



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:26 AM GMT

PDB ID : 3DKW
Title : Crystal Structure of DNR from Pseudomonas aeruginosa.
Authors : Giardina, G.
Deposited on : 2008-06-26
Resolution : 3.60 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>

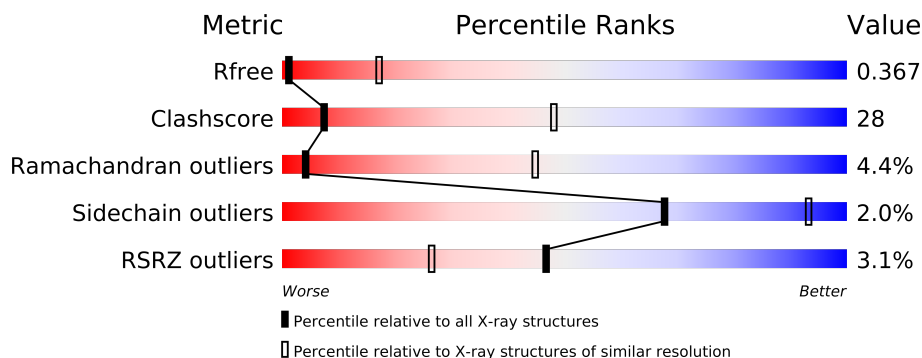
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.60 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	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)

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	227	
1	B	227	
1	C	227	
1	D	227	
1	E	227	
1	F	227	
1	G	227	
1	H	227	
1	I	227	
1	J	227	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18250 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 DNR protein.

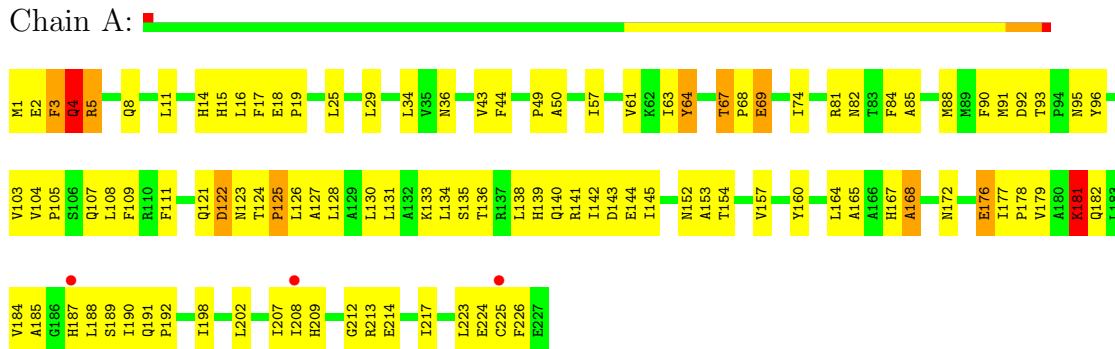
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	204	0	0
			1825	1158	325	334	8			
1	B	227	Total	C	N	O	S	354	0	0
			1825	1158	325	334	8			
1	C	227	Total	C	N	O	S	268	0	0
			1825	1158	325	334	8			
1	D	227	Total	C	N	O	S	483	0	0
			1825	1158	325	334	8			
1	E	227	Total	C	N	O	S	404	0	0
			1825	1158	325	334	8			
1	F	227	Total	C	N	O	S	417	0	0
			1825	1158	325	334	8			
1	G	227	Total	C	N	O	S	350	0	0
			1825	1158	325	334	8			
1	H	227	Total	C	N	O	S	352	0	0
			1825	1158	325	334	8			
1	I	227	Total	C	N	O	S	284	0	0
			1825	1158	325	334	8			
1	J	227	Total	C	N	O	S	206	0	0
			1825	1158	325	334	8			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

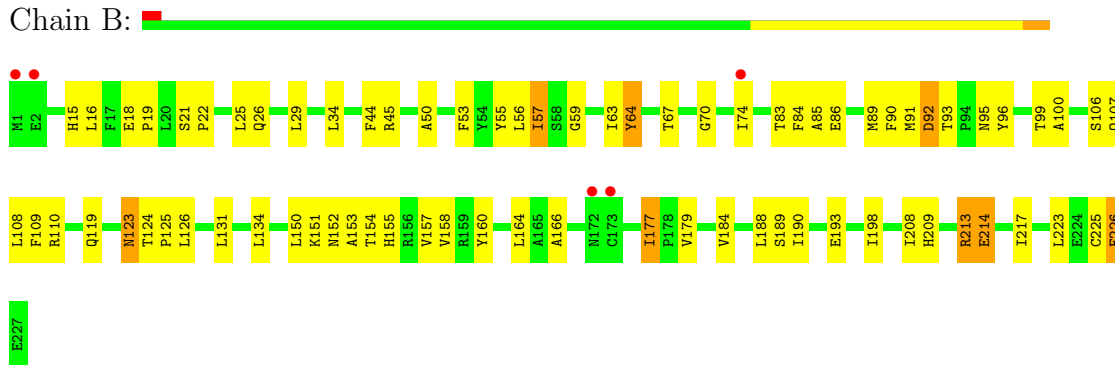
• Molecule 1: DNR protein

Chain A:



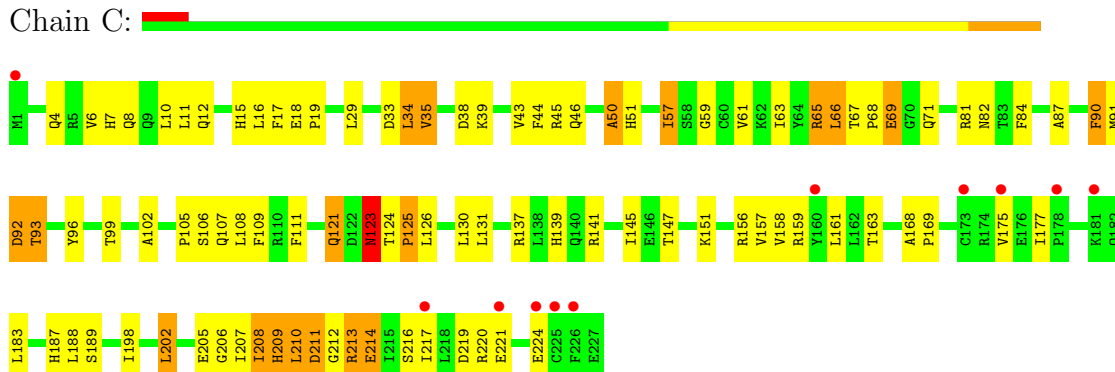
• Molecule 1: DNR protein

Chain B:



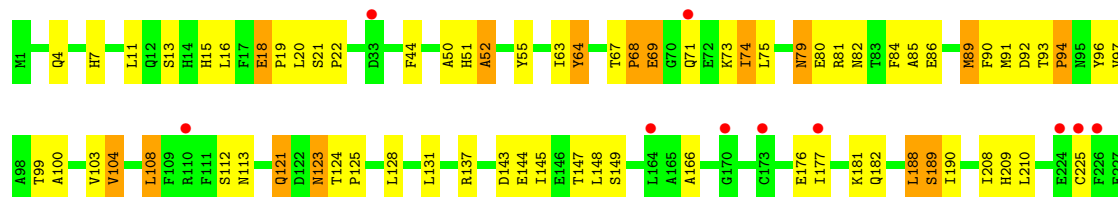
• Molecule 1: DNR protein

Chain C:



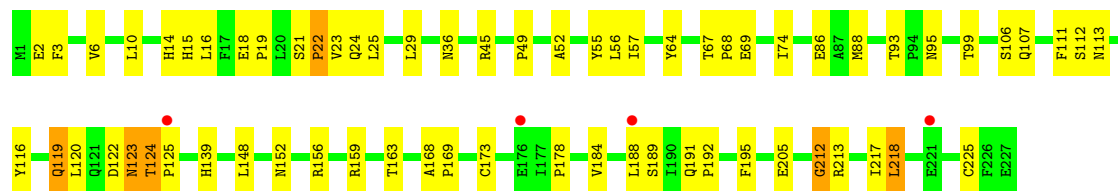
- Molecule 1: DNR protein

Chain D:



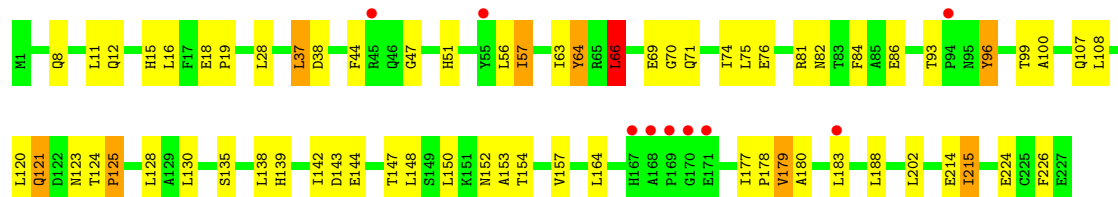
- Molecule 1: DNR protein

Chain E:



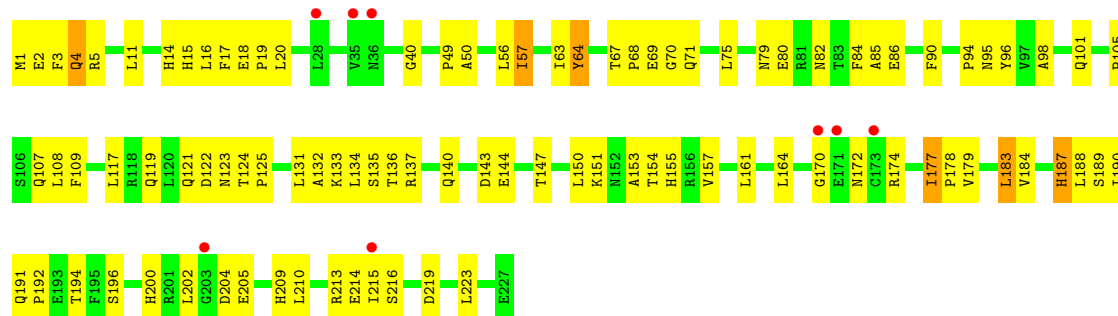
- Molecule 1: DNR protein

Chain F:



- Molecule 1: DNR protein

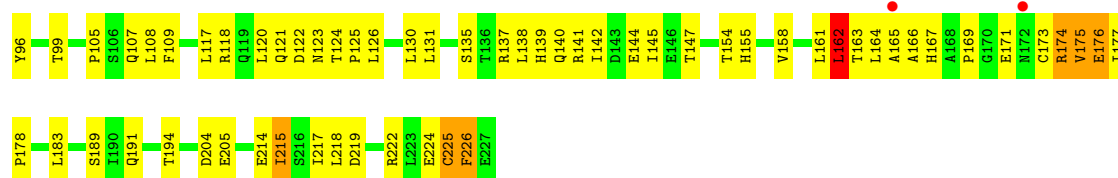
Chain G:



- Molecule 1: DNR protein

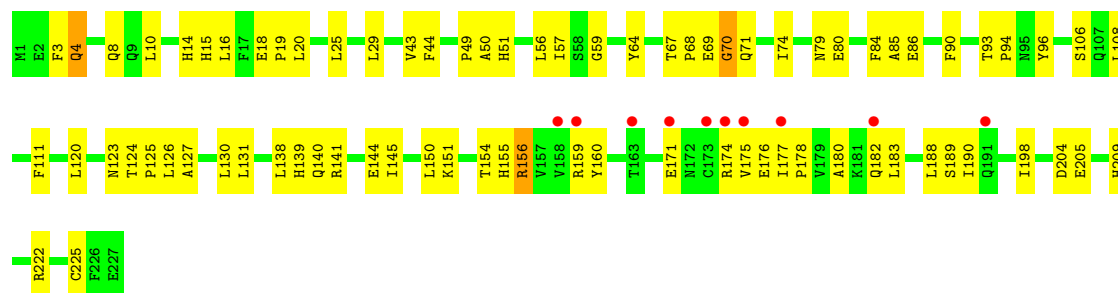
Chain H:





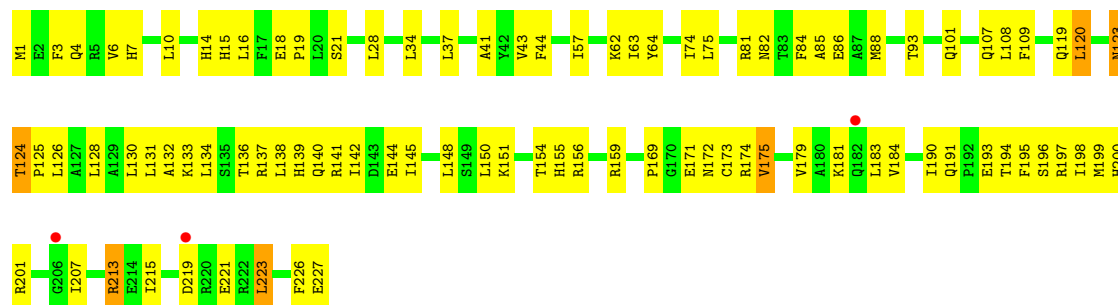
• Molecule 1: DNR protein

Chain I:



• Molecule 1: DNR protein

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.28Å 121.47Å 82.55Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	100.00 – 3.60 48.77 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (100.00-3.60) 96.7 (48.77-3.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.326 , 0.374 0.322 , 0.367	Depositor DCC
R_{free} test set	1359 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 34.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 27021 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	18250	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% 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	0.52	5/1861 (0.3%)	0.51	1/2520 (0.0%)
1	B	0.67	9/1861 (0.5%)	0.58	0/2520
1	C	0.50	3/1861 (0.2%)	0.60	4/2520 (0.2%)
1	D	0.55	3/1861 (0.2%)	0.56	0/2520
1	E	0.59	3/1861 (0.2%)	0.61	3/2520 (0.1%)
1	F	0.58	3/1861 (0.2%)	0.86	9/2520 (0.4%)
1	G	0.70	9/1861 (0.5%)	0.73	8/2520 (0.3%)
1	H	0.69	7/1861 (0.4%)	0.67	8/2520 (0.3%)
1	I	0.54	5/1861 (0.3%)	0.50	1/2520 (0.0%)
1	J	0.50	3/1861 (0.2%)	0.61	7/2520 (0.3%)
All	All	0.59	50/18610 (0.3%)	0.63	41/25200 (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	B	0	1
1	D	0	4
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	9

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	226	PHE	C-O	12.33	1.46	1.23
1	B	21	SER	CB-OG	-12.18	1.26	1.42
1	H	171	GLU	C-O	8.72	1.40	1.23
1	C	224	GLU	CG-CD	8.69	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	112	SER	CB-OG	-8.31	1.31	1.42
1	E	86	GLU	CB-CG	-8.25	1.36	1.52
1	G	135	SER	CB-OG	-8.18	1.31	1.42
1	G	187	HIS	CB-CG	-8.05	1.35	1.50
1	J	21	SER	CB-OG	-8.03	1.31	1.42
1	F	96	TYR	CB-CG	7.76	1.63	1.51
1	H	155	HIS	CB-CG	7.63	1.63	1.50
1	G	189	SER	CB-OG	7.55	1.52	1.42
1	H	73	LYS	CE-NZ	-7.39	1.30	1.49
1	J	219	ASP	CB-CG	7.32	1.67	1.51
1	H	163	THR	CB-OG1	-7.21	1.28	1.43
1	A	224	GLU	CB-CG	7.14	1.65	1.52
1	A	182	GLN	CB-CG	7.10	1.71	1.52
1	D	181	LYS	C-O	6.60	1.35	1.23
1	E	205	GLU	C-N	6.36	1.44	1.33
1	F	66	LEU	C-N	6.26	1.48	1.34
1	I	177	ILE	CB-CG1	-6.24	1.36	1.54
1	G	179	VAL	CB-CG1	-6.12	1.40	1.52
1	B	179	VAL	CB-CG2	-6.11	1.40	1.52
1	G	214	GLU	CB-CG	-5.90	1.41	1.52
1	G	177	ILE	C-N	5.89	1.45	1.34
1	B	213	ARG	CB-CG	5.87	1.68	1.52
1	C	205	GLU	CB-CG	5.71	1.62	1.52
1	H	173	CYS	CB-SG	5.63	1.91	1.82
1	G	107	GLN	CB-CG	-5.55	1.37	1.52
1	A	143	ASP	CB-CG	5.54	1.63	1.51
1	H	225	CYS	CB-SG	5.54	1.91	1.82
1	G	174	ARG	CB-CG	5.52	1.67	1.52
1	G	213	ARG	C-O	5.47	1.33	1.23
1	B	110	ARG	CB-CG	5.46	1.67	1.52
1	F	224	GLU	CB-CG	-5.44	1.41	1.52
1	B	198	ILE	CB-CG1	5.40	1.69	1.54
1	B	45	ARG	CB-CG	5.39	1.67	1.52
1	B	184	VAL	CB-CG2	5.38	1.64	1.52
1	A	209	HIS	CB-CG	-5.38	1.40	1.50
1	I	225	CYS	CB-SG	5.38	1.91	1.82
1	I	190	ILE	CB-CG1	5.36	1.69	1.54
1	J	137	ARG	CB-CG	5.35	1.67	1.52
1	I	222	ARG	C-O	-5.23	1.13	1.23
1	B	190	ILE	CB-CG2	5.21	1.69	1.52
1	D	121	GLN	CB-CG	5.21	1.66	1.52
1	B	193	GLU	CB-CG	-5.19	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	156	ARG	CB-CG	5.15	1.66	1.52
1	A	181	LYS	CB-CG	5.15	1.66	1.52
1	C	216	SER	CB-OG	-5.11	1.35	1.42
1	E	148	LEU	CB-CG	5.05	1.67	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	96	TYR	CB-CG-CD2	-20.12	108.93	121.00
1	F	96	TYR	CB-CG-CD1	19.25	132.55	121.00
1	F	28	LEU	CB-CG-CD1	10.63	129.06	111.00
1	C	183	LEU	CB-CG-CD1	-9.01	95.69	111.00
1	H	164	LEU	C-N-CA	8.12	142.01	121.70
1	J	226	PHE	CB-CG-CD1	-7.65	115.44	120.80
1	G	183	LEU	CB-CG-CD2	-7.53	98.19	111.00
1	G	5	ARG	N-CA-CB	7.40	123.92	110.60
1	C	137	ARG	CG-CD-NE	7.29	127.11	111.80
1	G	183	LEU	CA-CB-CG	7.24	131.96	115.30
1	H	164	LEU	O-C-N	-7.08	111.38	122.70
1	J	120	LEU	CA-CB-CG	7.01	131.43	115.30
1	H	215	ILE	O-C-N	-6.94	111.59	122.70
1	J	120	LEU	CB-CG-CD2	-6.86	99.34	111.00
1	G	223	LEU	CA-CB-CG	6.79	130.91	115.30
1	J	226	PHE	CB-CG-CD2	6.73	125.51	120.80
1	J	223	LEU	CA-CB-CG	6.67	130.65	115.30
1	H	225	CYS	O-C-N	-6.60	112.14	122.70
1	F	96	TYR	CA-CB-CG	-6.45	101.15	113.40
1	F	226	PHE	CB-CG-CD2	-6.36	116.35	120.80
1	A	67	THR	CA-CB-CG2	-6.30	103.58	112.40
1	E	29	LEU	CB-CG-CD1	6.13	121.42	111.00
1	H	174	ARG	CA-CB-CG	6.07	126.76	113.40
1	C	8	GLN	CA-CB-CG	6.05	126.70	113.40
1	G	214	GLU	CA-CB-CG	5.94	126.46	113.40
1	G	134	LEU	CA-CB-CG	5.93	128.94	115.30
1	H	161	LEU	CA-CB-CG	5.89	128.85	115.30
1	F	37	LEU	CD1-CG-CD2	5.79	127.86	110.50
1	G	183	LEU	CB-CG-CD1	5.78	120.82	111.00
1	E	218	LEU	CA-CB-CG	5.70	128.40	115.30
1	G	204	ASP	O-C-N	-5.68	113.61	122.70
1	F	38	ASP	CB-CG-OD2	5.57	123.31	118.30
1	H	155	HIS	CA-CB-CG	-5.42	104.39	113.60
1	J	120	LEU	CB-CG-CD1	5.28	119.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	182	GLN	CA-CB-CG	5.23	124.90	113.40
1	F	164	LEU	CA-CB-CG	5.19	127.23	115.30
1	C	175	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	J	219	ASP	CB-CG-OD1	5.09	122.88	118.30
1	H	162	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	E	205	GLU	O-C-N	5.01	131.71	123.20
1	F	226	PHE	CB-CG-CD1	5.00	124.30	120.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	ALA	Mainchain
1	D	182	GLN	Mainchain
1	D	208	ILE	Mainchain
1	D	209	HIS	Mainchain
1	D	210	LEU	Mainchain
1	F	93	THR	Mainchain
1	G	205	GLU	Mainchain
1	H	215	ILE	Mainchain
1	I	209	HIS	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	1825	0	1837	117	2
1	B	1825	0	1837	82	0
1	C	1825	0	1837	113	1
1	D	1825	0	1837	82	0
1	E	1825	0	1837	73	0
1	F	1825	0	1837	67	0
1	G	1825	0	1837	85	0
1	H	1825	0	1836	95	1
1	I	1825	0	1837	92	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1825	0	1837	103	0
All	All	18250	0	18369	806	4

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 28.

All (806) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:124:THR:OG1	1:J:125:PRO:HD3	1.24	1.34
1:E:22:PRO:O	1:E:25:LEU:HD13	1.12	1.30
1:D:103:VAL:O	1:D:104:VAL:CG1	1.81	1.28
1:A:152:ASN:OD1	1:B:152:ASN:OD1	1.56	1.24
1:I:138:LEU:HD13	1:J:138:LEU:CD2	1.69	1.22
1:C:67:THR:CG2	1:C:68:PRO:HD2	1.72	1.19
1:G:190:ILE:HG22	1:G:192:PRO:CD	1.75	1.16
1:A:131:LEU:HD23	1:B:131:LEU:CD2	1.76	1.15
1:F:179:VAL:HG12	1:F:180:ALA:H	1.07	1.14
1:E:21:SER:HB2	1:E:22:PRO:HD2	1.19	1.13
1:A:213:ARG:NH1	1:H:30:ALA:HA	1.63	1.13
1:D:103:VAL:O	1:D:104:VAL:HG12	0.96	1.13
1:A:131:LEU:HD23	1:B:131:LEU:HD23	1.30	1.12
1:A:131:LEU:CD2	1:B:131:LEU:HD23	1.78	1.12
1:A:131:LEU:CD2	1:B:131:LEU:CD2	2.26	1.12
1:G:131:LEU:CD2	1:H:131:LEU:HD23	1.80	1.12
1:G:131:LEU:HD23	1:H:131:LEU:CD2	1.80	1.12
1:C:131:LEU:HD23	1:D:131:LEU:HD23	1.30	1.12
1:C:145:ILE:HG12	1:D:145:ILE:HD11	1.22	1.11
1:J:123:ASN:ND2	1:J:126:LEU:HD12	1.67	1.10
1:J:123:ASN:O	1:J:124:THR:OG1	1.66	1.08
1:G:20:LEU:CD2	1:G:119:GLN:HE22	1.66	1.08
1:D:124:THR:OG1	1:D:125:PRO:HD3	1.50	1.08
1:G:20:LEU:HD21	1:G:119:GLN:HE22	1.18	1.08
1:C:67:THR:HG22	1:C:68:PRO:HD2	1.29	1.07
1:H:67:THR:HB	1:H:68:PRO:HD2	1.37	1.06
1:B:208:ILE:HG22	1:B:209:HIS:H	0.95	1.06
1:A:138:LEU:HD23	1:A:138:LEU:O	1.54	1.06
1:G:131:LEU:HD23	1:H:131:LEU:HD23	1.10	1.05
1:E:124:THR:HB	1:E:125:PRO:HD3	1.31	1.05
1:F:202:LEU:HD23	1:F:202:LEU:O	1.58	1.04
1:J:64:TYR:HB3	1:J:74:ILE:HD13	1.37	1.04
1:I:138:LEU:CD1	1:J:138:LEU:HD23	1.87	1.04
1:H:64:TYR:HB3	1:H:74:ILE:HD13	1.40	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:190:ILE:CG2	1:G:192:PRO:HD2	1.89	1.02
1:I:131:LEU:CD2	1:J:131:LEU:HD23	1.90	1.02
1:H:124:THR:N	1:H:125:PRO:HD2	1.75	1.01
1:E:22:PRO:O	1:E:25:LEU:CD1	2.08	1.01
1:E:152:ASN:OD1	1:F:152:ASN:ND2	1.95	1.00
1:J:14:HIS:O	1:J:18:GLU:HG3	1.59	1.00
1:H:158:VAL:O	1:H:162:LEU:HB2	1.62	0.99
1:B:208:ILE:HG22	1:B:209:HIS:N	1.77	0.99
1:I:138:LEU:HD13	1:J:138:LEU:HD23	1.03	0.99
1:C:107:GLN:C	1:C:108:LEU:HD12	1.83	0.99
1:G:131:LEU:CD2	1:H:131:LEU:CD2	2.38	0.98
1:C:145:ILE:CG1	1:D:145:ILE:HD11	1.93	0.98
1:J:123:ASN:HD22	1:J:126:LEU:HD12	1.19	0.98
1:B:99:THR:HG22	1:B:100:ALA:H	1.22	0.98
1:J:130:LEU:HD23	1:J:130:LEU:O	1.63	0.98
1:D:99:THR:HG22	1:D:100:ALA:H	1.28	0.97
1:F:107:GLN:C	1:F:108:LEU:HD12	1.84	0.97
1:H:66:LEU:O	1:H:67:THR:OG1	1.81	0.97
1:I:131:LEU:HD23	1:J:131:LEU:HD23	1.44	0.96
1:B:53:PHE:CE1	1:B:89:MET:CE	2.48	0.96
1:H:81:ARG:C	1:H:82:ASN:HD22	1.68	0.96
1:J:124:THR:OG1	1:J:125:PRO:CD	2.14	0.95
1:B:53:PHE:CE1	1:B:89:MET:HE1	2.01	0.95
1:F:99:THR:HG22	1:F:100:ALA:H	1.30	0.95
1:G:20:LEU:CD2	1:G:119:GLN:NE2	2.29	0.94
1:A:181:LYS:O	1:A:184:VAL:HG12	1.65	0.94
1:D:89:MET:HA	1:D:89:MET:HE3	1.46	0.94
1:A:107:GLN:C	1:A:108:LEU:HD12	1.88	0.94
1:C:131:LEU:HD23	1:D:131:LEU:CD2	1.98	0.94
1:C:18:GLU:HB3	1:C:19:PRO:HD3	1.47	0.94
1:D:148:LEU:HD12	1:D:149:SER:N	1.83	0.93
1:B:123:ASN:HD21	1:B:126:LEU:HB2	1.33	0.92
1:G:190:ILE:HG22	1:G:192:PRO:HD2	0.96	0.92
1:B:53:PHE:CD1	1:B:89:MET:CE	2.53	0.92
1:E:6:VAL:HG11	1:H:7:HIS:CE1	2.04	0.92
1:C:145:ILE:HG12	1:D:145:ILE:CD1	2.00	0.92
1:I:156:ARG:HB2	1:I:188:LEU:HD21	1.52	0.92
1:B:107:GLN:C	1:B:108:LEU:HD12	1.89	0.91
1:I:156:ARG:HB2	1:I:188:LEU:CD2	2.00	0.91
1:E:123:ASN:ND2	1:F:123:ASN:O	2.04	0.91
1:C:121:GLN:NE2	1:E:36:ASN:HD21	1.69	0.91
1:I:124:THR:N	1:I:125:PRO:HD2	1.86	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:147:THR:O	1:C:151:LYS:HG3	1.69	0.90
1:E:21:SER:HB2	1:E:22:PRO:CD	2.01	0.90
1:C:208:ILE:HD12	1:C:208:ILE:C	1.92	0.90
1:C:10:LEU:HD23	1:I:10:LEU:HD23	1.52	0.90
1:A:128:LEU:HD21	1:B:90:PHE:O	1.71	0.90
1:A:131:LEU:CD2	1:B:131:LEU:HD21	2.02	0.90
1:C:67:THR:HG22	1:C:68:PRO:CD	2.02	0.89
1:H:130:LEU:O	1:H:130:LEU:HD23	1.73	0.89
1:A:68:PRO:O	1:A:69:GLU:HB2	1.68	0.89
1:C:19:PRO:HG2	1:C:130:LEU:HD23	1.54	0.89
1:B:208:ILE:CG2	1:B:209:HIS:H	1.81	0.89
1:G:20:LEU:HD21	1:G:119:GLN:NE2	1.86	0.88
1:H:123:ASN:C	1:H:125:PRO:HD2	1.94	0.88
1:B:57:ILE:N	1:B:57:ILE:HD12	1.89	0.88
1:C:210:LEU:HD12	1:C:210:LEU:H	1.39	0.88
1:I:131:LEU:CD2	1:J:131:LEU:CD2	2.53	0.87
1:A:128:LEU:HD23	1:A:128:LEU:O	1.75	0.87
1:C:67:THR:HG23	1:C:68:PRO:HD2	1.53	0.87
1:E:23:VAL:O	1:E:25:LEU:N	2.08	0.87
1:A:131:LEU:HD21	1:B:131:LEU:CD2	2.04	0.87
1:D:103:VAL:C	1:D:104:VAL:HG12	1.95	0.87
1:C:10:LEU:HD23	1:I:10:LEU:CD2	2.05	0.86
1:J:10:LEU:HD23	1:J:10:LEU:H	1.41	0.86
1:F:179:VAL:HG12	1:F:180:ALA:N	1.89	0.86
1:C:131:LEU:CD2	1:D:131:LEU:HD23	2.05	0.86
1:F:64:TYR:HB3	1:F:74:ILE:HD13	1.57	0.86
1:B:124:THR:HG22	1:B:125:PRO:HD3	1.58	0.86
1:C:208:ILE:HG22	1:C:217:ILE:HA	1.57	0.86
1:B:124:THR:CG2	1:B:125:PRO:HD3	2.05	0.86
1:A:139:HIS:NE2	1:B:86:GLU:OE2	2.08	0.85
1:H:107:GLN:C	1:H:108:LEU:HD12	1.96	0.85
1:A:123:ASN:C	1:A:125:PRO:HD2	1.97	0.85
1:F:99:THR:HG22	1:F:100:ALA:N	1.93	0.84
1:I:124:THR:H	1:I:125:PRO:HD2	1.39	0.84
1:C:211:ASP:CG	1:C:214:GLU:O	2.15	0.84
1:C:139:HIS:CE1	1:D:86:GLU:OE2	2.30	0.84
1:B:99:THR:HG22	1:B:100:ALA:N	1.91	0.84
1:G:57:ILE:HD12	1:G:57:ILE:N	1.93	0.84
1:I:131:LEU:HD23	1:J:131:LEU:CD2	2.07	0.83
1:D:89:MET:HE1	1:D:113:ASN:HB3	1.60	0.83
1:B:91:MET:O	1:B:93:THR:HG23	1.77	0.83
1:F:57:ILE:HD12	1:F:57:ILE:N	1.93	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:131:LEU:CD2	1:D:131:LEU:CD2	2.57	0.83
1:F:124:THR:N	1:F:125:PRO:CD	2.41	0.83
1:E:6:VAL:HG11	1:H:7:HIS:HE1	1.43	0.82
1:C:57:ILE:HD12	1:C:57:ILE:N	1.95	0.82
1:A:131:LEU:HD23	1:B:131:LEU:HD21	1.60	0.82
1:D:99:THR:HG22	1:D:100:ALA:N	1.94	0.81
1:B:34:LEU:HD11	1:B:107:GLN:HE21	1.44	0.81
1:H:174:ARG:O	1:H:175:VAL:HB	1.81	0.81
1:A:138:LEU:HD23	1:A:138:LEU:C	2.01	0.81
1:H:124:THR:N	1:H:125:PRO:CD	2.44	0.81
1:E:21:SER:CB	1:E:22:PRO:HD2	2.07	0.80
1:A:128:LEU:HD23	1:A:128:LEU:C	2.02	0.80
1:C:123:ASN:O	1:C:124:THR:OG1	2.00	0.80
1:J:64:TYR:HB3	1:J:74:ILE:CD1	2.12	0.80
1:I:188:LEU:O	1:I:189:SER:OG	1.98	0.79
1:H:57:ILE:N	1:H:57:ILE:HD12	1.97	0.79
1:A:190:ILE:O	1:A:190:ILE:HD12	1.81	0.79
1:C:211:ASP:OD2	1:C:214:GLU:O	2.01	0.79
1:H:64:TYR:HB3	1:H:74:ILE:CD1	2.12	0.79
1:I:156:ARG:CB	1:I:188:LEU:CD2	2.61	0.79
1:G:191:GLN:N	1:G:192:PRO:HD2	1.98	0.78
1:E:124:THR:HB	1:E:125:PRO:CD	2.12	0.78
1:F:215:ILE:HD12	1:F:215:ILE:N	1.97	0.78
1:A:95:ASN:ND2	1:D:225:CYS:SG	2.57	0.78
1:C:10:LEU:CD2	1:I:10:LEU:CD2	2.62	0.77
1:C:67:THR:CG2	1:C:68:PRO:CD	2.57	0.77
1:C:10:LEU:CD2	1:I:10:LEU:HD23	2.14	0.77
1:I:156:ARG:CB	1:I:188:LEU:HD21	2.15	0.77
1:C:209:HIS:O	1:C:210:LEU:O	2.02	0.77
1:B:91:MET:O	1:B:93:THR:N	2.17	0.77
1:A:57:ILE:HD12	1:A:57:ILE:N	1.99	0.76
1:A:14:HIS:O	1:A:18:GLU:HG3	1.85	0.76
1:B:123:ASN:ND2	1:B:126:LEU:HB2	1.99	0.76
1:F:124:THR:N	1:F:125:PRO:HD2	1.99	0.76
1:D:89:MET:O	1:D:89:MET:HE2	1.84	0.75
1:A:190:ILE:C	1:A:190:ILE:HD12	2.06	0.75
1:E:21:SER:O	1:E:23:VAL:N	2.20	0.75
1:H:15:HIS:HB3	1:H:137:ARG:HD2	1.68	0.75
1:C:210:LEU:O	1:C:211:ASP:CB	2.34	0.75
1:C:208:ILE:O	1:C:209:HIS:HB3	1.87	0.75
1:D:89:MET:HA	1:D:89:MET:CE	2.18	0.74
1:J:194:THR:O	1:J:198:ILE:HG13	1.87	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:99:THR:CG2	1:B:100:ALA:H	2.00	0.74
1:H:81:ARG:O	1:H:82:ASN:ND2	2.19	0.74
1:F:19:PRO:HG2	1:F:130:LEU:HD23	1.70	0.74
1:C:139:HIS:HE1	1:D:86:GLU:OE2	1.69	0.74
1:I:69:GLU:O	1:I:69:GLU:OE1	2.05	0.74
1:H:66:LEU:C	1:H:67:THR:HG1	1.90	0.73
1:C:208:ILE:O	1:C:209:HIS:CB	2.35	0.73
1:J:140:GLN:O	1:J:144:GLU:HG3	1.88	0.73
1:C:210:LEU:O	1:C:211:ASP:HB2	1.86	0.73
1:H:67:THR:HB	1:H:68:PRO:CD	2.17	0.73
1:J:181:LYS:HB2	1:J:184:VAL:CG2	2.19	0.73
1:B:53:PHE:CD1	1:B:89:MET:HE2	2.23	0.73
1:G:20:LEU:HD23	1:G:119:GLN:NE2	2.03	0.73
1:I:131:LEU:HD21	1:J:131:LEU:HD23	1.70	0.72
1:C:156:ARG:HG2	1:C:188:LEU:HD13	1.70	0.72
1:I:131:LEU:HD21	1:J:131:LEU:CD2	2.19	0.72
1:I:124:THR:N	1:I:125:PRO:CD	2.52	0.72
1:B:64:TYR:HB3	1:B:74:ILE:HD13	1.72	0.72
1:J:207:ILE:HG22	1:J:207:ILE:O	1.89	0.71
1:H:34:LEU:HD21	1:H:107:GLN:HE21	1.54	0.71
1:E:18:GLU:HB3	1:E:19:PRO:HD3	1.73	0.71
1:J:123:ASN:ND2	1:J:126:LEU:CD1	2.52	0.71
1:C:121:GLN:NE2	1:E:36:ASN:ND2	2.39	0.71
1:D:108:LEU:O	1:D:108:LEU:HD12	1.90	0.71
1:F:177:ILE:N	1:F:178:PRO:HA	2.05	0.70
1:A:4:GLN:O	1:A:5:ARG:HB2	1.92	0.70
1:C:50:ALA:HA	1:C:96:TYR:CE2	2.26	0.70
1:A:64:TYR:HB3	1:A:74:ILE:HD13	1.74	0.70
1:I:70:GLY:O	1:I:71:GLN:HG2	1.92	0.70
1:C:208:ILE:C	1:C:208:ILE:CD1	2.59	0.70
1:D:21:SER:HB2	1:D:22:PRO:HD2	1.74	0.69
1:F:179:VAL:CG1	1:F:180:ALA:H	1.91	0.69
1:E:120:LEU:CD2	1:F:128:LEU:HD21	2.23	0.69
1:J:174:ARG:O	1:J:175:VAL:HB	1.92	0.69
1:J:10:LEU:CD2	1:J:10:LEU:H	2.06	0.69
1:G:184:VAL:HG22	1:G:194:THR:HG21	1.73	0.69
1:E:23:VAL:C	1:E:25:LEU:H	1.94	0.69
1:F:99:THR:CG2	1:F:100:ALA:H	2.04	0.69
1:A:124:THR:N	1:A:125:PRO:HD2	2.08	0.69
1:A:8:GLN:HG3	1:A:25:LEU:CD2	2.23	0.69
1:A:92:ASP:HB2	1:C:187:HIS:CD2	2.27	0.69
1:G:86:GLU:OE2	1:H:139:HIS:NE2	2.24	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:150:LEU:O	1:G:154:THR:HG23	1.93	0.68
1:G:124:THR:OG1	1:G:125:PRO:HD3	1.93	0.68
1:H:218:LEU:O	1:H:222:ARG:HG3	1.93	0.68
1:C:108:LEU:N	1:C:108:LEU:HD12	2.08	0.68
1:I:14:HIS:O	1:I:18:GLU:HG3	1.91	0.68
1:I:8:GLN:NE2	1:I:25:LEU:HD13	2.08	0.68
1:A:108:LEU:N	1:A:108:LEU:HD12	2.09	0.68
1:F:138:LEU:O	1:F:142:ILE:HG13	1.93	0.68
1:J:123:ASN:O	1:J:124:THR:CB	2.40	0.68
1:H:108:LEU:HD12	1:H:108:LEU:N	2.09	0.68
1:A:134:LEU:HD23	1:B:134:LEU:HD23	1.75	0.68
1:F:108:LEU:N	1:F:108:LEU:HD12	2.08	0.68
1:B:34:LEU:HD11	1:B:107:GLN:NE2	2.08	0.68
1:F:202:LEU:CD2	1:F:202:LEU:O	2.39	0.68
1:I:124:THR:H	1:I:125:PRO:CD	2.06	0.68
1:B:123:ASN:OD1	1:B:123:ASN:C	2.33	0.68
1:E:64:TYR:HB3	1:E:74:ILE:HD13	1.76	0.67
1:D:93:THR:N	1:D:94:PRO:HD3	2.10	0.67
1:A:213:ARG:HH11	1:H:30:ALA:HA	1.58	0.67
1:C:50:ALA:O	1:C:51:HIS:HB2	1.94	0.67
1:E:88:MET:CE	1:E:93:THR:HG21	2.24	0.67
1:J:64:TYR:CB	1:J:74:ILE:HD13	2.21	0.67
1:I:171:GLU:OE1	1:I:174:ARG:HD2	1.93	0.67
1:B:124:THR:N	1:B:125:PRO:CD	2.58	0.67
1:C:81:ARG:O	1:C:82:ASN:OD1	2.11	0.67
1:B:63:ILE:O	1:B:64:TYR:CG	2.48	0.67
1:J:75:LEU:N	1:J:75:LEU:HD12	2.09	0.67
1:H:64:TYR:CB	1:H:74:ILE:HD13	2.23	0.67
1:I:90:PHE:HB2	1:J:132:ALA:HB2	1.77	0.67
1:D:81:ARG:O	1:D:82:ASN:OD1	2.13	0.66
1:D:15:HIS:HB3	1:D:137:ARG:NE	2.11	0.66
1:A:131:LEU:HD21	1:B:131:LEU:HD23	1.62	0.66
1:E:122:ASP:OD1	1:E:123:ASN:N	2.27	0.66
1:J:181:LYS:HB2	1:J:184:VAL:HG23	1.77	0.66
1:G:131:LEU:HD21	1:H:131:LEU:CD2	2.24	0.66
1:D:143:ASP:O	1:D:147:THR:HG23	1.96	0.66
1:B:18:GLU:HB3	1:B:19:PRO:HD3	1.76	0.66
1:C:207:ILE:O	1:C:208:ILE:HG23	1.96	0.66
1:A:164:LEU:HD12	1:A:165:ALA:N	2.11	0.66
1:C:12:GLN:O	1:C:18:GLU:OE1	2.14	0.66
1:C:124:THR:HB	1:C:125:PRO:HD2	1.78	0.66
1:G:121:GLN:O	1:G:122:ASP:HB2	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:18:GLU:HB3	1:D:19:PRO:HD3	1.77	0.66
1:H:95:ASN:N	1:H:95:ASN:HD22	1.94	0.65
1:C:210:LEU:H	1:C:210:LEU:CD1	2.09	0.65
1:A:29:LEU:HD23	1:A:111:PHE:HE2	1.60	0.65
1:G:20:LEU:HD23	1:G:119:GLN:HE22	1.54	0.65
1:D:124:THR:HG1	1:D:125:PRO:HD3	1.57	0.65
1:J:107:GLN:C	1:J:108:LEU:HD12	2.16	0.65
1:D:99:THR:CG2	1:D:100:ALA:H	2.04	0.65
1:G:131:LEU:CD2	1:H:131:LEU:HD21	2.24	0.65
1:I:56:LEU:HA	1:I:108:LEU:HD23	1.77	0.65
1:D:123:ASN:HD22	1:D:125:PRO:HD2	1.61	0.65
1:E:52:ALA:HB2	1:E:112:SER:HA	1.78	0.65
1:C:208:ILE:CG2	1:C:217:ILE:HA	2.27	0.64
1:A:57:ILE:HD11	1:A:109:PHE:CD1	2.32	0.64
1:I:159:ARG:CZ	1:J:159:ARG:HD2	2.26	0.64
1:H:18:GLU:N	1:H:19:PRO:HD2	2.11	0.64
1:A:88:MET:HE1	1:A:93:THR:CB	2.28	0.64
1:I:138:LEU:CD1	1:J:138:LEU:CD2	2.57	0.64
1:C:207:ILE:O	1:C:208:ILE:CG2	2.45	0.64
1:J:18:GLU:OE1	1:J:133:LYS:HD2	1.97	0.64
1:E:23:VAL:C	1:E:25:LEU:N	2.51	0.64
1:B:57:ILE:N	1:B:57:ILE:CD1	2.59	0.63
1:I:20:LEU:HB2	1:I:25:LEU:HD21	1.79	0.63
1:I:64:TYR:HB3	1:I:74:ILE:HD13	1.78	0.63
1:G:40:GLY:HA2	1:G:101:GLN:HE21	1.62	0.63
1:E:52:ALA:HA	1:E:113:ASN:OD1	1.99	0.63
1:G:57:ILE:N	1:G:57:ILE:CD1	2.62	0.63
1:E:120:LEU:HD21	1:F:128:LEU:CD2	2.29	0.63
1:A:167:HIS:O	1:A:168:ALA:HB3	1.96	0.63
1:J:10:LEU:HD23	1:J:10:LEU:N	2.13	0.63
1:F:57:ILE:N	1:F:57:ILE:CD1	2.61	0.63
1:F:120:LEU:O	1:F:121:GLN:C	2.38	0.63
1:C:209:HIS:O	1:C:210:LEU:C	2.38	0.62
1:A:8:GLN:HG3	1:A:25:LEU:HD21	1.81	0.62
1:D:18:GLU:H	1:D:19:PRO:CD	2.13	0.62
1:A:152:ASN:CG	1:B:152:ASN:OD1	2.37	0.62
1:A:34:LEU:HD11	1:A:107:GLN:HE21	1.65	0.62
1:I:18:GLU:N	1:I:19:PRO:HD2	2.13	0.62
1:D:44:PHE:H	1:D:100:ALA:HB3	1.65	0.62
1:D:89:MET:CA	1:D:89:MET:CE	2.78	0.62
1:D:20:LEU:HD12	1:D:20:LEU:N	2.15	0.62
1:E:120:LEU:HD21	1:F:128:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:212:GLY:O	1:E:213:ARG:HB2	1.99	0.62
1:G:191:GLN:N	1:G:192:PRO:CD	2.62	0.62
1:H:34:LEU:HD21	1:H:107:GLN:NE2	2.15	0.61
1:A:164:LEU:C	1:A:164:LEU:HD12	2.21	0.61
1:I:124:THR:CG2	1:I:125:PRO:HD3	2.29	0.61
1:A:18:GLU:HB2	1:A:19:PRO:HD3	1.81	0.61
1:C:57:ILE:CD1	1:C:57:ILE:N	2.63	0.61
1:F:124:THR:H	1:F:125:PRO:CD	2.11	0.61
1:B:164:LEU:HD11	1:B:177:ILE:HB	1.81	0.61
1:H:94:PRO:C	1:H:95:ASN:HD22	2.03	0.61
1:I:120:LEU:HD11	1:I:127:ALA:HB2	1.82	0.61
1:I:138:LEU:HD13	1:J:138:LEU:HD21	1.74	0.61
1:F:177:ILE:H	1:F:178:PRO:HA	1.66	0.61
1:H:158:VAL:O	1:H:162:LEU:CB	2.44	0.61
1:E:88:MET:HE1	1:E:93:THR:HG21	1.82	0.60
1:J:84:PHE:O	1:J:85:ALA:HB3	2.00	0.60
1:C:123:ASN:N	1:C:123:ASN:HD22	1.99	0.60
1:G:11:LEU:O	1:G:17:PHE:HB2	2.00	0.60
1:G:153:ALA:O	1:G:157:VAL:HG23	2.02	0.60
1:A:153:ALA:O	1:A:157:VAL:HG23	2.00	0.60
1:J:156:ARG:HB2	1:J:191:GLN:NE2	2.16	0.60
1:J:108:LEU:HD12	1:J:108:LEU:N	2.15	0.60
1:J:151:LYS:O	1:J:155:HIS:CD2	2.54	0.60
1:A:36:ASN:OD1	1:A:107:GLN:HG3	2.02	0.60
1:A:124:THR:N	1:A:125:PRO:CD	2.63	0.60
1:E:52:ALA:HB1	1:E:111:PHE:O	2.01	0.60
1:I:159:ARG:NE	1:J:159:ARG:HD2	2.16	0.60
1:H:141:ARG:O	1:H:145:ILE:HG13	2.00	0.60
1:J:138:LEU:O	1:J:142:ILE:HG13	2.02	0.60
1:H:174:ARG:O	1:H:175:VAL:CB	2.47	0.60
1:A:15:HIS:CE1	1:A:16:LEU:HG	2.37	0.60
1:G:67:THR:HB	1:G:68:PRO:HD2	1.82	0.60
1:J:57:ILE:HD11	1:J:109:PHE:CE1	2.37	0.60
1:F:215:ILE:N	1:F:215:ILE:CD1	2.65	0.59
1:D:123:ASN:ND2	1:D:125:PRO:HD2	2.17	0.59
1:C:34:LEU:O	1:C:35:VAL:HB	2.02	0.59
1:C:157:VAL:HG11	1:C:198:ILE:HG21	1.84	0.59
1:I:29:LEU:HD23	1:I:111:PHE:HE2	1.68	0.59
1:I:156:ARG:HB2	1:I:188:LEU:HD22	1.82	0.59
1:A:57:ILE:HD11	1:A:109:PHE:HD1	1.67	0.59
1:G:15:HIS:CE1	1:G:16:LEU:HG	2.38	0.59
1:B:108:LEU:HD12	1:B:108:LEU:N	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:197:ARG:O	1:J:201:ARG:HG3	2.03	0.59
1:D:75:LEU:N	1:D:75:LEU:HD12	2.17	0.59
1:A:190:ILE:CD1	1:A:190:ILE:C	2.70	0.59
1:C:68:PRO:O	1:C:69:GLU:HB2	2.03	0.59
1:B:124:THR:H	1:B:125:PRO:HD3	1.67	0.59
1:B:150:LEU:O	1:B:154:THR:HG23	2.03	0.59
1:J:190:ILE:HG22	1:J:190:ILE:O	2.01	0.59
1:J:124:THR:HG1	1:J:125:PRO:HD3	1.61	0.59
1:A:88:MET:HE1	1:A:93:THR:OG1	2.03	0.59
1:E:68:PRO:HG2	1:E:69:GLU:OE1	2.03	0.59
1:J:34:LEU:HD11	1:J:107:GLN:HE21	1.67	0.58
1:D:84:PHE:O	1:D:85:ALA:HB3	2.03	0.58
1:E:188:LEU:O	1:E:189:SER:OG	2.21	0.58
1:E:107:GLN:HE22	1:H:6:VAL:HG22	1.67	0.58
1:A:128:LEU:CD2	1:A:128:LEU:C	2.71	0.58
1:A:67:THR:HB	1:A:68:PRO:HD2	1.85	0.58
1:B:124:THR:H	1:B:125:PRO:CD	2.16	0.58
1:A:19:PRO:HG2	1:A:130:LEU:HD23	1.85	0.58
1:E:57:ILE:O	1:H:9:GLN:NE2	2.36	0.58
1:A:81:ARG:O	1:A:82:ASN:OD1	2.21	0.58
1:F:56:LEU:C	1:F:57:ILE:HD12	2.24	0.58
1:J:179:VAL:O	1:J:179:VAL:HG12	2.04	0.58
1:J:141:ARG:O	1:J:145:ILE:HG13	2.04	0.57
1:F:66:LEU:HD12	1:F:66:LEU:C	2.24	0.57
1:A:57:ILE:CD1	1:A:57:ILE:N	2.67	0.57
1:G:14:HIS:O	1:G:18:GLU:HG3	2.04	0.57
1:B:123:ASN:ND2	1:B:126:LEU:CB	2.66	0.57
1:B:53:PHE:CD1	1:B:89:MET:HE3	2.36	0.57
1:G:210:LEU:HD11	1:G:215:ILE:HD12	1.87	0.57
1:G:190:ILE:CG2	1:G:192:PRO:CD	2.65	0.57
1:C:208:ILE:HD12	1:C:208:ILE:O	2.05	0.57
1:A:138:LEU:C	1:A:138:LEU:CD2	2.72	0.57
1:A:3:PHE:CD1	1:A:3:PHE:N	2.73	0.57
1:D:4:GLN:HB2	1:D:7:HIS:HD2	1.70	0.57
1:G:49:PRO:HA	1:G:95:ASN:HD22	1.68	0.57
1:F:153:ALA:O	1:F:157:VAL:HG23	2.05	0.57
1:I:139:HIS:CE1	1:J:86:GLU:OE2	2.58	0.57
1:J:124:THR:CB	1:J:125:PRO:HD3	2.32	0.56
1:G:70:GLY:O	1:G:71:GLN:HB2	2.04	0.56
1:E:156:ARG:O	1:E:188:LEU:HD13	2.06	0.56
1:B:217:ILE:HD13	1:B:223:LEU:HD11	1.86	0.56
1:I:50:ALA:HA	1:I:96:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:21:SER:C	1:E:23:VAL:N	2.59	0.56
1:I:138:LEU:HB2	1:J:138:LEU:HD21	1.86	0.56
1:A:213:ARG:HH12	1:H:30:ALA:HA	1.66	0.56
1:I:69:GLU:O	1:I:70:GLY:C	2.43	0.56
1:I:123:ASN:HD22	1:I:126:LEU:HD12	1.70	0.56
1:A:124:THR:O	1:A:126:LEU:N	2.39	0.56
1:G:132:ALA:O	1:G:136:THR:HG23	2.06	0.56
1:A:133:LYS:HA	1:A:136:THR:HG22	1.88	0.56
1:F:66:LEU:CD1	1:F:66:LEU:O	2.53	0.56
1:G:124:THR:N	1:G:125:PRO:CD	2.69	0.56
1:J:62:LYS:HZ2	1:J:101:GLN:HB3	1.70	0.56
1:I:67:THR:OG1	1:I:68:PRO:HD2	2.06	0.56
1:D:63:ILE:O	1:D:64:TYR:CD1	2.60	0.55
1:B:63:ILE:O	1:B:64:TYR:CD1	2.59	0.55
1:G:18:GLU:N	1:G:19:PRO:CD	2.69	0.55
1:D:188:LEU:O	1:D:189:SER:C	2.45	0.55
1:H:154:THR:O	1:H:158:VAL:HG23	2.06	0.55
1:B:119:GLN:O	1:B:126:LEU:HD23	2.07	0.55
1:F:18:GLU:HB3	1:F:19:PRO:HD3	1.88	0.55
1:A:63:ILE:O	1:A:64:TYR:O	2.24	0.55
1:H:217:ILE:HG22	1:H:218:LEU:HG	1.87	0.55
1:H:138:LEU:O	1:H:142:ILE:HG13	2.06	0.55
1:E:21:SER:C	1:E:23:VAL:H	2.10	0.55
1:B:124:THR:CG2	1:B:125:PRO:CD	2.84	0.55
1:I:8:GLN:HE22	1:I:25:LEU:HD13	1.70	0.55
1:I:140:GLN:O	1:I:144:GLU:HG3	2.06	0.55
1:H:214:GLU:N	1:H:214:GLU:OE1	2.40	0.55
1:A:140:GLN:O	1:A:144:GLU:HG3	2.06	0.55
1:H:175:VAL:HG12	1:H:176:GLU:N	2.21	0.55
1:G:151:LYS:O	1:G:155:HIS:CD2	2.59	0.55
1:A:84:PHE:O	1:A:85:ALA:HB3	2.06	0.55
1:F:150:LEU:O	1:F:154:THR:HG23	2.06	0.55
1:H:144:GLU:HA	1:H:147:THR:HG22	1.88	0.55
1:C:39:LYS:HB3	1:C:105:PRO:HD3	1.89	0.55
1:C:131:LEU:CD2	1:D:131:LEU:HD21	2.36	0.54
1:H:140:GLN:O	1:H:144:GLU:HG3	2.07	0.54
1:G:79:ASN:CG	1:G:80:GLU:H	2.10	0.54
1:G:57:ILE:HD11	1:G:109:PHE:HD1	1.72	0.54
1:H:89:MET:HG2	1:H:117:LEU:HD21	1.89	0.54
1:I:124:THR:HG22	1:I:125:PRO:HD3	1.89	0.54
1:D:108:LEU:C	1:D:108:LEU:HD12	2.28	0.54
1:D:18:GLU:H	1:D:19:PRO:HD2	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:18:GLU:N	1:J:19:PRO:HD2	2.23	0.54
1:A:4:GLN:O	1:A:5:ARG:CB	2.56	0.54
1:E:45:ARG:HA	1:E:99:THR:HG23	1.88	0.54
1:I:131:LEU:CD2	1:J:131:LEU:HD21	2.36	0.54
1:A:8:GLN:HG3	1:A:25:LEU:HD23	1.90	0.54
1:H:45:ARG:HA	1:H:99:THR:HG23	1.88	0.54
1:J:196:SER:O	1:J:200:HIS:CD2	2.61	0.54
1:F:108:LEU:N	1:F:108:LEU:CD1	2.70	0.53
1:D:15:HIS:CE1	1:D:16:LEU:HG	2.43	0.53
1:J:43:VAL:HG12	1:J:44:PHE:HD1	1.73	0.53
1:H:108:LEU:N	1:H:108:LEU:CD1	2.71	0.53
1:J:57:ILE:HD11	1:J:109:PHE:CD1	2.43	0.53
1:C:207:ILE:C	1:C:208:ILE:HG23	2.29	0.53
1:I:8:GLN:HE22	1:I:25:LEU:HB3	1.73	0.53
1:I:43:VAL:HG12	1:I:44:PHE:HD1	1.73	0.53
1:A:141:ARG:O	1:A:145:ILE:HG13	2.09	0.53
1:C:65:ARG:HD3	1:C:65:ARG:O	2.09	0.53
1:E:21:SER:HB3	1:G:191:GLN:CD	2.29	0.53
1:D:148:LEU:C	1:D:148:LEU:HD12	2.27	0.53
1:B:50:ALA:HA	1:B:96:TYR:CE2	2.44	0.53
1:E:6:VAL:CG1	1:H:7:HIS:HE1	2.17	0.53
1:G:57:ILE:HD11	1:G:109:PHE:CD1	2.44	0.53
1:E:119:GLN:H	1:E:119:GLN:NE2	2.07	0.53
1:D:64:TYR:HA	1:D:74:ILE:HA	1.91	0.53
1:H:122:ASP:O	1:H:123:ASN:HB2	2.09	0.53
1:H:57:ILE:N	1:H:57:ILE:CD1	2.65	0.53
1:C:212:GLY:O	1:C:214:GLU:N	2.42	0.53
1:H:18:GLU:N	1:H:19:PRO:CD	2.72	0.53
1:C:124:THR:C	1:C:126:LEU:H	2.13	0.52
1:E:14:HIS:HD2	1:E:16:LEU:H	1.56	0.52
1:H:167:HIS:HB3	1:H:219:ASP:HB2	1.92	0.52
1:F:63:ILE:O	1:F:64:TYR:O	2.27	0.52
1:F:18:GLU:N	1:F:19:PRO:CD	2.71	0.52
1:B:59:GLY:HA3	1:B:106:SER:OG	2.09	0.52
1:C:210:LEU:N	1:C:210:LEU:HD12	2.17	0.52
1:H:175:VAL:CG1	1:H:176:GLU:N	2.72	0.52
1:I:3:PHE:O	1:I:4:GLN:HB2	2.10	0.52
1:J:130:LEU:C	1:J:130:LEU:HD23	2.30	0.52
1:E:217:ILE:HG12	1:E:218:LEU:N	2.25	0.52
1:F:75:LEU:N	1:F:75:LEU:HD12	2.25	0.52
1:J:195:PHE:O	1:J:199:MET:HG2	2.10	0.52
1:C:50:ALA:HA	1:C:96:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:75:LEU:HD12	1:G:75:LEU:N	2.24	0.52
1:C:19:PRO:CG	1:C:130:LEU:HD23	2.33	0.52
1:A:128:LEU:HD21	1:B:90:PHE:C	2.29	0.52
1:D:15:HIS:HB3	1:D:137:ARG:CD	2.40	0.52
1:C:38:ASP:OD1	1:C:39:LYS:N	2.36	0.52
1:D:74:ILE:C	1:D:75:LEU:HD12	2.30	0.52
1:B:124:THR:HG23	1:B:125:PRO:HD3	1.90	0.52
1:A:88:MET:CE	1:A:93:THR:OG1	2.57	0.52
1:J:156:ARG:HB2	1:J:191:GLN:HE22	1.73	0.52
1:D:89:MET:HE2	1:D:89:MET:C	2.30	0.51
1:C:108:LEU:CD1	1:C:108:LEU:N	2.72	0.51
1:E:120:LEU:HD23	1:F:128:LEU:HD21	1.92	0.51
1:D:20:LEU:H	1:D:20:LEU:CD1	2.22	0.51
1:E:14:HIS:CD2	1:E:16:LEU:H	2.28	0.51
1:F:44:PHE:HE1	1:F:84:PHE:HE2	1.58	0.51
1:B:217:ILE:HD13	1:B:223:LEU:CD1	2.39	0.51
1:G:84:PHE:O	1:G:85:ALA:HB3	2.09	0.51
1:A:207:ILE:HG21	1:A:223:LEU:HD21	1.92	0.51
1:H:65:ARG:O	1:H:66:LEU:HB2	2.09	0.51
1:D:51:HIS:O	1:D:52:ALA:HB3	2.11	0.51
1:G:50:ALA:HA	1:G:96:TYR:CE2	2.45	0.51
1:J:174:ARG:O	1:J:175:VAL:CB	2.57	0.51
1:E:67:THR:HB	1:E:68:PRO:HD2	1.91	0.51
1:C:4:GLN:HB2	1:C:7:HIS:HD2	1.74	0.51
1:B:53:PHE:CE1	1:B:89:MET:HE2	2.39	0.51
1:C:10:LEU:HD21	1:I:10:LEU:HG	1.93	0.51
1:B:57:ILE:HD11	1:B:109:PHE:HD1	1.76	0.51
1:G:124:THR:N	1:G:125:PRO:HD2	2.25	0.51
1:D:63:ILE:O	1:D:64:TYR:O	2.29	0.51
1:A:108:LEU:CD1	1:A:108:LEU:N	2.73	0.51
1:C:33:ASP:OD1	1:C:34:LEU:N	2.43	0.51
1:I:131:LEU:HD22	1:J:130:LEU:HD22	1.92	0.51
1:D:20:LEU:HD12	1:D:20:LEU:H	1.76	0.51
1:G:132:ALA:HB2	1:H:90:PHE:HB2	1.93	0.51
1:I:150:LEU:O	1:I:154:THR:HG23	2.11	0.51
1:H:20:LEU:HD23	1:H:126:LEU:HD11	1.92	0.51
1:D:124:THR:OG1	1:D:125:PRO:CD	2.41	0.51
1:C:11:LEU:O	1:C:17:PHE:HB2	2.11	0.51
1:A:202:LEU:HD13	1:A:208:ILE:HD12	1.93	0.51
1:E:88:MET:HE3	1:E:93:THR:HG21	1.92	0.50
1:F:143:ASP:O	1:F:147:THR:HG23	2.10	0.50
1:J:19:PRO:HD3	1:J:133:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:10:LEU:HD23	1:I:10:LEU:HD21	1.89	0.50
1:G:190:ILE:HG22	1:G:191:GLN:N	2.26	0.50
1:I:18:GLU:N	1:I:19:PRO:CD	2.74	0.50
1:H:75:LEU:N	1:H:75:LEU:HD12	2.26	0.50
1:D:97:VAL:HG22	1:D:97:VAL:O	2.10	0.50
1:C:131:LEU:HG	1:D:131:LEU:HD21	1.93	0.50
1:C:141:ARG:O	1:C:145:ILE:HG13	2.11	0.50
1:J:18:GLU:N	1:J:19:PRO:CD	2.75	0.50
1:C:29:LEU:HD23	1:C:111:PHE:HE2	1.76	0.50
1:E:25:LEU:HD12	1:E:25:LEU:N	2.26	0.50
1:F:202:LEU:HD23	1:F:202:LEU:C	2.29	0.50
1:F:124:THR:H	1:F:125:PRO:HD3	1.77	0.50
1:D:144:GLU:O	1:D:148:LEU:HG	2.12	0.50
1:J:75:LEU:N	1:J:75:LEU:CD1	2.75	0.50
1:G:202:LEU:HD21	1:G:209:HIS:HB2	1.93	0.50
1:E:123:ASN:O	1:E:124:THR:C	2.50	0.50
1:J:7:HIS:HA	1:J:10:LEU:HD21	1.94	0.50
1:G:151:LYS:O	1:G:155:HIS:HD2	1.93	0.50
1:I:3:PHE:HB2	1:I:4:GLN:OE1	2.12	0.50
1:I:84:PHE:O	1:I:85:ALA:HB3	2.11	0.50
1:C:202:LEU:C	1:C:202:LEU:HD12	2.32	0.50
1:H:88:MET:HA	1:H:91:MET:HB2	1.94	0.50
1:A:131:LEU:CG	1:B:131:LEU:HD21	2.42	0.49
1:H:63:ILE:O	1:H:64:TYR:O	2.30	0.49
1:I:155:HIS:CA	1:I:159:ARG:NH1	2.75	0.49
1:D:91:MET:O	1:D:92:ASP:HB2	2.12	0.49
1:H:189:SER:OG	1:H:194:THR:HG23	2.12	0.49
1:F:177:ILE:HB	1:F:178:PRO:C	2.32	0.49
1:F:177:ILE:HG21	1:F:179:VAL:O	2.12	0.49
1:G:67:THR:CB	1:G:68:PRO:HD2	2.42	0.49
1:A:172:ASN:HB2	1:A:217:ILE:HB	1.94	0.49
1:G:63:ILE:HG22	1:G:98:ALA:HB1	1.93	0.49
1:E:152:ASN:CG	1:F:152:ASN:ND2	2.66	0.49
1:D:15:HIS:HB3	1:D:137:ARG:HD2	1.94	0.49
1:G:140:GLN:O	1:G:144:GLU:HG2	2.13	0.49
1:A:212:GLY:O	1:A:213:ARG:HB3	2.13	0.49
1:B:50:ALA:H	1:B:95:ASN:HA	1.76	0.49
1:J:150:LEU:O	1:J:154:THR:HG23	2.12	0.49
1:B:124:THR:HG23	1:B:125:PRO:CD	2.42	0.49
1:A:185:ALA:HB1	1:A:190:ILE:HD11	1.95	0.49
1:J:221:GLU:OE1	1:J:221:GLU:N	2.45	0.49
1:F:63:ILE:O	1:F:64:TYR:CG	2.66	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:124:THR:HB	1:C:125:PRO:CD	2.41	0.49
1:I:15:HIS:CE1	1:I:16:LEU:HG	2.47	0.49
1:B:158:VAL:O	1:B:158:VAL:HG12	2.13	0.49
1:G:57:ILE:H	1:G:57:ILE:HD12	1.75	0.49
1:A:49:PRO:HA	1:A:95:ASN:OD1	2.13	0.49
1:C:157:VAL:HG13	1:C:158:VAL:N	2.28	0.49
1:C:59:GLY:HA3	1:C:106:SER:OG	2.12	0.49
1:C:57:ILE:HD13	1:C:107:GLN:O	2.13	0.48
1:J:130:LEU:CD2	1:J:130:LEU:O	2.51	0.48
1:I:124:THR:HG23	1:I:125:PRO:HD3	1.95	0.48
1:I:19:PRO:HG3	1:I:130:LEU:HD23	1.94	0.48
1:G:144:GLU:OE2	1:H:145:ILE:CG1	2.61	0.48
1:G:164:LEU:HD13	1:G:172:ASN:HB3	1.95	0.48
1:D:176:GLU:O	1:D:177:ILE:C	2.52	0.48
1:A:50:ALA:HA	1:A:96:TYR:CE2	2.49	0.48
1:G:131:LEU:HD22	1:H:130:LEU:HD22	1.96	0.48
1:A:34:LEU:HD11	1:A:107:GLN:NE2	2.28	0.48
1:I:151:LYS:O	1:I:155:HIS:CD2	2.66	0.48
1:A:154:THR:HA	1:A:198:ILE:HD13	1.94	0.48
1:C:91:MET:O	1:C:93:THR:HG23	2.13	0.48
1:B:44:PHE:H	1:B:100:ALA:HB3	1.79	0.48
1:D:93:THR:H	1:D:94:PRO:HD3	1.75	0.48
1:F:66:LEU:CD1	1:F:66:LEU:C	2.82	0.48
1:D:93:THR:N	1:D:94:PRO:CD	2.76	0.48
1:E:52:ALA:CB	1:E:112:SER:HA	2.44	0.48
1:B:213:ARG:O	1:B:214:GLU:O	2.31	0.48
1:G:68:PRO:O	1:G:69:GLU:HB2	2.13	0.47
1:G:19:PRO:HG3	1:G:133:LYS:HG3	1.95	0.47
1:B:188:LEU:O	1:B:189:SER:OG	2.28	0.47
1:A:167:HIS:O	1:A:168:ALA:CB	2.62	0.47
1:C:208:ILE:CD1	1:C:209:HIS:N	2.77	0.47
1:A:88:MET:HE1	1:A:93:THR:HG21	1.97	0.47
1:J:123:ASN:C	1:J:125:PRO:HD2	2.35	0.47
1:J:151:LYS:O	1:J:155:HIS:HD2	1.96	0.47
1:C:6:VAL:HG22	1:I:57:ILE:HD13	1.97	0.47
1:J:3:PHE:HE2	1:J:34:LEU:HD22	1.79	0.47
1:G:18:GLU:HB2	1:G:19:PRO:HD3	1.96	0.47
1:C:43:VAL:HG12	1:C:44:PHE:HD1	1.80	0.47
1:H:204:ASP:O	1:H:205:GLU:HB2	2.14	0.47
1:H:80:GLU:O	1:H:81:ARG:HB2	2.15	0.47
1:F:44:PHE:H	1:F:100:ALA:HB3	1.80	0.47
1:C:213:ARG:O	1:C:214:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:20:LEU:N	1:D:20:LEU:CD1	2.76	0.47
1:F:66:LEU:HD13	1:F:66:LEU:O	2.14	0.47
1:I:86:GLU:OE1	1:I:86:GLU:N	2.38	0.47
1:D:75:LEU:N	1:D:75:LEU:CD1	2.78	0.47
1:C:210:LEU:N	1:C:210:LEU:CD1	2.77	0.47
1:G:63:ILE:O	1:G:64:TYR:CG	2.68	0.47
1:D:73:LYS:HD2	1:D:75:LEU:HD11	1.97	0.47
1:C:124:THR:C	1:C:126:LEU:N	2.68	0.47
1:J:108:LEU:CD1	1:J:108:LEU:N	2.78	0.47
1:C:124:THR:O	1:C:126:LEU:N	2.47	0.46
1:G:40:GLY:HA2	1:G:101:GLN:NE2	2.27	0.46
1:G:94:PRO:O	1:G:95:ASN:ND2	2.47	0.46
1:E:15:HIS:ND1	1:E:16:LEU:HG	2.30	0.46
1:J:123:ASN:O	1:J:125:PRO:HD3	2.15	0.46
1:F:177:ILE:HB	1:F:178:PRO:CA	2.45	0.46
1:H:135:SER:O	1:H:139:HIS:HD2	1.98	0.46
1:G:18:GLU:OE1	1:G:133:LYS:HD2	2.15	0.46
1:F:135:SER:O	1:F:139:HIS:HD2	1.97	0.46
1:B:91:MET:O	1:B:92:ASP:C	2.51	0.46
1:G:117:LEU:O	1:G:121:GLN:HG3	2.16	0.46
1:H:88:MET:CE	1:H:96:TYR:HA	2.45	0.46
1:J:88:MET:CE	1:J:93:THR:OG1	2.63	0.46
1:I:127:ALA:O	1:I:131:LEU:HG	2.15	0.46
1:A:135:SER:O	1:A:139:HIS:CD2	2.69	0.46
1:B:18:GLU:N	1:B:19:PRO:CD	2.79	0.46
1:G:1:MET:O	1:G:2:GLU:HB2	2.16	0.46
1:A:177:ILE:C	1:A:179:VAL:H	2.19	0.46
1:A:188:LEU:O	1:A:189:SER:OG	2.30	0.46
1:A:207:ILE:HG21	1:A:223:LEU:CD2	2.46	0.46
1:I:69:GLU:C	1:I:69:GLU:OE1	2.53	0.46
1:A:64:TYR:CB	1:A:74:ILE:HD13	2.43	0.46
1:G:196:SER:O	1:G:200:HIS:ND1	2.49	0.46
1:F:16:LEU:HD11	1:F:86:GLU:OE1	2.16	0.46
1:A:124:THR:C	1:A:126:LEU:N	2.69	0.46
1:F:214:GLU:C	1:F:215:ILE:HD12	2.34	0.46
1:I:56:LEU:HD13	1:I:108:LEU:HD21	1.98	0.46
1:E:116:TYR:HA	1:E:119:GLN:HE22	1.80	0.46
1:J:6:VAL:HG22	1:J:6:VAL:O	2.14	0.46
1:J:81:ARG:O	1:J:82:ASN:OD1	2.34	0.46
1:I:59:GLY:HA3	1:I:106:SER:OG	2.16	0.46
1:A:124:THR:O	1:A:127:ALA:N	2.49	0.45
1:H:123:ASN:C	1:H:125:PRO:CD	2.78	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:123:ASN:CA	1:H:125:PRO:HD2	2.46	0.45
1:J:132:ALA:O	1:J:136:THR:HG23	2.16	0.45
1:H:84:PHE:O	1:H:85:ALA:HB3	2.15	0.45
1:F:177:ILE:N	1:F:178:PRO:CA	2.78	0.45
1:B:56:LEU:C	1:B:57:ILE:HD12	2.36	0.45
1:A:190:ILE:HD13	1:A:191:GLN:O	2.16	0.45
1:G:216:SER:OG	1:G:219:ASP:OD1	2.34	0.45
1:A:138:LEU:O	1:A:142:ILE:HG13	2.15	0.45
1:H:63:ILE:O	1:H:64:TYR:CD1	2.69	0.45
1:D:18:GLU:N	1:D:19:PRO:CD	2.77	0.45
1:F:47:GLY:HA2	1:H:224:GLU:HG2	1.97	0.45
1:A:131:LEU:HD21	1:B:131:LEU:CG	2.47	0.45
1:J:18:GLU:HB2	1:J:19:PRO:HD3	1.98	0.45
1:H:158:VAL:HG21	1:H:225:CYS:HB3	1.98	0.45
1:J:15:HIS:CE1	1:J:16:LEU:HG	2.52	0.45
1:B:99:THR:CG2	1:B:100:ALA:N	2.63	0.45
1:E:184:VAL:HG21	1:E:195:PHE:CZ	2.51	0.45
1:E:159:ARG:O	1:E:163:THR:HG23	2.16	0.45
1:H:63:ILE:O	1:H:64:TYR:CG	2.70	0.45
1:A:164:LEU:CD1	1:A:164:LEU:C	2.84	0.45
1:J:213:ARG:O	1:J:215:ILE:N	2.42	0.45
1:H:25:LEU:O	1:H:29:LEU:HG	2.17	0.45
1:I:124:THR:CG2	1:I:125:PRO:CD	2.95	0.45
1:H:57:ILE:HD11	1:H:109:PHE:HD1	1.82	0.45
1:F:202:LEU:CD2	1:F:202:LEU:C	2.85	0.44
1:E:88:MET:HE3	1:E:93:THR:CG2	2.47	0.44
1:E:15:HIS:CE1	1:E:16:LEU:HG	2.52	0.44
1:I:93:THR:HA	1:I:94:PRO:HD3	1.87	0.44
1:A:43:VAL:HG12	1:A:44:PHE:HD1	1.81	0.44
1:F:11:LEU:HD22	1:F:11:LEU:N	2.32	0.44
1:B:84:PHE:O	1:B:85:ALA:HB3	2.15	0.44
1:A:212:GLY:C	1:A:214:GLU:H	2.21	0.44
1:A:18:GLU:N	1:A:19:PRO:CD	2.80	0.44
1:D:108:LEU:CD1	1:D:108:LEU:C	2.86	0.44
1:J:34:LEU:HD11	1:J:107:GLN:NE2	2.30	0.44
1:G:137:ARG:HB2	1:H:138:LEU:HD13	1.99	0.44
1:C:63:ILE:HD11	1:C:84:PHE:CD2	2.52	0.44
1:H:177:ILE:HA	1:H:178:PRO:HD3	1.85	0.44
1:I:90:PHE:HD2	1:J:128:LEU:HB3	1.83	0.44
1:I:155:HIS:HB3	1:I:159:ARG:NH1	2.32	0.44
1:B:22:PRO:O	1:B:26:GLN:HG2	2.17	0.44
1:H:43:VAL:HG12	1:H:44:PHE:HD1	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:183:LEU:HD22	1:J:193:GLU:HB3	2.00	0.44
1:C:61:VAL:HG22	1:C:102:ALA:HB2	2.00	0.44
1:D:103:VAL:O	1:D:103:VAL:HG23	2.17	0.44
1:C:90:PHE:HB3	1:D:128:LEU:HB3	1.99	0.44
1:B:108:LEU:CD1	1:B:108:LEU:N	2.80	0.44
1:C:87:ALA:O	1:C:91:MET:HB2	2.18	0.44
1:A:67:THR:CB	1:A:68:PRO:HD2	2.48	0.44
1:E:55:TYR:CE1	1:E:57:ILE:HD13	2.52	0.44
1:B:57:ILE:HD12	1:B:57:ILE:H	1.79	0.43
1:D:79:ASN:ND2	1:D:80:GLU:H	2.16	0.43
1:G:3:PHE:O	1:G:4:GLN:HB2	2.18	0.43
1:J:172:ASN:O	1:J:173:CYS:C	2.57	0.43
1:A:124:THR:O	1:A:125:PRO:C	2.55	0.43
1:D:68:PRO:O	1:D:69:GLU:C	2.56	0.43
1:J:144:GLU:O	1:J:148:LEU:HG	2.19	0.43
1:G:137:ARG:CB	1:H:138:LEU:HD13	2.47	0.43
1:J:88:MET:HE3	1:J:93:THR:OG1	2.18	0.43
1:C:57:ILE:HD11	1:C:109:PHE:CD1	2.53	0.43
1:E:124:THR:CB	1:E:125:PRO:HD3	2.20	0.43
1:C:67:THR:HG22	1:C:68:PRO:N	2.33	0.43
1:G:121:GLN:O	1:G:122:ASP:CB	2.65	0.43
1:E:212:GLY:O	1:E:213:ARG:CB	2.63	0.43
1:J:57:ILE:HD11	1:J:109:PHE:HE1	1.83	0.43
1:G:79:ASN:H	1:G:82:ASN:HD21	1.66	0.43
1:E:139:HIS:HE1	1:F:86:GLU:HG2	1.83	0.43
1:H:95:ASN:ND2	1:H:95:ASN:N	2.64	0.43
1:E:49:PRO:HA	1:E:95:ASN:HD22	1.84	0.43
1:G:143:ASP:O	1:G:147:THR:HG23	2.18	0.43
1:E:18:GLU:N	1:E:19:PRO:CD	2.81	0.43
1:D:67:THR:OG1	1:D:68:PRO:HD2	2.18	0.43
1:C:45:ARG:HA	1:C:99:THR:HG23	2.00	0.43
1:I:80:GLU:OE1	1:I:80:GLU:N	2.41	0.43
1:C:212:GLY:O	1:C:213:ARG:C	2.57	0.43
1:A:3:PHE:HB2	1:A:4:GLN:H	1.53	0.43
1:I:19:PRO:CG	1:I:130:LEU:HD23	2.49	0.43
1:D:11:LEU:HD23	1:D:55:TYR:CZ	2.54	0.43
1:A:131:LEU:HG	1:B:131:LEU:HD21	2.00	0.43
1:C:57:ILE:H	1:C:57:ILE:HD12	1.79	0.43
1:F:63:ILE:HG23	1:F:99:THR:O	2.19	0.43
1:C:208:ILE:HD12	1:C:209:HIS:N	2.34	0.43
1:A:14:HIS:HB3	1:A:17:PHE:HD1	1.84	0.43
1:I:8:GLN:NE2	1:I:25:LEU:CD1	2.78	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:LEU:HD21	1:A:142:ILE:HD11	2.00	0.42
1:D:73:LYS:HA	1:J:74:ILE:HB	2.01	0.42
1:C:38:ASP:OD1	1:C:105:PRO:HG3	2.18	0.42
1:B:151:LYS:O	1:B:155:HIS:ND1	2.52	0.42
1:C:15:HIS:CE1	1:C:16:LEU:HG	2.55	0.42
1:C:65:ARG:O	1:C:66:LEU:HB2	2.18	0.42
1:J:227:GLU:C	1:J:227:GLU:CD	2.78	0.42
1:J:134:LEU:O	1:J:138:LEU:HG	2.17	0.42
1:A:207:ILE:CG2	1:A:223:LEU:HD21	2.49	0.42
1:I:86:GLU:OE2	1:J:139:HIS:CE1	2.72	0.42
1:D:148:LEU:HD12	1:D:149:SER:H	1.78	0.42
1:I:159:ARG:NH2	1:J:159:ARG:HD2	2.33	0.42
1:A:61:VAL:HG21	1:A:108:LEU:HD21	2.02	0.42
1:C:18:GLU:CB	1:C:19:PRO:HD3	2.27	0.42
1:C:159:ARG:O	1:C:163:THR:HG23	2.18	0.42
1:D:89:MET:O	1:D:89:MET:CE	2.59	0.42
1:C:206:GLY:O	1:C:219:ASP:OD2	2.37	0.42
1:B:55:TYR:CE1	1:B:57:ILE:HG13	2.54	0.42
1:G:187:HIS:O	1:G:188:LEU:HB2	2.20	0.42
1:A:187:HIS:HD2	1:C:91:MET:HA	1.84	0.42
1:D:50:ALA:HA	1:D:96:TYR:CE2	2.55	0.42
1:J:28:LEU:HB2	1:J:119:GLN:HE22	1.84	0.42
1:D:89:MET:HE1	1:D:113:ASN:CB	2.41	0.42
1:C:220:ARG:O	1:C:221:GLU:HB2	2.20	0.42
1:E:21:SER:HB3	1:G:191:GLN:OE1	2.20	0.42
1:F:15:HIS:CE1	1:F:16:LEU:HG	2.54	0.42
1:B:15:HIS:CE1	1:B:16:LEU:HG	2.55	0.42
1:H:21:SER:HB2	1:H:22:PRO:HD2	2.01	0.42
1:J:37:LEU:HB3	1:J:41:ALA:HB3	2.02	0.42
1:A:91:MET:O	1:A:92:ASP:HB2	2.20	0.42
1:I:155:HIS:HA	1:I:159:ARG:HH12	1.84	0.42
1:J:63:ILE:HD11	1:J:84:PHE:CD2	2.55	0.42
1:C:157:VAL:O	1:C:161:LEU:HG	2.20	0.42
1:C:29:LEU:HD23	1:C:111:PHE:CE2	2.54	0.42
1:A:103:VAL:HG23	1:A:104:VAL:HG13	2.02	0.42
1:B:55:TYR:HD2	1:B:83:THR:HG22	1.85	0.41
1:G:75:LEU:CD1	1:G:75:LEU:N	2.83	0.41
1:H:75:LEU:CD1	1:H:75:LEU:N	2.83	0.41
1:J:223:LEU:O	1:J:227:GLU:HB3	2.20	0.41
1:H:88:MET:HE1	1:H:96:TYR:HA	2.03	0.41
1:B:25:LEU:O	1:B:29:LEU:HG	2.20	0.41
1:C:19:PRO:HG2	1:C:130:LEU:CD2	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:LEU:O	1:A:17:PHE:HB2	2.21	0.41
1:G:11:LEU:HB3	1:G:17:PHE:CG	2.56	0.41
1:E:69:GLU:OE1	1:E:69:GLU:N	2.50	0.41
1:I:180:ALA:HB3	1:I:183:LEU:HG	2.03	0.41
1:I:204:ASP:OD1	1:I:205:GLU:N	2.53	0.41
1:E:21:SER:CA	1:G:191:GLN:OE1	2.69	0.41
1:C:10:LEU:HD21	1:I:10:LEU:CD2	2.49	0.41
1:I:154:THR:HA	1:I:198:ILE:HD13	2.02	0.41
1:I:80:GLU:H	1:I:80:GLU:CD	2.22	0.41
1:B:55:TYR:HD2	1:B:83:THR:CG2	2.32	0.41
1:I:141:ARG:O	1:I:145:ILE:HG13	2.20	0.41
1:F:8:GLN:O	1:F:12:GLN:HG3	2.20	0.41
1:I:49:PRO:HB2	1:I:51:HIS:CD2	2.56	0.41
1:I:155:HIS:HA	1:I:159:ARG:NH1	2.36	0.41
1:A:88:MET:HE1	1:A:93:THR:CG2	2.51	0.41
1:I:86:GLU:OE2	1:J:139:HIS:NE2	2.53	0.41
1:A:178:PRO:HG2	1:H:3:PHE:H	1.85	0.41
1:E:10:LEU:HD13	1:H:10:LEU:HD13	2.03	0.41
1:A:3:PHE:O	1:A:4:GLN:O	2.38	0.41
1:I:29:LEU:HD23	1:I:111:PHE:CE2	2.51	0.41
1:E:225:CYS:HB3	1:G:95:ASN:OD1	2.20	0.41
1:G:56:LEU:HD23	1:G:79:ASN:O	2.21	0.41
1:E:191:GLN:HA	1:E:192:PRO:HD3	1.93	0.41
1:E:56:LEU:HD11	1:E:106:SER:HB3	2.01	0.41
1:E:120:LEU:CD2	1:F:128:LEU:CD2	2.92	0.41
1:C:46:GLN:OE1	1:C:66:LEU:HD12	2.21	0.41
1:F:144:GLU:O	1:F:148:LEU:HG	2.20	0.41
1:F:81:ARG:O	1:F:82:ASN:ND2	2.54	0.41
1:E:25:LEU:CD1	1:E:25:LEU:N	2.84	0.41
1:E:6:VAL:CG1	1:H:7:HIS:CE1	2.90	0.41
1:C:207:ILE:HA	1:C:219:ASP:HB2	2.03	0.41
1:H:34:LEU:HD12	1:H:108:LEU:O	2.20	0.41
1:I:8:GLN:HE22	1:I:25:LEU:CB	2.32	0.41
1:G:157:VAL:O	1:G:161:LEU:HG	2.21	0.41
1:E:139:HIS:HB3	1:F:76:GLU:OE1	2.21	0.41
1:F:70:GLY:O	1:F:71:GLN:HB2	2.21	0.41
1:J:123:ASN:O	1:J:125:PRO:CD	2.68	0.41
1:A:123:ASN:C	1:A:125:PRO:CD	2.78	0.41
1:D:13:SER:O	1:D:137:ARG:NH2	2.54	0.41
1:J:84:PHE:O	1:J:85:ALA:CB	2.65	0.41
1:H:166:ALA:O	1:H:167:HIS:HB2	2.21	0.41
1:D:67:THR:O	1:D:68:PRO:C	2.58	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:50:ALA:HA	1:G:96:TYR:CZ	2.55	0.40
1:H:15:HIS:CE1	1:H:16:LEU:HG	2.56	0.40
1:G:155:HIS:HB3	1:G:187:HIS:HB2	2.01	0.40
1:A:50:ALA:HA	1:A:96:TYR:CZ	2.56	0.40
1:B:225:CYS:O	1:B:226:PHE:O	2.39	0.40
1:B:153:ALA:O	1:B:157:VAL:HG23	2.21	0.40
1:H:120:LEU:O	1:H:121:GLN:C	2.59	0.40
1:D:89:MET:CE	1:D:89:MET:C	2.90	0.40
1:A:122:ASP:O	1:A:123:ASN:HB2	2.22	0.40
1:A:191:GLN:HA	1:A:192:PRO:HD3	1.85	0.40
1:J:179:VAL:CG1	1:J:179:VAL:O	2.70	0.40
1:G:57:ILE:H	1:G:57:ILE:CD1	2.30	0.40
1:A:176:GLU:O	1:A:177:ILE:HB	2.20	0.40
1:A:160:TYR:HE2	1:A:177:ILE:CD1	2.35	0.40
1:A:225:CYS:SG	1:A:226:PHE:N	2.94	0.40
1:C:92:ASP:O	1:C:93:THR:C	2.60	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:MET:N	1:A:122:ASP:OD2[2_555]	1.58	0.62
1:C:210:LEU:CB	1:C:210:LEU:CD2[2_556]	1.76	0.44
1:A:2:GLU:OE2	1:A:121:GLN:OE1[2_555]	1.77	0.43
1:H:69:GLU:OE2	1:I:79:ASN:OD1[4_456]	2.11	0.09

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	225/227 (99%)	197 (88%)	18 (8%)	10 (4%)	4	45
1	B	225/227 (99%)	202 (90%)	17 (8%)	6 (3%)	8	59
1	C	225/227 (99%)	183 (81%)	21 (9%)	21 (9%)	1	20
1	D	225/227 (99%)	189 (84%)	23 (10%)	13 (6%)	3	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	225/227 (99%)	197 (88%)	17 (8%)	11 (5%)	3	41
1	F	225/227 (99%)	193 (86%)	25 (11%)	7 (3%)	7	57
1	G	225/227 (99%)	197 (88%)	22 (10%)	6 (3%)	8	59
1	H	225/227 (99%)	195 (87%)	16 (7%)	14 (6%)	2	34
1	I	225/227 (99%)	207 (92%)	13 (6%)	5 (2%)	10	64
1	J	225/227 (99%)	198 (88%)	21 (9%)	6 (3%)	8	59
All	All	2250/2270 (99%)	1958 (87%)	193 (9%)	99 (4%)	4	45

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	TYR
1	B	92	ASP
1	B	214	GLU
1	B	226	PHE
1	C	34	LEU
1	C	50	ALA
1	C	209	HIS
1	C	210	LEU
1	C	211	ASP
1	D	64	TYR
1	D	94	PRO
1	E	2	GLU
1	E	24	GLN
1	E	169	PRO
1	E	173	CYS
1	F	64	TYR
1	F	121	GLN
1	H	64	TYR
1	H	68	PRO
1	H	71	GLN
1	H	165	ALA
1	H	175	VAL
1	H	226	PHE
1	J	124	THR
1	A	4	GLN
1	A	176	GLU
1	B	70	GLY
1	C	123	ASN
1	C	213	ARG

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Mol	Chain	Res	Type
1	C	214	GLU
1	D	166	ALA
1	D	190	ILE
1	F	188	LEU
1	G	64	TYR
1	G	178	PRO
1	H	70	GLY
1	H	169	PRO
1	I	70	GLY
1	I	176	GLU
1	J	123	ASN
1	A	69	GLU
1	B	64	TYR
1	C	92	ASP
1	C	121	GLN
1	C	168	ALA
1	D	68	PRO
1	D	121	GLN
1	E	3	PHE
1	E	22	PRO
1	E	124	THR
1	H	69	GLU
1	J	175	VAL
1	A	5	ARG
1	A	122	ASP
1	A	181	LYS
1	B	177	ILE
1	C	35	VAL
1	C	189	SER
1	D	18	GLU
1	D	71	GLN
1	D	189	SER
1	E	123	ASN
1	F	51	HIS
1	F	125	PRO
1	G	4	GLN
1	I	175	VAL
1	J	4	GLN
1	A	105	PRO
1	C	66	LEU
1	C	69	GLU
1	C	71	GLN

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Mol	Chain	Res	Type
1	D	74	ILE
1	D	104	VAL
1	E	168	ALA
1	E	178	PRO
1	F	69	GLU
1	H	66	LEU
1	H	176	GLU
1	H	191	GLN
1	I	4	GLN
1	J	213	ARG
1	C	93	THR
1	C	208	ILE
1	D	52	ALA
1	D	69	GLU
1	G	105	PRO
1	G	123	ASN
1	H	105	PRO
1	A	125	PRO
1	C	125	PRO
1	C	177	ILE
1	I	178	PRO
1	H	67	THR
1	C	169	PRO
1	E	212	GLY
1	F	179	VAL
1	G	170	GLY
1	J	169	PRO
1	A	168	ALA

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	199/199 (100%)	196 (98%)	3 (2%)	76	95
1	B	199/199 (100%)	195 (98%)	4 (2%)	68	93
1	C	199/199 (100%)	194 (98%)	5 (2%)	60	91
1	D	199/199 (100%)	193 (97%)	6 (3%)	53	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	199/199 (100%)	198 (100%)	1 (0%)	94	98
1	F	199/199 (100%)	193 (97%)	6 (3%)	53	90
1	G	199/199 (100%)	194 (98%)	5 (2%)	60	91
1	H	199/199 (100%)	193 (97%)	6 (3%)	53	90
1	I	199/199 (100%)	198 (100%)	1 (0%)	94	98
1	J	199/199 (100%)	196 (98%)	3 (2%)	76	95
All	All	1990/1990 (100%)	1950 (98%)	40 (2%)	68	93

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	4	GLN
1	A	90	PHE
1	B	57	ILE
1	B	67	THR
1	B	123	ASN
1	B	160	TYR
1	C	57	ILE
1	C	65	ARG
1	C	90	PHE
1	C	123	ASN
1	C	202	LEU
1	D	79	ASN
1	D	89	MET
1	D	90	PHE
1	D	108	LEU
1	D	123	ASN
1	D	188	LEU
1	E	119	GLN
1	F	37	LEU
1	F	57	ILE
1	F	66	LEU
1	F	96	TYR
1	F	183	LEU
1	F	215	ILE
1	G	57	ILE
1	G	90	PHE
1	G	108	LEU
1	G	177	ILE

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Mol	Chain	Res	Type
1	G	183	LEU
1	H	57	ILE
1	H	82	ASN
1	H	95	ASN
1	H	118	ARG
1	H	162	LEU
1	H	183	LEU
1	I	160	TYR
1	J	1	MET
1	J	120	LEU
1	J	171	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	95	ASN
1	A	107	GLN
1	A	155	HIS
1	B	12	GLN
1	B	26	GLN
1	B	107	GLN
1	C	9	GLN
1	C	12	GLN
1	C	121	GLN
1	C	123	ASN
1	C	139	HIS
1	D	7	HIS
1	D	79	ASN
1	D	95	ASN
1	D	123	ASN
1	E	14	HIS
1	E	95	ASN
1	E	107	GLN
1	E	119	GLN
1	F	26	GLN
1	F	82	ASN
1	F	101	GLN
1	F	139	HIS
1	F	152	ASN
1	F	155	HIS
1	G	101	GLN

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Mol	Chain	Res	Type
1	G	119	GLN
1	G	155	HIS
1	H	4	GLN
1	H	7	HIS
1	H	12	GLN
1	H	82	ASN
1	H	95	ASN
1	H	107	GLN
1	H	167	HIS
1	I	8	GLN
1	I	26	GLN
1	I	123	ASN
1	I	155	HIS
1	I	200	HIS
1	J	8	GLN
1	J	101	GLN
1	J	107	GLN
1	J	123	ASN
1	J	155	HIS
1	J	200	HIS

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	225/227 (99%)	0.16	3 (1%) 74 47	20, 55, 94, 100	47 (20%)
1	B	216/227 (95%)	0.32	5 (2%) 57 33	20, 62, 100, 100	70 (32%)
1	C	221/227 (97%)	0.40	11 (4%) 28 15	20, 57, 100, 100	57 (25%)
1	D	199/227 (87%)	0.27	10 (5%) 28 15	22, 58, 100, 100	66 (33%)
1	E	211/227 (92%)	0.25	4 (1%) 64 37	20, 68, 100, 100	75 (35%)
1	F	212/227 (93%)	0.46	9 (4%) 35 19	24, 72, 100, 100	76 (35%)
1	G	216/227 (95%)	0.34	8 (3%) 39 22	28, 66, 100, 100	66 (30%)
1	H	210/227 (92%)	0.28	3 (1%) 72 45	23, 63, 100, 100	54 (25%)
1	I	213/227 (93%)	0.39	10 (4%) 30 17	24, 63, 100, 100	46 (21%)
1	J	222/227 (97%)	0.30	3 (1%) 72 45	27, 70, 99, 100	43 (19%)
All	All	2145/2270 (94%)	0.32	66 (3%) 47 26	20, 63, 100, 100	600 (27%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	CYS	6.9
1	C	225	CYS	6.0
1	F	171	GLU	5.6
1	D	173	CYS	5.3
1	C	221	GLU	4.6
1	D	170	GLY	4.0
1	F	170	GLY	4.0
1	H	165	ALA	3.7
1	F	167	HIS	3.5
1	I	175	VAL	3.3
1	I	182	GLN	3.3
1	C	175	VAL	3.1
1	B	173	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	172	ASN	3.1
1	C	226	PHE	3.0
1	C	1	MET	3.0
1	F	55	TYR	3.0
1	G	203	GLY	3.0
1	D	177	ILE	2.9
1	B	2	GLU	2.9
1	I	159	ARG	2.9
1	C	178	PRO	2.8
1	I	173	CYS	2.8
1	I	177	ILE	2.8
1	H	172	ASN	2.7
1	F	169	PRO	2.7
1	J	219	ASP	2.6
1	F	94	PRO	2.6
1	I	174	ARG	2.6
1	I	171	GLU	2.5
1	G	36	ASN	2.5
1	A	208	ILE	2.4
1	A	225	CYS	2.4
1	D	164	LEU	2.4
1	G	215	ILE	2.4
1	H	3	PHE	2.4
1	G	28	LEU	2.4
1	C	160	TYR	2.3
1	E	125	PRO	2.3
1	G	170	GLY	2.3
1	D	33	ASP	2.3
1	F	45	ARG	2.3
1	D	225	CYS	2.3
1	C	224	GLU	2.3
1	G	35	VAL	2.3
1	D	226	PHE	2.2
1	F	168	ALA	2.2
1	D	71	GLN	2.2
1	I	191	GLN	2.2
1	G	171	GLU	2.2
1	J	206	GLY	2.2
1	E	176	GLU	2.1
1	D	224	GLU	2.1
1	F	183	LEU	2.1
1	I	163	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	2.1
1	C	217	ILE	2.1
1	G	173	CYS	2.1
1	I	158	VAL	2.1
1	J	182	GLN	2.1
1	B	74	ILE	2.1
1	C	181	LYS	2.1
1	E	221	GLU	2.1
1	E	188	LEU	2.0
1	D	110	ARG	2.0
1	A	187	HIS	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.