE:HG22	1.45	1.12
1:B:18:LEU:HD12	1:B:30:LEU:HD11	1.42	0.99
1:D:38:ARG:HH12	1:D:48:LEU:HD21	1.27	0.99
1:C:187:THR:HG22	1:C:188:ASP:H	1.26	0.98
1:C:174:PHE:HA	1:C:178:LEU:HB2	1.44	0.96
1:C:60:VAL:HG12	1:C:60:VAL:O	1.65	0.95
1:B:71:LYS:HE3	1:B:74:GLN:HE21	1.28	0.95
1:A:50:LEU:HD13	1:A:115:GLU:HG3	1.51	0.93
1:C:60:VAL:C	1:C:61:ILE:HG22	1.82	0.90
1:D:18:LEU:HD12	1:D:30:LEU:HD11	1.52	0.89
1:C:59:ASP:C	1:C:61:ILE:H	1.70	0.89
1:A:85:VAL:HG13	1:A:86:THR:N	1.88	0.86
1:B:178:LEU:HB3	1:B:201:MSE:HE1	1.57	0.86
1:B:50:LEU:HD13	1:B:115:GLU:HG3	1.58	0.86
1:A:47:ASN:HD22	1:A:50:LEU:HB2	1.39	0.86
1:D:105:SER:HA	1:D:110:GLN:HE22	1.40	0.85
1:C:60:VAL:C	1:C:61:ILE:CG2	2.44	0.85
1:C:10:ILE:HG23	1:C:57:LEU:HD21	1.59	0.84
1:A:40:LEU:HB3	1:A:118:VAL:HG13	1.60	0.84
1:B:47:ASN:ND2	1:B:50:LEU:HB2	1.94	0.83
1:C:47:ASN:HD22	1:C:50:LEU:HB2	1.44	0.82
1:B:15:LEU:HD22	1:B:27:ARG:HG2	1.59	0.82
1:B:35:ARG:HD2	1:C:215:ASP:C	2.01	0.81
1:C:124:ARG:HD3	1:C:181:LEU:HD22	1.60	0.81
1:C:59:ASP:C	1:C:61:ILE:N	2.25	0.81
1:D:120:GLN:NE2	1:D:186:ASN:HD21	1.80	0.80
1:D:61:ILE:HG13	1:D:62:ASP:N	1.96	0.79
1:D:2:ILE:HD12	1:D:50:LEU:HA	1.65	0.79
1:C:94:PHE:O	1:C:98:ASP:HB2	1.83	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:61:ILE:O	1:C:62:ASP:CB	2.26	0.79
1:D:125:LEU:HD22	1:D:193:LEU:HD23	1.65	0.79
1:B:115:GLU:O	1:B:119:VAL:HG23	1.84	0.77
1:B:18:LEU:CD1	1:B:30:LEU:HD11	2.14	0.77
1:B:155:ARG:CZ	1:B:158:MSE:HE3	2.15	0.76
1:D:159:THR:OG1	1:D:162:GLN:HG3	1.85	0.76
1:B:47:ASN:HD22	1:B:50:LEU:HB2	1.50	0.76
1:D:73:HIS:O	1:D:77:ILE:HD12	1.85	0.76
1:C:54:ALA:HA	1:C:97:ILE:HD11	1.68	0.75
1:A:12:THR:HG23	1:A:16:GLN:HE22	1.51	0.75
1:A:47:ASN:ND2	1:A:50:LEU:HB2	2.01	0.75
1:B:35:ARG:HD2	1:C:215:ASP:O	1.87	0.75
1:A:85:VAL:HG13	1:A:86:THR:H	1.50	0.75
1:C:71:LYS:HE2	1:C:75:ASP:OD2	1.87	0.75
1:C:61:ILE:O	1:C:62:ASP:HB2	1.85	0.74
1:A:94:PHE:O	1:A:98:ASP:HB2	1.87	0.74
1:C:40:LEU:HB3	1:C:118:VAL:HG13	1.69	0.74
1:B:47:ASN:HD22	1:B:50:LEU:CB	2.01	0.74
1:A:182:ALA:HA	1:A:185:MSE:HE2	1.71	0.73
1:C:120:GLN:NE2	1:C:186:ASN:HD21	1.86	0.73
1:D:18:LEU:O	1:D:21:ASP:HB2	1.89	0.72
1:C:12:THR:HG23	1:C:16:GLN:HE22	1.51	0.72
1:C:60:VAL:O	1:C:61:ILE:CG2	2.32	0.72
1:B:2:ILE:HD12	1:B:50:LEU:HA	1.72	0.71
1:C:58:HIS:HA	1:C:97:ILE:HG23	1.72	0.71
1:C:12:THR:CG2	1:C:16:GLN:HE22	2.02	0.71
1:B:85:VAL:CG1	1:B:90:GLN:HG3	2.20	0.71
1:D:61:ILE:HG13	1:D:62:ASP:H	1.55	0.70
1:B:137:LEU:HD22	1:C:134:ALA:HA	1.71	0.70
1:A:145:GLU:HG2	1:A:168:GLY:O	1.92	0.70
1:B:152:ILE:HG12	1:D:146:LYS:HE2	1.72	0.69
1:B:79:GLN:HE22	1:B:83:GLN:HE21	1.39	0.69
1:C:155:ARG:CZ	1:C:158:MSE:HE2	2.22	0.69
1:C:155:ARG:HD3	1:C:176:GLU:OE2	1.92	0.69
1:B:80:LEU:HB3	1:B:85:VAL:HG11	1.74	0.69
1:D:6:GLN:O	1:D:10:ILE:HG13	1.93	0.69
1:D:114:LEU:O	1:D:118:VAL:HG23	1.93	0.69
1:A:57:LEU:HB2	1:A:97:ILE:HD11	1.74	0.68
1:D:105:SER:HA	1:D:110:GLN:NE2	2.06	0.68
1:B:106:PHE:CE2	1:B:158:MSE:HB2	2.29	0.68
1:D:38:ARG:NH1	1:D:48:LEU:HD21	2.04	0.68
1:D:128:ILE:HA	1:D:201:MSE:CE	2.24	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:VAL:HG11	1:A:90:GLN:OE1	1.94	0.67
1:C:187:THR:HG22	1:C:188:ASP:N	2.05	0.67
1:A:57:LEU:HD13	1:A:76:LEU:HD11	1.75	0.67
1:C:149:ASP:OD1	1:C:151:ALA:HB3	1.93	0.67
1:D:115:GLU:CD	1:D:115:GLU:H	1.98	0.67
1:D:80:LEU:HD13	1:D:90:GLN:HG3	1.77	0.66
1:A:85:VAL:C	1:A:86:THR:HG22	2.16	0.66
1:D:57:LEU:HA	1:D:60:VAL:CG2	2.26	0.66
1:C:61:ILE:HG12	1:C:62:ASP:N	2.10	0.66
1:B:85:VAL:HG13	1:B:90:GLN:HG3	1.78	0.65
1:B:71:LYS:HE3	1:B:74:GLN:NE2	2.08	0.65
1:D:47:ASN:HD22	1:D:50:LEU:HB2	1.60	0.65
1:B:3:THR:OG1	1:B:6:GLN:HG3	1.97	0.65
1:B:61:ILE:CD1	1:B:97:ILE:HG21	2.27	0.65
1:D:102:PHE:HB2	1:D:177:LYS:HE3	1.78	0.65
1:B:27:ARG:O	1:B:31:GLN:HG3	1.95	0.65
1:A:86:THR:HG23	1:A:89:ASP:HB2	1.78	0.65
1:A:148:TYR:HB2	1:A:171:ILE:HG13	1.78	0.64
1:C:103:SER:HB2	1:C:160:ARG:HH11	1.61	0.64
1:D:92:ALA:C	1:D:94:PHE:N	2.49	0.64
1:C:80:LEU:O	1:C:85:VAL:HB	1.98	0.64
1:D:143:VAL:O	1:D:143:VAL:HG12	1.96	0.63
1:A:159:THR:OG1	1:A:162:GLN:HG3	1.98	0.63
1:D:120:GLN:HE21	1:D:186:ASN:HD21	1.44	0.63
1:D:106:PHE:CE1	1:D:158:MSE:HB2	2.34	0.63
1:A:178:LEU:HD13	1:A:201:MSE:HE1	1.81	0.62
1:C:129:GLY:O	1:C:133:ILE:HG13	2.00	0.62
1:B:58:HIS:HA	1:B:97:ILE:HG23	1.81	0.62
1:B:165:HIS:O	1:B:167:PRO:HD3	1.99	0.62
1:A:81:ASN:C	1:A:83:GLN:H	2.01	0.62
1:A:6:GLN:O	1:A:10:ILE:HG13	1.99	0.62
1:D:79:GLN:O	1:D:83:GLN:CG	2.48	0.62
1:C:115:GLU:H	1:C:115:GLU:CD	2.04	0.62
1:D:201:MSE:O	1:D:205:VAL:HG23	2.00	0.61
1:C:100:MSE:HG3	1:C:101:SER:N	2.15	0.61
1:C:61:ILE:HG12	1:C:62:ASP:H	1.63	0.61
1:B:158:MSE:HE1	1:B:163:TYR:HD1	1.65	0.61
1:D:155:ARG:NE	1:D:158:MSE:HE3	2.16	0.61
1:B:172:ASN:HB3	1:B:176:GLU:OE2	2.00	0.61
1:D:79:GLN:NE2	1:D:83:GLN:HG3	2.15	0.61
1:C:81:ASN:O	1:C:83:GLN:N	2.34	0.61
1:C:59:ASP:O	1:C:61:ILE:N	2.33	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:155:ARG:NH2	1:A:166:GLN:O	2.34	0.60
1:B:47:ASN:ND2	1:B:50:LEU:H	2.00	0.60
1:A:57:LEU:HB2	1:A:97:ILE:CD1	2.31	0.60
1:C:47:ASN:ND2	1:C:50:LEU:HB2	2.14	0.60
1:D:207:GLN:OE1	1:D:207:GLN:HA	2.01	0.60
1:D:3:THR:OG1	1:D:6:GLN:HG3	2.01	0.60
1:C:81:ASN:C	1:C:83:GLN:H	2.05	0.60
1:D:128:ILE:HA	1:D:201:MSE:HE3	1.84	0.60
1:A:11:GLN:HG3	1:A:56:TRP:CZ2	2.37	0.60
1:D:47:ASN:ND2	1:D:50:LEU:HB2	2.17	0.59
1:A:75:ASP:O	1:A:78:VAL:HG23	2.02	0.59
1:B:196:HIS:ND1	1:B:196:HIS:O	2.34	0.59
1:B:102:PHE:CD2	1:B:177:LYS:HD2	2.37	0.59
1:B:65:LEU:N	1:B:65:LEU:HD23	2.17	0.59
1:D:77:ILE:HG23	1:D:90:GLN:HE22	1.67	0.59
1:C:29:HIS:O	1:C:33:VAL:HG23	2.03	0.59
1:D:125:LEU:HD13	1:D:193:LEU:CD2	2.33	0.59
1:C:186:ASN:O	1:C:187:THR:O	2.21	0.59
1:A:115:GLU:O	1:A:119:VAL:HG23	2.03	0.59
1:A:131:ILE:O	1:A:135:ARG:HG3	2.03	0.59
1:A:125:LEU:HD22	1:A:193:LEU:HD23	1.85	0.58
1:C:58:HIS:HA	1:C:97:ILE:CG2	2.31	0.58
1:C:155:ARG:CZ	1:C:158:MSE:CE	2.80	0.58
1:C:125:LEU:CD2	1:C:185:MSE:HE3	2.33	0.58
1:D:120:GLN:HE21	1:D:186:ASN:ND2	2.01	0.58
1:D:92:ALA:C	1:D:94:PHE:H	2.05	0.58
1:D:187:THR:O	1:D:191:LYS:HG3	2.03	0.58
1:A:11:GLN:HE21	1:A:15:LEU:HD11	1.68	0.58
1:D:57:LEU:HD13	1:D:76:LEU:HD21	1.84	0.58
1:C:47:ASN:HD22	1:C:50:LEU:CB	2.15	0.58
1:D:90:GLN:C	1:D:92:ALA:H	2.07	0.58
1:D:48:LEU:O	1:D:52:LEU:HG	2.04	0.58
1:D:104:LYS:HD3	1:D:160:ARG:NH1	2.18	0.58
1:D:125:LEU:CD2	1:D:193:LEU:HD23	2.33	0.57
1:C:18:LEU:HD12	1:C:30:LEU:HD11	1.86	0.57
1:A:148:TYR:HB2	1:A:171:ILE:CG1	2.34	0.57
1:C:60:VAL:CG1	1:C:60:VAL:O	2.43	0.57
1:C:100:MSE:HG3	1:C:101:SER:H	1.70	0.57
1:B:207:GLN:HG3	1:C:200:VAL:HG21	1.87	0.57
1:B:11:GLN:HG3	1:B:56:TRP:CZ2	2.40	0.57
1:C:57:LEU:HB2	1:C:97:ILE:CD1	2.35	0.57
1:D:160:ARG:O	1:D:164:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:187:THR:CG2	1:C:188:ASP:H	2.03	0.57
1:A:80:LEU:O	1:A:85:VAL:HB	2.05	0.57
1:A:81:ASN:O	1:A:83:GLN:N	2.37	0.57
1:B:104:LYS:HB3	1:B:110:GLN:HE22	1.70	0.56
1:C:90:GLN:O	1:C:93:ILE:HB	2.04	0.56
1:B:192:ALA:O	1:B:195:ALA:HB3	2.06	0.56
1:A:47:ASN:HD22	1:A:50:LEU:CB	2.16	0.56
1:D:179:PHE:CZ	1:D:205:VAL:HG21	2.41	0.56
1:A:12:THR:HG23	1:A:16:GLN:NE2	2.21	0.56
1:D:19:ALA:O	1:D:20:HIS:HB2	2.06	0.56
1:A:160:ARG:NH1	1:A:164:ARG:HE	2.02	0.56
1:C:203:GLU:O	1:C:207:GLN:HB2	2.06	0.56
1:D:79:GLN:O	1:D:83:GLN:HG2	2.06	0.55
1:D:155:ARG:CZ	1:D:158:MSE:HE3	2.37	0.55
1:A:127:ALA:O	1:A:178:LEU:HD22	2.07	0.55
1:B:200:VAL:HG21	1:C:207:GLN:NE2	2.22	0.55
1:B:106:PHE:C	1:B:108:GLY:H	2.11	0.55
1:B:65:LEU:HB2	1:B:66:MSE:HE2	1.89	0.55
1:D:11:GLN:HG3	1:D:56:TRP:CZ2	2.42	0.55
1:D:103:SER:HB3	1:D:163:TYR:CD2	2.41	0.54
1:C:6:GLN:O	1:C:9:ALA:HB3	2.07	0.54
1:A:85:VAL:CG1	1:A:86:THR:N	2.60	0.54
1:A:12:THR:CG2	1:A:16:GLN:HE22	2.19	0.54
1:C:201:MSE:O	1:C:205:VAL:HG23	2.08	0.54
1:B:16:GLN:HB3	2:B:3005:HOH:O	2.07	0.54
1:B:85:VAL:HG11	1:B:90:GLN:HG3	1.90	0.53
1:D:182:ALA:HA	1:D:185:MSE:HE2	1.89	0.53
1:C:71:LYS:O	1:C:75:ASP:OD2	2.27	0.53
1:A:174:PHE:HA	1:A:178:LEU:HB2	1.90	0.53
1:A:47:ASN:ND2	1:A:50:LEU:H	2.07	0.53
1:D:100:MSE:HG3	1:D:101:SER:N	2.22	0.53
1:D:57:LEU:HD12	1:D:93:ILE:HG21	1.91	0.53
1:D:165:HIS:ND1	1:D:166:GLN:N	2.56	0.53
1:C:5:THR:HG22	1:C:5:THR:O	2.08	0.53
1:D:57:LEU:HA	1:D:60:VAL:HG21	1.89	0.53
1:A:187:THR:HG22	1:A:189:THR:H	1.74	0.53
1:C:103:SER:HB2	1:C:160:ARG:NH1	2.25	0.52
1:A:61:ILE:HG12	1:A:62:ASP:N	2.24	0.52
1:B:96:ILE:HG22	1:B:97:ILE:N	2.25	0.52
1:C:85:VAL:HG11	1:C:90:GLN:OE1	2.10	0.52
1:D:16:GLN:O	1:D:19:ALA:HB3	2.09	0.52
1:B:47:ASN:ND2	1:B:50:LEU:CB	2.65	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:VAL:HG22	1:A:86:THR:H	1.74	0.52
1:B:79:GLN:NE2	1:B:83:GLN:HE21	2.08	0.52
1:C:48:LEU:O	1:C:51:THR:N	2.42	0.52
1:D:90:GLN:C	1:D:92:ALA:N	2.62	0.51
1:D:125:LEU:HD13	1:D:193:LEU:HD23	1.91	0.51
1:D:115:GLU:O	1:D:119:VAL:HG23	2.10	0.51
1:D:121:ASP:O	1:D:125:LEU:HG	2.10	0.51
1:C:18:LEU:CD1	1:C:30:LEU:HD11	2.41	0.51
1:A:213:THR:C	1:A:215:ASP:H	2.13	0.51
1:B:80:LEU:HB3	1:B:85:VAL:CG1	2.40	0.51
1:D:50:LEU:O	1:D:50:LEU:HD23	2.10	0.51
1:B:71:LYS:CE	1:B:74:GLN:HE21	2.12	0.51
1:D:103:SER:HB3	1:D:163:TYR:HD2	1.75	0.51
1:A:103:SER:O	1:A:106:PHE:HD2	1.94	0.51
1:D:143:VAL:O	1:D:143:VAL:CG1	2.58	0.51
1:A:11:GLN:HG3	1:A:56:TRP:CH2	2.46	0.51
1:C:143:VAL:O	1:C:143:VAL:HG12	2.10	0.51
1:B:155:ARG:NH2	1:B:166:GLN:O	2.44	0.51
1:B:61:ILE:CD1	1:B:97:ILE:CG2	2.89	0.51
1:A:85:VAL:CG1	1:A:90:GLN:OE1	2.59	0.50
1:C:160:ARG:HH11	1:C:160:ARG:HG3	1.76	0.50
1:D:182:ALA:HA	1:D:185:MSE:CE	2.41	0.50
1:D:85:VAL:HG12	1:D:86:THR:N	2.25	0.50
1:A:128:ILE:HA	1:A:201:MSE:CE	2.41	0.50
1:B:205:VAL:O	1:B:209:LYS:HG3	2.12	0.50
1:C:54:ALA:CA	1:C:97:ILE:HD11	2.38	0.50
1:D:128:ILE:HA	1:D:201:MSE:HE1	1.92	0.50
1:A:212:TRP:O	1:A:215:ASP:O	2.30	0.50
1:A:185:MSE:HB3	1:A:191:LYS:HG2	1.94	0.50
1:D:85:VAL:O	1:D:86:THR:O	2.29	0.50
1:D:38:ARG:NH2	1:D:52:LEU:HD11	2.27	0.50
1:A:96:ILE:O	1:A:98:ASP:N	2.44	0.50
1:B:89:ASP:O	1:B:93:ILE:HG13	2.11	0.50
1:C:120:GLN:O	1:C:124:ARG:HG3	2.12	0.50
1:D:92:ALA:O	1:D:94:PHE:N	2.45	0.49
1:B:207:GLN:HG3	1:C:200:VAL:CG2	2.42	0.49
1:A:12:THR:CG2	1:A:16:GLN:NE2	2.75	0.49
1:B:148:TYR:CE2	1:B:150:PRO:HD3	2.47	0.49
1:B:167:PRO:HD2	1:D:167:PRO:HD3	1.95	0.49
1:A:7:LEU:O	1:A:10:ILE:N	2.45	0.49
1:A:213:THR:C	1:A:215:ASP:N	2.65	0.49
1:A:58:HIS:HA	1:A:97:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:ARG:HD2	1:A:181:LEU:HD22	1.93	0.49
1:C:12:THR:CG2	1:C:16:GLN:NE2	2.74	0.49
1:A:155:ARG:NE	1:A:158:MSE:HE3	2.28	0.49
1:A:11:GLN:O	1:A:12:THR:C	2.51	0.49
1:B:161:GLU:O	1:B:162:GLN:C	2.51	0.48
1:D:57:LEU:O	1:D:60:VAL:HB	2.13	0.48
1:B:61:ILE:HD12	1:B:97:ILE:HG21	1.94	0.48
1:C:40:LEU:HD22	1:C:122:ALA:HB2	1.94	0.48
1:D:61:ILE:HD11	1:D:97:ILE:HG22	1.95	0.48
1:D:80:LEU:O	1:D:83:GLN:HB2	2.14	0.48
1:A:185:MSE:HG3	1:A:190:ALA:CB	2.43	0.48
1:D:12:THR:HG23	1:D:16:GLN:HE22	1.77	0.48
1:B:57:LEU:HD22	1:B:76:LEU:HD13	1.95	0.48
1:A:85:VAL:CG1	1:A:86:THR:H	2.20	0.48
1:D:57:LEU:HB2	1:D:97:ILE:CD1	2.43	0.48
1:D:187:THR:HB	1:D:190:ALA:CB	2.43	0.48
1:D:61:ILE:O	1:D:62:ASP:O	2.32	0.48
1:A:18:LEU:HD12	1:A:30:LEU:HD11	1.95	0.48
1:D:179:PHE:HZ	1:D:205:VAL:HG21	1.77	0.48
1:D:19:ALA:O	1:D:20:HIS:CB	2.61	0.47
1:D:199:ALA:O	1:D:203:GLU:N	2.43	0.47
1:C:10:ILE:CG2	1:C:57:LEU:HD21	2.35	0.47
1:C:89:ASP:O	1:C:93:ILE:HG13	2.14	0.47
1:A:81:ASN:C	1:A:83:GLN:N	2.68	0.47
1:D:154:PRO:HD3	1:D:172:ASN:OD1	2.15	0.47
1:C:27:ARG:HH11	1:C:27:ARG:HB3	1.79	0.47
1:A:85:VAL:C	1:A:86:THR:CG2	2.83	0.47
1:B:115:GLU:H	1:B:115:GLU:CD	2.16	0.47
1:B:152:ILE:CG1	1:D:146:LYS:HE2	2.43	0.47
1:D:147:ILE:O	1:D:169:THR:HB	2.13	0.47
1:C:66:MSE:HE2	1:C:66:MSE:CA	2.44	0.47
1:C:159:THR:OG1	1:C:162:GLN:HG3	2.14	0.47
1:B:121:ASP:OD2	1:B:186:ASN:HB2	2.14	0.47
1:C:20:HIS:HA	1:C:22:HIS:CE1	2.50	0.47
1:C:97:ILE:HG22	1:C:97:ILE:O	2.14	0.47
1:D:77:ILE:HG23	1:D:90:GLN:NE2	2.30	0.47
1:D:41:ALA:O	1:D:45:GLY:N	2.47	0.47
1:D:76:LEU:O	1:D:80:LEU:HG	2.15	0.47
1:C:212:TRP:C	1:C:212:TRP:CD1	2.88	0.47
1:A:4:GLU:HA	1:A:49:ASN:HD21	1.79	0.47
1:B:213:THR:O	1:B:214:ALA:C	2.53	0.47
1:A:147:ILE:O	1:A:171:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:81:ASN:C	1:C:83:GLN:N	2.69	0.46
1:A:85:VAL:O	1:A:86:THR:HG22	2.15	0.46
1:D:47:ASN:HD22	1:D:50:LEU:H	1.63	0.46
1:B:159:THR:OG1	1:B:162:GLN:HG3	2.15	0.46
1:B:67:ALA:O	1:B:69:PRO:HD3	2.16	0.46
1:D:112:LEU:HB3	1:D:117:GLN:HG3	1.97	0.46
1:B:193:LEU:HA	1:B:193:LEU:HD12	1.72	0.46
1:C:6:GLN:NE2	1:C:85:VAL:HA	2.30	0.46
1:D:182:ALA:O	1:D:185:MSE:HB2	2.16	0.46
1:D:196:HIS:O	1:D:196:HIS:CG	2.69	0.46
2:A:3008:HOH:O	1:B:203:GLU:HG2	2.13	0.46
1:B:73:HIS:O	1:B:77:ILE:HD13	2.15	0.46
1:D:127:ALA:O	1:D:178:LEU:HD22	2.15	0.46
1:B:208:PHE:HA	1:C:130:ALA:HB3	1.98	0.46
1:D:46:ALA:HA	1:D:114:LEU:HD23	1.98	0.46
1:D:16:GLN:OE1	1:D:16:GLN:N	2.48	0.46
1:A:21:ASP:O	1:A:22:HIS:HB2	2.15	0.46
1:A:120:GLN:NE2	1:A:186:ASN:HD21	2.13	0.46
1:C:158:MSE:SE	1:C:163:TYR:HB2	2.66	0.46
1:A:48:LEU:HD21	1:A:52:LEU:HD12	1.96	0.46
1:A:107:ASN:ND2	1:B:202:HIS:HB3	2.30	0.46
1:B:137:LEU:CD2	1:C:134:ALA:HB1	2.45	0.46
1:C:112:LEU:HG	1:C:113:SER:N	2.30	0.46
1:B:130:ALA:HB3	1:C:208:PHE:HA	1.98	0.46
1:D:120:GLN:HG2	1:D:124:ARG:HD2	1.97	0.46
1:C:1:MSE:HA	1:C:89:ASP:OD1	2.16	0.46
1:B:13:TYR:CG	1:B:79:GLN:HG2	2.52	0.45
1:D:12:THR:HG23	1:D:16:GLN:NE2	2.31	0.45
1:B:47:ASN:HD22	1:B:50:LEU:HB3	1.81	0.45
1:D:58:HIS:C	1:D:60:VAL:H	2.18	0.45
1:C:148:TYR:OH	1:C:209:LYS:HD2	2.16	0.45
1:A:128:ILE:HA	1:A:201:MSE:HE3	1.98	0.45
1:D:146:LYS:O	1:D:169:THR:HA	2.16	0.45
1:C:12:THR:HG22	1:C:16:GLN:HE22	1.82	0.45
1:A:108:GLY:O	1:A:110:GLN:NE2	2.50	0.45
1:B:141:GLY:HA3	1:C:138:TYR:O	2.16	0.45
1:C:74:GLN:O	1:C:77:ILE:N	2.49	0.45
1:A:155:ARG:CZ	1:A:158:MSE:HE1	2.46	0.45
1:C:120:GLN:NE2	1:C:186:ASN:ND2	2.60	0.45
1:D:76:LEU:HG	1:D:80:LEU:HD11	1.98	0.45
1:B:96:ILE:O	1:B:97:ILE:C	2.54	0.45
1:D:185:MSE:HE3	1:D:194:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:39:ARG:O	1:D:39:ARG:HG2	2.17	0.45
1:B:174:PHE:CE2	1:B:201:MSE:HE2	2.51	0.45
1:D:40:LEU:HD21	1:D:190:ALA:HB2	1.99	0.45
1:B:80:LEU:HD13	1:B:90:GLN:HG2	1.98	0.45
1:B:138:TYR:O	1:C:141:GLY:HA3	2.16	0.45
1:B:61:ILE:HG12	1:B:61:ILE:O	2.16	0.45
1:C:54:ALA:HB1	1:C:97:ILE:HG13	1.99	0.44
1:B:103:SER:O	1:B:106:PHE:HD1	2.00	0.44
1:A:61:ILE:O	1:A:62:ASP:O	2.36	0.44
1:C:142:HIS:O	1:C:142:HIS:CG	2.71	0.44
1:C:61:ILE:HG21	1:C:61:ILE:HD12	1.64	0.44
1:C:76:LEU:O	1:C:80:LEU:HG	2.18	0.44
1:A:48:LEU:C	1:A:48:LEU:HD23	2.37	0.44
1:B:10:ILE:HG23	1:B:57:LEU:HD21	1.99	0.44
1:D:140:SER:HB3	1:D:145:GLU:HB3	2.00	0.44
1:C:121:ASP:OD1	1:C:186:ASN:N	2.45	0.44
1:C:71:LYS:NZ	1:C:74:GLN:NE2	2.66	0.44
1:B:113:SER:O	1:B:117:GLN:HG3	2.17	0.44
1:C:12:THR:HG22	1:C:16:GLN:NE2	2.32	0.44
1:D:93:ILE:O	1:D:97:ILE:HB	2.17	0.44
1:D:187:THR:HB	1:D:190:ALA:HB2	1.99	0.44
1:D:148:TYR:CD1	1:D:171:ILE:HG13	2.53	0.44
1:A:6:GLN:NE2	1:A:84:ASN:O	2.51	0.43
1:A:149:ASP:HB3	1:A:152:ILE:HB	2.00	0.43
1:C:146:LYS:O	1:C:169:THR:HA	2.18	0.43
1:C:193:LEU:O	1:C:197:ARG:HG3	2.18	0.43
1:A:85:VAL:HG22	1:A:86:THR:N	2.33	0.43
1:C:54:ALA:O	1:C:97:ILE:HD11	2.18	0.43
1:C:214:ALA:O	1:C:215:ASP:O	2.36	0.43
1:C:74:GLN:HG2	1:C:75:ASP:N	2.33	0.43
1:A:61:ILE:HA	1:A:72:ALA:HB1	2.00	0.43
1:D:60:VAL:HG12	1:D:60:VAL:O	2.17	0.43
1:B:166:GLN:HE22	1:D:143:VAL:HG12	1.84	0.43
1:C:73:HIS:O	1:C:74:GLN:C	2.56	0.43
1:A:161:GLU:O	1:A:162:GLN:C	2.57	0.43
1:B:165:HIS:ND1	1:B:165:HIS:C	2.71	0.43
1:A:143:VAL:HG12	1:A:145:GLU:HB2	1.99	0.43
1:D:96:ILE:HG23	1:D:116:GLY:HA2	2.00	0.43
1:C:205:VAL:O	1:C:209:LYS:HG3	2.19	0.43
1:A:48:LEU:O	1:A:52:LEU:HG	2.18	0.43
1:C:165:HIS:C	1:C:165:HIS:ND1	2.72	0.43
1:C:1:MSE:HE2	1:C:1:MSE:N	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:LEU:HD11	1:A:52:LEU:HB2	2.01	0.43
1:C:28:ASP:HB3	1:C:32:ARG:HH12	1.83	0.43
1:D:37:ALA:HB2	1:D:122:ALA:CB	2.48	0.43
1:B:158:MSE:HE2	1:B:163:TYR:HA	2.01	0.43
1:C:28:ASP:HB3	1:C:32:ARG:NH1	2.33	0.43
1:D:213:THR:O	1:D:214:ALA:C	2.57	0.43
1:D:92:ALA:O	1:D:93:ILE:C	2.56	0.43
1:A:147:ILE:HA	1:A:170:ALA:HB3	2.01	0.43
1:B:77:ILE:HG22	1:B:81:ASN:HD22	1.82	0.43
1:B:182:ALA:HA	1:B:185:MSE:HE2	2.00	0.43
1:B:174:PHE:HA	1:B:178:LEU:HB2	2.01	0.42
1:C:149:ASP:C	1:C:151:ALA:H	2.22	0.42
1:C:81:ASN:HA	1:C:85:VAL:HG12	2.01	0.42
1:C:125:LEU:HD21	1:C:185:MSE:HE3	2.00	0.42
1:B:115:GLU:N	1:B:115:GLU:CD	2.72	0.42
1:D:54:ALA:O	1:D:97:ILE:HD11	2.20	0.42
1:B:77:ILE:N	1:B:77:ILE:HD12	2.35	0.42
1:B:149:ASP:O	1:B:152:ILE:N	2.51	0.42
1:C:28:ASP:O	1:C:32:ARG:HG3	2.20	0.42
1:C:61:ILE:HA	1:C:66:MSE:HE3	2.00	0.42
1:A:118:VAL:O	1:A:121:ASP:HB2	2.20	0.42
1:C:178:LEU:HA	1:C:178:LEU:HD23	1.83	0.42
1:C:103:SER:CB	1:C:160:ARG:NH1	2.82	0.42
1:B:50:LEU:CD1	1:B:115:GLU:HG3	2.40	0.42
1:B:125:LEU:HA	1:B:125:LEU:HD23	1.92	0.42
1:D:47:ASN:HD22	1:D:50:LEU:CB	2.29	0.41
1:C:13:TYR:CD1	1:C:79:GLN:HG2	2.55	0.41
1:C:155:ARG:NH1	1:C:158:MSE:CE	2.83	0.41
1:B:138:TYR:CG	1:C:147:ILE:HD11	2.55	0.41
1:D:74:GLN:O	1:D:78:VAL:HG23	2.20	0.41
1:C:53:ALA:O	1:C:57:LEU:HG	2.19	0.41
1:D:159:THR:O	1:D:161:GLU:N	2.53	0.41
1:B:137:LEU:HD22	1:C:134:ALA:CA	2.45	0.41
1:A:102:PHE:CB	1:A:177:LYS:HE3	2.50	0.41
1:C:174:PHE:O	1:C:179:PHE:N	2.53	0.41
1:D:85:VAL:O	1:D:86:THR:C	2.58	0.41
1:B:38:ARG:O	1:B:42:LYS:HG3	2.20	0.41
1:C:13:TYR:CG	1:C:79:GLN:HG2	2.55	0.41
1:C:96:ILE:HA	1:C:112:LEU:HD11	2.01	0.41
1:C:208:PHE:CD1	1:C:208:PHE:C	2.93	0.41
1:B:104:LYS:O	1:B:106:PHE:N	2.53	0.41
1:C:100:MSE:O	1:C:101:SER:C	2.58	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:PRO:O	1:C:72:ALA:HB3	2.19	0.41
1:D:120:GLN:NE2	1:D:186:ASN:ND2	2.57	0.41
1:A:178:LEU:HD13	1:A:201:MSE:CE	2.49	0.41
1:D:191:LYS:O	1:D:192:ALA:C	2.58	0.41
1:A:103:SER:O	1:A:106:PHE:CD2	2.73	0.41
1:B:57:LEU:HD13	1:B:76:LEU:HD11	2.03	0.41
1:C:7:LEU:O	1:C:10:ILE:HB	2.21	0.40
1:C:179:PHE:CZ	1:C:205:VAL:HG21	2.56	0.40
1:B:121:ASP:CG	1:B:186:ASN:H	2.24	0.40
1:A:112:LEU:O	1:A:113:SER:O	2.40	0.40
1:C:171:ILE:HA	1:C:171:ILE:HD13	1.94	0.40
1:C:2:ILE:HG22	1:C:3:THR:N	2.36	0.40
1:C:119:VAL:O	1:C:120:GLN:C	2.59	0.40
1:C:98:ASP:O	1:C:99:HIS:ND1	2.54	0.40
1:D:29:HIS:O	1:D:33:VAL:HG23	2.22	0.40
1:D:29:HIS:NE2	1:D:59:ASP:OD2	2.49	0.40
1:A:145:GLU:CG	1:A:168:GLY:O	2.66	0.40
1:C:83:GLN:O	1:C:84:ASN:C	2.59	0.40
1:A:185:MSE:HG3	1:A:190:ALA:HB1	2.03	0.40
1:C:166:GLN:HA	1:C:167:PRO:HD3	1.77	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	202/231 (87%)	171 (85%)	23 (11%)	8 (4%)	5	14
1	B	208/231 (90%)	179 (86%)	24 (12%)	5 (2%)	9	29
1	C	208/231 (90%)	172 (83%)	24 (12%)	12 (6%)	3	7
1	D	197/231 (85%)	163 (83%)	32 (16%)	2 (1%)	22	60
All	All	815/924 (88%)	685 (84%)	103 (13%)	27 (3%)	6	19

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	97	ILE
1	A	113	SER
1	C	82	ALA
1	C	187	THR
1	D	84	ASN
1	A	75	ASP
1	A	82	ALA
1	B	97	ILE
1	B	105	SER
1	C	48	LEU
1	C	60	VAL
1	C	61	ILE
1	C	156	GLU
1	B	107	ASN
1	D	46	ALA
1	A	11	GLN
1	B	178	LEU
1	C	49	ASN
1	C	101	SER
1	C	103	SER
1	C	177	LYS
1	A	96	ILE
1	B	96	ILE
1	C	74	GLN
1	A	152	ILE
1	C	109	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	165/178 (93%)	151 (92%)	14 (8%)	15	41
1	B	169/178 (95%)	156 (92%)	13 (8%)	18	45
1	C	169/178 (95%)	156 (92%)	13 (8%)	18	45
1	D	163/178 (92%)	156 (96%)	7 (4%)	40	76
All	All	666/712 (94%)	619 (93%)	47 (7%)	21	51

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	7	LEU
1	A	8	THR
1	A	16	GLN
1	A	40	LEU
1	A	50	LEU
1	A	61	ILE
1	A	78	VAL
1	A	86	THR
1	A	115	GLU
1	A	143	VAL
1	A	157	HIS
1	A	160	ARG
1	A	207	GLN
1	B	4	GLU
1	B	7	LEU
1	B	16	GLN
1	B	27	ARG
1	B	40	LEU
1	B	50	LEU
1	B	61	ILE
1	B	66	MSE
1	B	71	LYS
1	B	74	GLN
1	B	115	GLU
1	B	157	HIS
1	B	187	THR
1	C	7	LEU
1	C	27	ARG
1	C	50	LEU
1	C	58	HIS
1	C	59	ASP
1	C	61	ILE
1	C	62	ASP
1	C	71	LYS
1	C	113	SER
1	C	137	LEU
1	C	157	HIS
1	C	188	ASP
1	C	209	LYS
1	D	4	GLU
1	D	7	LEU

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Mol	Chain	Res	Type
1	D	16	GLN
1	D	86	THR
1	D	137	LEU
1	D	155	ARG
1	D	157	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	16	GLN
1	A	47	ASN
1	A	49	ASN
1	A	58	HIS
1	A	79	GLN
1	A	99	HIS
1	A	120	GLN
1	A	162	GLN
1	B	25	HIS
1	B	47	ASN
1	B	58	HIS
1	B	74	GLN
1	B	79	GLN
1	B	81	ASN
1	B	90	GLN
1	B	99	HIS
1	B	110	GLN
1	B	120	GLN
1	B	162	GLN
1	C	6	GLN
1	C	16	GLN
1	C	29	HIS
1	C	47	ASN
1	C	74	GLN
1	C	79	GLN
1	C	120	GLN
1	C	162	GLN
1	C	186	ASN
1	D	47	ASN
1	D	79	GLN
1	D	90	GLN
1	D	99	HIS

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Mol	Chain	Res	Type
1	D	110	GLN
1	D	120	GLN
1	D	162	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	206/231 (89%)	0.04	7 (3%) 43 44	2, 17, 46, 63	0
1	B	212/231 (91%)	0.15	13 (6%) 21 20	1, 19, 82, 97	0
1	C	212/231 (91%)	0.71	31 (14%) 3 3	3, 37, 78, 101	0
1	D	203/231 (87%)	0.96	40 (19%) 2 1	3, 38, 83, 89	0
All	All	833/924 (90%)	0.46	91 (10%) 6 5	1, 26, 80, 101	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	108	GLY	10.9
1	B	164	ARG	7.6
1	C	110	GLN	6.5
1	C	107	ASN	6.0
1	D	74	GLN	5.7
1	C	115	GLU	5.5
1	A	215	ASP	5.5
1	D	101	SER	5.5
1	D	62	ASP	5.4
1	C	109	PRO	5.3
1	A	214	ALA	5.2
1	B	157	HIS	5.2
1	D	93	ILE	5.0
1	D	1	MSE	5.0
1	D	157	HIS	4.8
1	D	37	ALA	4.6
1	B	160	ARG	4.6
1	D	104	LYS	4.5
1	D	110	GLN	4.4
1	D	53	ALA	4.1
1	D	80	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	1	MSE	3.9
1	B	110	GLN	3.9
1	A	213	THR	3.8
1	D	76	LEU	3.6
1	D	60	VAL	3.5
1	C	164	ARG	3.5
1	D	167	PRO	3.5
1	D	57	LEU	3.4
1	C	114	LEU	3.3
1	A	188	ASP	3.3
1	A	72	ALA	3.3
1	B	107	ASN	3.3
1	C	161	GLU	3.2
1	D	85	VAL	3.2
1	C	104	LYS	3.1
1	D	49	ASN	3.1
1	A	62	ASP	3.1
1	D	10	ILE	3.1
1	C	99	HIS	3.0
1	D	4	GLU	3.0
1	C	44	GLU	3.0
1	D	41	ALA	2.9
1	D	165	HIS	2.9
1	C	118	VAL	2.9
1	B	106	PHE	2.8
1	B	108	GLY	2.8
1	C	119	VAL	2.8
1	D	59	ASP	2.8
1	D	160	ARG	2.8
1	B	111	LYS	2.8
1	D	61	ILE	2.8
1	B	196	HIS	2.7
1	C	93	ILE	2.7
1	D	6	GLN	2.7
1	C	50	LEU	2.7
1	A	73	HIS	2.7
1	B	163	TYR	2.6
1	D	54	ALA	2.6
1	D	50	LEU	2.6
1	C	105	SER	2.6
1	D	103	SER	2.5
1	B	109	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	55	ALA	2.5
1	D	98	ASP	2.5
1	C	48	LEU	2.5
1	C	38	ARG	2.5
1	C	96	ILE	2.5
1	D	18	LEU	2.4
1	C	13	TYR	2.4
1	D	27	ARG	2.4
1	D	111	LYS	2.4
1	C	79	GLN	2.4
1	D	109	PRO	2.4
1	C	196	HIS	2.4
1	D	2	ILE	2.3
1	C	165	HIS	2.3
1	C	53	ALA	2.2
1	D	72	ALA	2.2
1	D	44	GLU	2.2
1	D	7	LEU	2.2
1	C	189	THR	2.1
1	C	2	ILE	2.1
1	D	96	ILE	2.1
1	D	94	PHE	2.1
1	C	18	LEU	2.1
1	C	35	ARG	2.1
1	C	92	ALA	2.1
1	D	73	HIS	2.0
1	B	112	LEU	2.0
1	C	98	ASP	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.