



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:37 PM GMT

PDB ID : 1DBR
Title : HYPOXANTHINE GUANINE XANTHINE
Authors : Schumacher, M.A.; Carter, D.; Roos, D.; Ullman, B.; Brennan, R.G.
Deposited on : 1996-02-13
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

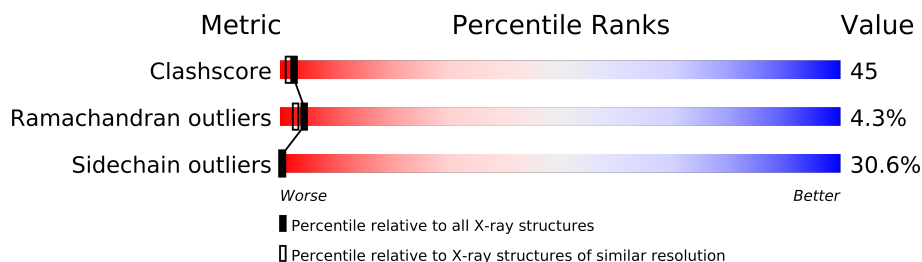
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	231	
1	B	231	
1	C	231	
1	D	231	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7494 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 HYPOXANTHINE GUANINE XANTHINE PHOSPHORIBOSYLTRANSFERASE.

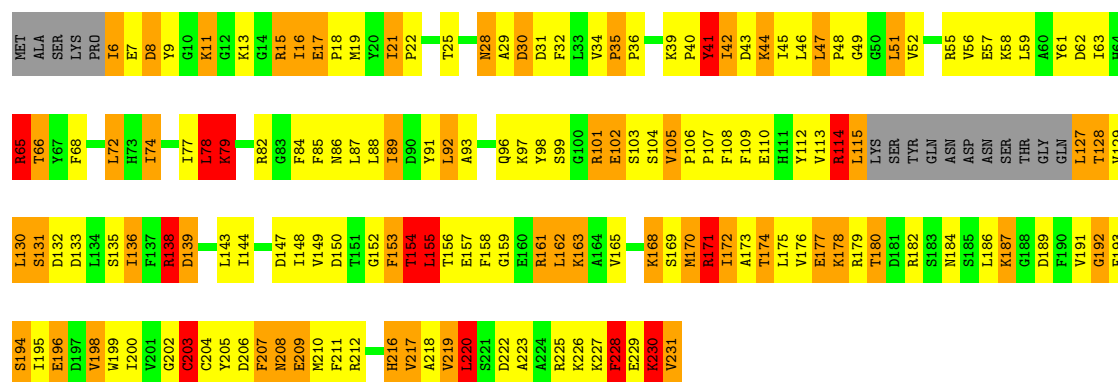
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1834	1180	306	341	7			
1	B	219	Total	C	N	O	S	0	0	0
			1775	1149	294	325	7			
1	C	215	Total	C	N	O	S	0	0	0
			1746	1130	289	320	7			
1	D	215	Total	C	N	O	S	0	0	0
			1748	1132	289	320	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

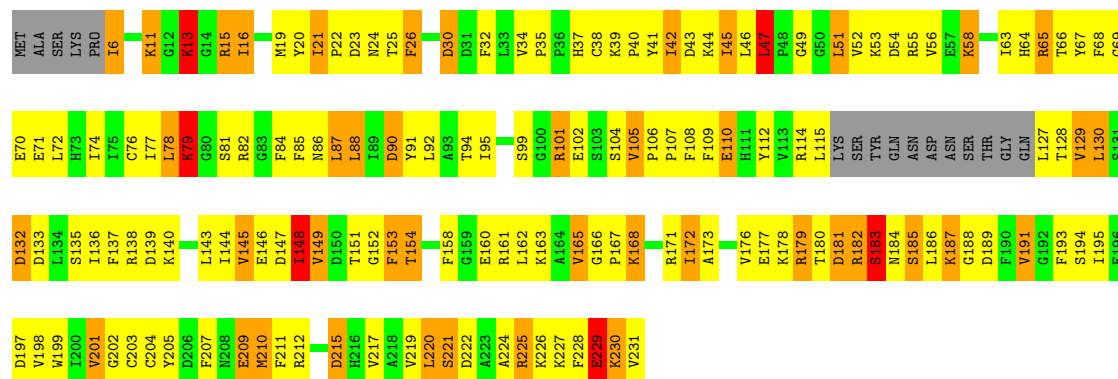
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	97	Total	O	0	0
			97	97		
3	C	95	Total	O	0	0
			95	95		
3	D	88	Total	O	0	0
			88	88		



• Molecule 1: HYPOXANTHINE GUANINE XANTHINE PHOSPHORIBOSYLTRANSFERASE

Chain D:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.15Å 109.22Å 79.74Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	90.0 (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7494	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.24	4/1876 (0.2%)	1.51	23/2530 (0.9%)
1	B	1.12	1/1817 (0.1%)	1.59	33/2450 (1.3%)
1	C	0.96	1/1787 (0.1%)	1.47	23/2409 (1.0%)
1	D	1.10	3/1789 (0.2%)	1.45	16/2412 (0.7%)
All	All	1.11	9/7269 (0.1%)	1.51	95/9801 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	1
1	D	0	1
All	All	2	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	CYS	CB-SG	20.10	2.16	1.82
1	A	120	ASN	N-CA	16.18	1.78	1.46
1	A	203	CYS	CA-CB	12.74	1.81	1.53
1	C	203	CYS	CB-SG	10.24	1.99	1.82
1	D	76	CYS	CB-SG	7.68	1.95	1.82
1	B	204	CYS	CA-CB	-6.59	1.39	1.53
1	A	204	CYS	CB-SG	6.35	1.93	1.82
1	D	229	GLU	CG-CD	5.99	1.60	1.51
1	D	229	GLU	CD-OE2	5.09	1.31	1.25

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	PRO	C-N-CD	-11.74	94.78	120.60
1	A	15	ARG	NE-CZ-NH2	10.06	125.33	120.30
1	A	120	ASN	N-CA-CB	9.42	127.56	110.60
1	A	15	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	B	204	CYS	CA-CB-SG	-8.88	98.01	114.00
1	C	55	ARG	CG-CD-NE	-8.65	93.63	111.80
1	A	162	LEU	CA-CB-CG	8.65	135.19	115.30
1	D	54	ASP	CB-CG-OD1	8.56	126.01	118.30
1	B	47	LEU	CB-CG-CD1	-8.45	96.63	111.00
1	B	23	ASP	CB-CG-OD1	8.39	125.85	118.30
1	B	184	ASN	N-CA-C	-8.31	88.56	111.00
1	A	179	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	B	46	LEU	CB-CG-CD1	7.71	124.11	111.00
1	B	78	LEU	N-CA-C	7.59	131.48	111.00
1	C	31	ASP	CB-CA-C	7.48	125.36	110.40
1	D	65	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	182	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	C	65	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	65	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	C	228	PHE	N-CA-C	7.17	130.35	111.00
1	C	138	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	C	41	TYR	N-CA-C	6.94	129.75	111.00
1	B	161	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	A	138	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	B	5	PRO	O-C-N	6.85	133.66	122.70
1	C	155	LEU	CA-CB-CG	-6.83	99.58	115.30
1	A	203	CYS	CA-CB-SG	6.82	126.28	114.00
1	D	47	LEU	CA-CB-CG	6.70	130.70	115.30
1	D	92	LEU	CA-CB-CG	-6.67	99.95	115.30
1	B	189	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	B	212	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	C	219	VAL	N-CA-C	-6.65	93.05	111.00
1	D	54	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	B	225	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	A	115	LEU	CA-CB-CG	-6.52	100.29	115.30
1	B	55	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	A	144	ILE	CA-CB-CG2	6.35	123.61	110.90
1	B	183	SER	N-CA-C	6.33	128.09	111.00
1	C	114	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	B	78	LEU	C-N-CA	6.24	137.31	121.70
1	C	172	ILE	CB-CA-C	-6.22	99.15	111.60
1	A	19	MET	CG-SD-CE	-6.22	90.25	100.20
1	C	78	LEU	N-CA-C	6.21	127.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	D	16	ILE	N-CA-C	-6.17	94.35	111.00
1	C	220	LEU	CB-CG-CD2	-6.12	100.60	111.00
1	D	101	ARG	N-CA-C	-6.03	94.71	111.00
1	B	30	ASP	CB-CA-C	-6.02	98.36	110.40
1	B	210	MET	CG-SD-CE	5.95	109.72	100.20
1	B	78	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	D	210	MET	CG-SD-CE	5.89	109.63	100.20
1	C	21	ILE	CG1-CB-CG2	-5.88	98.46	111.40
1	A	78	LEU	O-C-N	5.87	132.09	122.70
1	B	82	ARG	CB-CA-C	5.86	122.12	110.40
1	B	187	LYS	N-CA-C	-5.86	95.19	111.00
1	D	46	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	C	34	VAL	C-N-CD	-5.77	107.90	120.60
1	C	15	ARG	N-CA-C	5.75	126.52	111.00
1	A	170	MET	CG-SD-CE	5.69	109.30	100.20
1	C	228	PHE	CB-CG-CD2	5.67	124.77	120.80
1	D	55	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	B	46	LEU	CB-CG-CD2	5.65	120.61	111.00
1	D	16	ILE	CB-CA-C	-5.59	100.42	111.60
1	A	103	SER	N-CA-CB	5.59	118.88	110.50
1	A	55	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	B	186	LEU	CA-CB-CG	-5.54	102.56	115.30
1	D	191	VAL	CG1-CB-CG2	5.51	119.71	110.90
1	B	198	VAL	CG1-CB-CG2	5.45	119.61	110.90
1	C	130	LEU	CA-CB-CG	-5.44	102.80	115.30
1	B	203	CYS	CA-CB-SG	-5.40	104.27	114.00
1	B	3	SER	O-C-N	5.39	131.33	122.70
1	B	127	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	143	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	B	74	ILE	CB-CA-C	5.34	122.28	111.60
1	A	78	LEU	C-N-CA	5.29	134.92	121.70
1	D	92	LEU	CB-CA-C	-5.28	100.16	110.20
1	B	103	SER	N-CA-C	-5.28	96.74	111.00
1	D	15	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	C	231	VAL	CA-C-O	-5.24	109.09	120.10
1	A	123	SER	N-CA-C	5.20	125.05	111.00
1	A	55	ARG	CG-CD-NE	-5.18	100.93	111.80
1	A	78	LEU	CA-C-N	-5.17	105.82	117.20
1	B	78	LEU	CA-C-N	-5.17	105.82	117.20
1	C	180	THR	N-CA-C	5.17	124.97	111.00
1	B	130	LEU	CB-CG-CD2	-5.17	102.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	109	PHE	N-CA-C	-5.12	97.17	111.00
1	B	78	LEU	O-C-N	5.11	130.87	122.70
1	B	167	PRO	N-CA-C	-5.11	98.83	112.10
1	A	7	GLU	N-CA-C	5.05	124.64	111.00
1	A	144	ILE	N-CA-CB	5.05	122.42	110.80
1	D	13	LYS	N-CA-C	5.03	124.57	111.00
1	B	182	ARG	N-CA-C	5.02	124.56	111.00
1	D	42	ILE	CB-CA-C	5.01	121.61	111.60
1	C	194	SER	N-CA-CB	5.00	118.00	110.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	78	LEU	CA
1	C	228	PHE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	230	LYS	Peptide
1	D	179	ARG	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1834	0	1813	152	0
1	B	1775	0	1766	147	0
1	C	1746	0	1729	198	0
1	D	1748	0	1736	164	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	107	0	0	10	0
3	B	97	0	0	13	0
3	C	95	0	0	5	0
3	D	88	0	0	6	0
All	All	7494	0	7044	639	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 45.

All (639) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:CYS:CA	1:A:203:CYS:CB	1.82	1.57
1:A:120:ASN:N	1:A:120:ASN:CA	1.78	1.44
1:A:203:CYS:CB	1:A:203:CYS:SG	2.16	1.34
1:C:115:LEU:HD13	1:C:130:LEU:HB2	1.32	1.08
1:C:78:LEU:HD22	1:C:79:LYS:H	1.17	1.04
1:D:151:THR:HG22	1:D:153:PHE:H	1.22	1.01
1:C:28:ASN:N	1:C:28:ASN:HD22	1.56	1.01
1:B:105:VAL:HG23	1:B:106:PRO:HD2	1.42	1.01
1:D:129:VAL:HG13	1:D:158:PHE:HB2	1.41	1.00
1:C:203:CYS:HB2	1:C:217:VAL:HG12	1.43	1.00
1:D:180:THR:HG22	1:D:181:ASP:H	1.27	1.00
1:D:11:LYS:HD2	1:D:13:LYS:HA	1.45	0.98
1:C:96:GLN:HG3	1:C:107:PRO:HB3	1.45	0.97
1:D:19:MET:HE3	1:D:21:ILE:HD11	1.50	0.93
1:C:28:ASN:H	1:C:28:ASN:HD22	1.10	0.93
1:C:42:ILE:HD11	1:C:45:ILE:HD11	1.51	0.93
1:D:11:LYS:NZ	1:D:13:LYS:HD2	1.84	0.92
1:A:114:ARG:NE	1:A:130:LEU:HD11	1.83	0.92
1:A:49:GLY:H	1:A:216:HIS:HD2	1.12	0.91
1:D:172:ILE:HG12	1:D:188:GLY:HA2	1.52	0.91
1:D:229:GLU:HA	1:D:229:GLU:OE1	1.71	0.91
1:C:115:LEU:CD1	1:C:130:LEU:HB2	2.01	0.89
1:C:171:ARG:HG3	1:C:171:ARG:HH11	1.36	0.89
1:C:28:ASN:H	1:C:28:ASN:ND2	1.71	0.89
1:C:128:THR:HA	1:C:154:THR:HG22	1.55	0.89
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.38	0.88
1:A:144:ILE:HD11	1:A:155:LEU:HD11	1.55	0.88
1:C:42:ILE:HD13	1:C:218:ALA:CB	2.03	0.88
1:C:143:LEU:HD11	1:C:173:ALA:HB2	1.55	0.88
1:A:6:ILE:HD12	1:A:170:MET:HG2	1.57	0.87
1:D:105:VAL:HG22	1:D:106:PRO:HD2	1.56	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:178:LYS:HD2	1:D:197:ASP:HA	1.55	0.86
1:C:156:THR:CG2	1:C:186:LEU:HD21	2.05	0.86
1:B:152:GLY:O	1:B:156:THR:HG23	1.77	0.85
1:C:155:LEU:HB3	1:C:186:LEU:CD1	2.06	0.85
1:A:34:VAL:HG22	1:A:39:LYS:HG2	1.56	0.85
1:A:73:HIS:CD2	1:A:140:LYS:HG2	2.12	0.85
1:D:11:LYS:HD2	1:D:13:LYS:CA	2.08	0.83
1:B:147:ASP:HB2	1:B:205:TYR:CE1	2.12	0.83
1:C:42:ILE:HD13	1:C:218:ALA:HB2	1.60	0.82
1:D:19:MET:CE	1:D:21:ILE:HD11	2.09	0.82
1:A:78:LEU:HD21	1:B:78:LEU:HD11	1.62	0.82
1:A:52:VAL:O	1:A:56:VAL:HG13	1.79	0.81
1:C:136:ILE:O	1:C:136:ILE:HD13	1.80	0.81
1:D:39:LYS:HB3	1:D:40:PRO:HD3	1.62	0.81
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.46	0.81
1:B:63:ILE:HD11	1:B:72:LEU:HD11	1.62	0.80
1:A:225:ARG:HD2	3:A:309:HOH:O	1.81	0.80
1:B:18:PRO:HB3	1:B:191:VAL:HG22	1.64	0.80
1:C:89:ILE:HG22	1:C:108:PHE:CD2	2.15	0.80
1:B:159:GLY:O	1:B:163:LYS:HG3	1.81	0.80
1:B:15:ARG:NH2	1:B:187:LYS:HD2	1.96	0.80
1:A:49:GLY:H	1:A:216:HIS:CD2	1.99	0.80
1:A:113:VAL:HG12	1:A:131:SER:HB3	1.65	0.78
1:A:41:TYR:HE2	1:A:227:LYS:HG3	1.48	0.78
1:D:107:PRO:HB2	1:D:108:PHE:HD1	1.47	0.78
1:A:226:LYS:HD3	1:A:227:LYS:N	1.99	0.78
1:C:163:LYS:NZ	1:C:163:LYS:HB2	1.96	0.78
1:D:105:VAL:CG2	1:D:106:PRO:HD2	2.14	0.77
1:B:6:ILE:O	1:B:6:ILE:HG13	1.83	0.77
1:D:207:PHE:CE2	1:D:225:ARG:HA	2.20	0.77
1:C:29:ALA:HA	1:C:45:ILE:HD13	1.66	0.77
1:B:41:TYR:HB3	1:B:224:ALA:HB2	1.66	0.77
1:C:28:ASN:ND2	1:C:28:ASN:N	2.29	0.77
1:B:149:VAL:HG21	1:B:186:LEU:HB2	1.66	0.77
1:A:41:TYR:CE2	1:A:227:LYS:HG3	2.20	0.77
1:C:222:ASP:HB3	1:C:226:LYS:HZ2	1.50	0.77
1:B:180:THR:CG2	1:B:182:ARG:HD3	2.15	0.77
1:C:155:LEU:HB3	1:C:186:LEU:HD12	1.66	0.76
1:B:174:THR:O	1:B:191:VAL:HA	1.86	0.76
1:B:142:VAL:HG12	1:B:169:SER:O	1.85	0.76
1:D:127:LEU:O	1:D:154:THR:HB	1.86	0.76
1:A:133:ASP:O	1:A:136:ILE:HG22	1.86	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:42:ILE:HD11	1:C:45:ILE:CD1	2.16	0.75
1:D:133:ASP:OD2	1:D:135:SER:HB2	1.86	0.75
1:C:128:THR:HG23	1:C:157:GLU:OE2	1.87	0.75
1:C:19:MET:HE1	1:C:51:LEU:HD11	1.69	0.75
1:B:11:LYS:HB3	3:B:311:HOH:O	1.87	0.74
1:C:222:ASP:HA	1:C:225:ARG:HD3	1.69	0.74
1:A:34:VAL:HG22	1:A:39:LYS:CG	2.18	0.74
1:D:107:PRO:HB2	1:D:108:PHE:CD1	2.23	0.74
1:B:62:ASP:O	1:B:66:THR:HG22	1.88	0.73
1:D:11:LYS:HD2	1:D:13:LYS:N	2.03	0.73
1:C:207:PHE:CZ	1:C:225:ARG:HA	2.23	0.73
1:D:78:LEU:HD23	1:D:79:LYS:H	1.53	0.73
1:A:90:ASP:O	1:A:94:THR:HG22	1.89	0.72
1:A:110:GLU:OE1	1:B:82:ARG:HD2	1.88	0.72
1:A:119:GLN:CD	1:A:120:ASN:H	1.92	0.72
1:B:47:LEU:HD12	1:B:217:VAL:HG21	1.70	0.72
1:B:63:ILE:CD1	1:B:72:LEU:HD11	2.20	0.72
1:A:11:LYS:HD3	3:A:281:HOH:O	1.89	0.72
1:D:22:PRO:O	1:D:25:THR:HG23	1.90	0.72
1:C:210:MET:HB3	1:C:211:PHE:CD2	2.25	0.72
1:D:47:LEU:HB2	1:D:217:VAL:HB	1.70	0.72
1:D:91:TYR:O	1:D:95:ILE:HG13	1.90	0.72
1:C:210:MET:HB3	1:C:211:PHE:CE2	2.25	0.71
1:A:44:LYS:HE2	3:A:264:HOH:O	1.89	0.71
1:A:181:ASP:O	1:A:182:ARG:HB2	1.89	0.71
1:D:149:VAL:O	1:D:149:VAL:HG22	1.89	0.71
1:D:78:LEU:HD23	1:D:79:LYS:N	2.04	0.71
1:C:203:CYS:CB	1:C:217:VAL:HG12	2.20	0.71
1:A:49:GLY:N	1:A:216:HIS:HD2	1.86	0.71
1:C:207:PHE:O	1:C:210:MET:HB2	1.91	0.71
1:B:75:ILE:O	1:B:75:ILE:HD13	1.90	0.71
1:B:158:PHE:HD1	1:B:161:ARG:NH1	1.88	0.71
1:A:129:VAL:HG11	1:A:158:PHE:HB2	1.73	0.70
1:B:15:ARG:HD3	1:B:17:GLU:OE2	1.90	0.70
1:B:105:VAL:CG2	1:B:106:PRO:HD2	2.21	0.70
1:C:158:PHE:CE2	1:C:162:LEU:HD21	2.27	0.69
1:D:230:LYS:CD	1:D:231:VAL:H	2.05	0.69
1:B:199:TRP:CD1	1:B:220:LEU:HB2	2.28	0.69
1:D:180:THR:CG2	1:D:182:ARG:HG3	2.22	0.69
1:C:230:LYS:O	1:C:231:VAL:HB	1.91	0.69
1:B:43:ASP:HA	3:B:254:HOH:O	1.91	0.69
3:B:247:HOH:O	1:D:19:MET:HG3	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:101:ARG:HG3	3:D:252:HOH:O	1.91	0.68
1:A:19:MET:HE2	1:A:21:ILE:HD11	1.75	0.68
1:A:71:GLU:HG2	1:A:109:PHE:HE2	1.58	0.68
1:B:180:THR:HG21	1:B:182:ARG:HD3	1.75	0.68
1:B:68:PHE:CE2	1:B:101:ARG:HG2	2.28	0.68
1:A:225:ARG:HG2	1:A:225:ARG:NH1	2.08	0.68
1:D:130:LEU:C	1:D:130:LEU:HD13	2.14	0.68
1:C:79:LYS:HZ2	1:D:112:TYR:HD1	1.42	0.68
1:D:151:THR:HG22	1:D:153:PHE:N	2.02	0.67
1:A:136:ILE:HG13	1:A:136:ILE:O	1.93	0.67
1:D:16:ILE:HG12	3:D:234:HOH:O	1.95	0.67
1:B:65:ARG:HG2	1:B:65:ARG:HH11	1.59	0.67
1:C:148:ILE:HD11	1:C:178:LYS:HD2	1.76	0.67
1:C:178:LYS:HA	1:C:195:ILE:O	1.95	0.67
1:D:209:GLU:OE1	1:D:209:GLU:HA	1.93	0.67
1:C:174:THR:HG22	1:C:191:VAL:HG23	1.75	0.66
1:C:8:ASP:OD1	1:C:8:ASP:N	2.28	0.66
1:D:129:VAL:CG1	1:D:158:PHE:HB2	2.22	0.66
1:C:171:ARG:NH1	1:C:171:ARG:HG3	2.10	0.66
1:C:56:VAL:HG22	1:C:84:PHE:HE1	1.60	0.66
1:A:15:ARG:NH1	1:A:191:VAL:HG11	2.08	0.66
1:B:142:VAL:HG13	1:B:170:MET:HA	1.77	0.66
1:C:222:ASP:O	1:C:226:LYS:HD2	1.95	0.66
1:C:153:PHE:O	1:C:154:THR:HG23	1.95	0.66
1:A:37:HIS:CE1	1:B:96:GLN:HE22	2.14	0.66
1:C:89:ILE:H	1:C:89:ILE:HD12	1.59	0.66
1:B:63:ILE:HD11	1:B:72:LEU:CD1	2.26	0.66
1:D:11:LYS:CE	1:D:13:LYS:HD2	2.26	0.66
1:C:42:ILE:HD13	1:C:218:ALA:HB1	1.76	0.66
1:B:147:ASP:OD1	1:B:147:ASP:N	2.29	0.65
1:B:210:MET:HB3	1:B:211:PHE:CD2	2.31	0.65
1:C:78:LEU:HD22	1:C:79:LYS:N	2.02	0.65
1:C:131:SER:HB3	1:C:161:ARG:NH2	2.11	0.65
1:C:207:PHE:HZ	1:C:225:ARG:HA	1.62	0.65
1:D:180:THR:HG22	1:D:182:ARG:HG3	1.77	0.65
1:C:202:GLY:HA2	1:C:211:PHE:O	1.97	0.65
1:D:220:LEU:HD22	1:D:225:ARG:HG2	1.77	0.65
1:A:113:VAL:CG1	1:A:131:SER:HB3	2.26	0.65
1:D:220:LEU:HD23	1:D:224:ALA:HB3	1.77	0.65
1:B:161:ARG:CG	1:B:161:ARG:HH11	2.08	0.65
1:B:15:ARG:HG2	1:B:16:ILE:N	2.12	0.65
1:D:71:GLU:CG	1:D:109:PHE:HE2	2.09	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:114:ARG:HE	1:A:130:LEU:HD11	1.62	0.65
1:A:77:ILE:HD12	1:A:146:GLU:HG2	1.78	0.64
1:B:147:ASP:HB2	1:B:205:TYR:HE1	1.58	0.64
1:C:89:ILE:HG22	1:C:108:PHE:CE2	2.32	0.64
1:C:35:PRO:HB2	1:C:36:PRO:HD2	1.79	0.64
1:A:215:ASP:OD1	1:A:215:ASP:N	2.30	0.64
1:D:149:VAL:O	1:D:149:VAL:CG2	2.45	0.64
1:B:180:THR:HG23	1:B:182:ARG:HD3	1.80	0.64
1:B:26:PHE:HB2	3:B:257:HOH:O	1.95	0.64
1:C:68:PHE:CZ	1:C:101:ARG:HG2	2.32	0.64
1:C:155:LEU:HB3	1:C:186:LEU:HD11	1.79	0.64
1:D:11:LYS:HZ2	1:D:13:LYS:HD2	1.62	0.64
1:B:162:LEU:O	1:B:165:VAL:HG22	1.98	0.64
1:C:48:PRO:HA	1:C:216:HIS:HD2	1.63	0.64
1:B:40:PRO:HG2	1:B:41:TYR:CE2	2.33	0.64
1:D:138:ARG:HA	1:D:165:VAL:HG23	1.80	0.63
3:A:329:HOH:O	1:B:114:ARG:HD3	1.98	0.63
1:A:110:GLU:OE2	1:B:82:ARG:NH1	2.30	0.63
1:C:28:ASN:HB2	1:C:30:ASP:OD1	1.99	0.63
1:D:107:PRO:HG2	1:D:108:PHE:CE1	2.32	0.63
1:C:136:ILE:C	1:C:136:ILE:HD13	2.19	0.62
1:D:19:MET:HE2	1:D:193:PHE:HD1	1.63	0.62
1:D:178:LYS:HD3	1:D:195:ILE:HG13	1.81	0.62
1:C:131:SER:HB3	1:C:161:ARG:HH22	1.64	0.62
1:C:158:PHE:HD1	1:C:161:ARG:NH1	1.98	0.62
1:C:105:VAL:HG13	1:C:106:PRO:O	1.99	0.62
1:A:19:MET:CE	1:A:21:ILE:HD11	2.29	0.62
1:C:82:ARG:HD2	1:C:86:ASN:HD22	1.65	0.61
1:C:105:VAL:HG22	1:C:106:PRO:HD2	1.81	0.61
1:D:163:LYS:HD3	3:D:313:HOH:O	2.00	0.61
1:D:105:VAL:HG22	1:D:106:PRO:CD	2.29	0.61
1:C:209:GLU:OE1	1:C:212:ARG:HD2	2.00	0.61
1:C:86:ASN:HA	1:C:89:ILE:HD11	1.83	0.61
1:C:158:PHE:O	1:C:162:LEU:HD22	2.01	0.61
1:A:207:PHE:O	1:A:210:MET:HB2	2.00	0.61
1:C:29:ALA:HA	1:C:45:ILE:CD1	2.30	0.61
1:C:222:ASP:HB3	1:C:226:LYS:NZ	2.14	0.61
1:C:6:ILE:HG23	1:C:7:GLU:CD	2.20	0.60
1:C:207:PHE:O	1:C:208:ASN:HB3	2.01	0.60
1:C:89:ILE:HD12	1:C:89:ILE:N	2.16	0.60
1:A:226:LYS:HD3	1:A:227:LYS:H	1.67	0.60
1:C:129:VAL:HG11	1:C:158:PHE:HB2	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:201:VAL:HG13	1:D:220:LEU:HD12	1.83	0.60
1:C:156:THR:HG22	1:C:186:LEU:HD21	1.80	0.60
1:A:142:VAL:HB	3:A:296:HOH:O	2.02	0.59
1:C:110:GLU:HG3	3:C:272:HOH:O	2.01	0.59
1:D:19:MET:HE2	1:D:193:PHE:CD1	2.37	0.59
1:C:198:VAL:HG13	1:C:199:TRP:N	2.17	0.59
1:B:161:ARG:NH1	1:B:161:ARG:HG3	2.10	0.59
1:B:199:TRP:HD1	1:B:220:LEU:HB2	1.66	0.59
1:C:115:LEU:HB3	1:C:128:THR:O	2.03	0.59
1:D:35:PRO:HB2	1:D:37:HIS:CE1	2.38	0.59
1:A:49:GLY:O	1:A:53:LYS:HG3	2.02	0.58
1:C:19:MET:CE	1:C:51:LEU:HD11	2.33	0.58
1:D:82:ARG:HD2	1:D:82:ARG:O	2.03	0.58
1:C:19:MET:HE1	1:C:51:LEU:HD21	1.85	0.58
1:A:151:THR:HG22	1:A:153:PHE:H	1.67	0.58
1:C:143:LEU:HD11	1:C:173:ALA:CB	2.33	0.58
1:C:78:LEU:HD11	1:D:112:TYR:CD2	2.39	0.58
1:C:18:PRO:HB3	1:C:191:VAL:HG13	1.85	0.58
1:C:39:LYS:N	1:C:40:PRO:HD2	2.18	0.58
1:D:11:LYS:HE3	1:D:13:LYS:CD	2.34	0.57
1:B:142:VAL:CG1	1:B:170:MET:HA	2.34	0.57
1:D:32:PHE:CD1	1:D:45:ILE:HD13	2.40	0.57
1:D:74:ILE:HG22	1:D:85:PHE:HE1	1.68	0.57
1:D:147:ASP:O	1:D:148:ILE:HB	2.05	0.57
1:D:19:MET:HE1	1:D:193:PHE:HE1	1.68	0.57
1:B:129:VAL:HG13	1:B:158:PHE:HB2	1.86	0.57
1:A:28:ASN:OD1	1:A:30:ASP:HB2	2.04	0.57
1:C:19:MET:HE3	1:C:21:ILE:HD11	1.86	0.57
1:A:182:ARG:CZ	1:A:182:ARG:HB2	2.34	0.57
1:C:115:LEU:HB2	1:C:130:LEU:H	1.69	0.57
1:C:78:LEU:CD2	1:C:79:LYS:H	2.05	0.57
1:D:172:ILE:CG1	1:D:188:GLY:HA2	2.31	0.57
1:B:32:PHE:C	1:D:58:LYS:HD3	2.24	0.57
1:C:22:PRO:O	1:C:25:THR:HG23	2.04	0.57
1:D:180:THR:HG22	1:D:181:ASP:N	2.09	0.56
1:C:6:ILE:HG23	1:C:7:GLU:N	2.19	0.56
1:B:222:ASP:HB2	3:B:316:HOH:O	2.05	0.56
1:A:119:GLN:HB3	1:A:125:GLY:N	2.20	0.56
1:C:127:LEU:O	1:C:154:THR:HG21	2.06	0.56
1:D:11:LYS:HZ1	1:D:13:LYS:HD2	1.70	0.56
1:A:146:GLU:HG3	1:A:155:LEU:HD21	1.88	0.56
1:B:156:THR:HG22	1:B:186:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:ILE:HG22	1:A:145:VAL:HG12	1.87	0.56
1:D:11:LYS:HE3	1:D:13:LYS:HD2	1.86	0.56
1:D:78:LEU:HD12	1:D:112:TYR:HD2	1.71	0.56
1:D:71:GLU:HG2	1:D:109:PHE:HE2	1.71	0.56
1:B:75:ILE:HG12	1:B:113:VAL:HG22	1.87	0.56
1:D:6:ILE:HG21	1:D:163:LYS:HD2	1.88	0.56
1:C:180:THR:HG23	1:C:182:ARG:H	1.69	0.56
1:C:186:LEU:N	1:C:186:LEU:HD23	2.21	0.56
1:C:89:ILE:H	1:C:89:ILE:CD1	2.16	0.56
1:C:162:LEU:O	1:C:165:VAL:HG22	2.06	0.56
1:A:114:ARG:HE	1:A:130:LEU:HD21	1.70	0.56
1:B:15:ARG:HH22	1:B:187:LYS:HD2	1.69	0.56
1:C:115:LEU:HD13	1:C:130:LEU:CB	2.22	0.56
1:A:225:ARG:O	1:A:229:GLU:HB3	2.06	0.56
1:C:82:ARG:HD2	1:C:86:ASN:ND2	2.19	0.55
1:B:41:TYR:OH	1:B:227:LYS:HE3	2.06	0.55
1:C:49:GLY:HA2	1:C:52:VAL:HG13	1.87	0.55
1:A:120:ASN:N	1:A:120:ASN:C	2.57	0.55
1:D:230:LYS:HD2	1:D:231:VAL:O	2.06	0.55
1:B:223:ALA:O	1:B:227:LYS:HB3	2.06	0.55
1:A:175:LEU:O	1:A:175:LEU:HG	2.07	0.55
1:B:74:ILE:HG13	1:B:145:VAL:CG1	2.36	0.55
1:A:126:GLN:HA	1:A:153:PHE:CE2	2.41	0.55
1:B:47:LEU:HD12	1:B:217:VAL:CG2	2.36	0.55
1:A:105:VAL:CG2	1:A:106:PRO:HD2	2.37	0.55
1:C:153:PHE:O	1:C:153:PHE:CG	2.60	0.55
1:B:63:ILE:HD12	1:B:67:TYR:CD2	2.41	0.55
1:D:229:GLU:O	1:D:230:LYS:HB2	2.07	0.55
1:C:61:TYR:HE2	1:C:65:ARG:HH11	1.55	0.55
1:B:134:LEU:HD23	1:B:137:PHE:HE2	1.72	0.55
1:D:81:SER:OG	1:D:146:GLU:HA	2.06	0.55
1:A:199:TRP:CE3	1:A:220:LEU:HD22	2.42	0.55
1:C:128:THR:HA	1:C:154:THR:CG2	2.33	0.55
1:B:65:ARG:NH1	1:B:65:ARG:HG2	2.22	0.55
1:C:199:TRP:HB3	1:C:220:LEU:HD21	1.89	0.55
1:C:17:GLU:CG	1:C:18:PRO:HD2	2.37	0.54
1:D:138:ARG:CA	1:D:165:VAL:HG23	2.37	0.54
1:A:151:THR:HG22	1:A:153:PHE:CB	2.37	0.54
1:A:74:ILE:HG22	1:A:145:VAL:CG1	2.38	0.54
1:B:19:MET:HE2	1:B:21:ILE:HD11	1.87	0.54
1:A:88:LEU:O	1:A:92:LEU:HB2	2.06	0.54
1:C:199:TRP:HB3	1:C:220:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:186:LEU:O	3:D:243:HOH:O	2.18	0.54
1:A:105:VAL:HG23	1:A:106:PRO:HD2	1.90	0.54
1:A:196:GLU:HG2	3:A:272:HOH:O	2.07	0.54
1:B:129:VAL:HG13	3:B:293:HOH:O	2.07	0.54
1:B:17:GLU:HG2	3:B:295:HOH:O	2.08	0.54
1:C:19:MET:CE	1:C:21:ILE:HD11	2.38	0.54
1:D:138:ARG:HA	1:D:165:VAL:O	2.08	0.54
1:A:151:THR:C	1:A:153:PHE:H	2.10	0.54
1:C:102:GLU:HB3	3:C:258:HOH:O	2.08	0.54
1:C:222:ASP:O	1:C:225:ARG:HB2	2.08	0.54
1:B:75:ILE:CG1	1:B:113:VAL:HG22	2.38	0.54
1:A:6:ILE:HG22	1:A:6:ILE:O	2.07	0.54
1:D:6:ILE:CG2	1:D:163:LYS:HD2	2.38	0.54
1:A:63:ILE:HD11	1:A:190:PHE:CG	2.42	0.53
1:D:20:TYR:CE2	1:D:179:ARG:NH2	2.76	0.53
1:D:11:LYS:HG3	1:D:13:LYS:H	1.73	0.53
1:A:181:ASP:O	1:A:181:ASP:CG	2.45	0.53
1:A:203:CYS:C	1:A:203:CYS:CB	2.74	0.53
1:B:63:ILE:HD13	1:B:143:LEU:HD22	1.90	0.53
1:B:134:LEU:CD2	1:B:137:PHE:HE2	2.21	0.53
1:C:175:LEU:HD12	1:C:175:LEU:O	2.08	0.53
1:B:71:GLU:O	1:B:141:HIS:HB2	2.08	0.53
1:D:67:TYR:OH	1:D:171:ARG:HD2	2.08	0.53
1:D:130:LEU:HD13	1:D:130:LEU:O	2.09	0.53
1:D:178:LYS:HE2	1:D:198:VAL:H	1.74	0.53
1:D:71:GLU:HG2	1:D:109:PHE:CE2	2.43	0.53
1:A:138:ARG:HG2	1:A:139:ASP:OD2	2.09	0.53
1:C:48:PRO:HA	1:C:216:HIS:CD2	2.44	0.53
1:B:178:LYS:HG3	1:B:195:ILE:HG13	1.91	0.53
1:C:139:ASP:O	1:C:168:LYS:HB2	2.09	0.53
1:C:85:PHE:HE2	1:C:112:TYR:HH	1.56	0.53
1:A:114:ARG:CD	1:A:130:LEU:HD11	2.38	0.52
1:C:79:LYS:NZ	1:D:112:TYR:HD1	2.05	0.52
1:A:159:GLY:O	1:A:163:LYS:HG3	2.09	0.52
1:C:158:PHE:CD1	1:C:161:ARG:NH1	2.78	0.52
1:D:85:PHE:HB2	1:D:145:VAL:HG21	1.92	0.52
1:A:144:ILE:HD11	1:A:155:LEU:CD1	2.34	0.52
1:A:141:HIS:CE1	1:A:168:LYS:HD3	2.44	0.52
1:B:8:ASP:O	1:B:11:LYS:HG3	2.09	0.52
1:D:34:VAL:CG1	1:D:39:LYS:HA	2.39	0.52
1:B:133:ASP:OD1	1:B:135:SER:HB3	2.10	0.52
1:B:173:ALA:HA	1:B:190:PHE:O	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:VAL:CG2	1:A:219:VAL:HG13	2.39	0.52
1:D:19:MET:HE1	1:D:193:PHE:CE1	2.43	0.51
1:C:82:ARG:NH1	1:D:110:GLU:OE1	2.43	0.51
1:B:32:PHE:O	1:D:58:LYS:HD3	2.09	0.51
1:B:129:VAL:CG1	1:B:158:PHE:HB2	2.39	0.51
1:B:155:LEU:HB3	1:B:186:LEU:CD1	2.41	0.51
1:C:207:PHE:HD2	1:C:211:PHE:HE2	1.59	0.51
1:A:171:ARG:HG2	1:A:189:ASP:CG	2.30	0.51
1:A:76:CYS:HB2	1:A:85:PHE:CD1	2.45	0.51
1:A:100:GLY:HA3	1:D:65:ARG:NH2	2.26	0.51
1:A:34:VAL:CG2	1:A:39:LYS:HG2	2.34	0.51
1:C:8:ASP:O	1:C:11:LYS:HB2	2.11	0.51
1:A:182:ARG:HD2	1:A:185:SER:HB2	1.93	0.51
1:D:87:LEU:O	1:D:90:ASP:HB3	2.11	0.51
1:A:67:TYR:OH	1:A:171:ARG:HD2	2.10	0.51
1:D:49:GLY:O	1:D:52:VAL:HB	2.11	0.51
1:A:38:CYS:HB3	1:A:42:ILE:HD12	1.93	0.50
1:B:115:LEU:HD12	1:B:129:VAL:HA	1.94	0.50
1:B:57:GLU:OE2	1:C:98:TYR:OH	2.21	0.50
1:C:77:ILE:HD13	1:C:113:VAL:HG22	1.93	0.50
1:A:114:ARG:O	1:A:115:LEU:HB2	2.10	0.50
1:D:11:LYS:HE3	1:D:13:LYS:HB2	1.93	0.50
1:B:128:THR:HG22	1:B:129:VAL:O	2.12	0.50
1:B:89:ILE:HB	1:B:108:PHE:CZ	2.46	0.50
1:C:114:ARG:O	1:C:115:LEU:HB2	2.10	0.50
1:D:129:VAL:HG13	1:D:158:PHE:CB	2.28	0.50
1:B:68:PHE:CD2	1:B:101:ARG:NH1	2.79	0.50
1:D:202:GLY:HA2	1:D:211:PHE:O	2.12	0.50
1:C:17:GLU:HG3	1:C:18:PRO:HD2	1.94	0.50
1:D:13:LYS:O	1:D:13:LYS:HG3	2.10	0.49
1:B:206:ASP:HB3	1:B:212:ARG:HG2	1.94	0.49
1:C:174:THR:CG2	1:C:191:VAL:HG23	2.41	0.49
1:C:99:SER:C	1:C:101:ARG:H	2.16	0.49
1:C:147:ASP:O	1:C:175:LEU:HB3	2.12	0.49
1:C:177:GLU:OE1	3:C:321:HOH:O	2.20	0.49
1:B:42:ILE:HD12	1:B:218:ALA:CB	2.42	0.49
1:D:129:VAL:HG22	1:D:158:PHE:CD1	2.46	0.49
1:B:174:THR:HG23	1:B:191:VAL:HB	1.94	0.49
1:A:129:VAL:HG22	1:A:129:VAL:O	2.12	0.49
1:B:71:GLU:HA	3:B:287:HOH:O	2.11	0.49
1:B:158:PHE:HD1	1:B:161:ARG:HH12	1.61	0.49
1:C:220:LEU:HD23	1:C:220:LEU:N	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:229:GLU:CG	1:B:230:LYS:N	2.75	0.49
1:B:142:VAL:HG13	1:B:142:VAL:O	2.13	0.49
1:A:137:PHE:O	1:A:167:PRO:HA	2.13	0.49
1:B:199:TRP:CD1	1:B:220:LEU:CB	2.96	0.49
1:D:165:VAL:HG23	1:D:165:VAL:O	2.11	0.49
1:C:128:THR:CG2	1:C:129:VAL:N	2.76	0.49
1:C:129:VAL:HG11	1:C:158:PHE:CD1	2.48	0.49
1:C:62:ASP:O	1:C:66:THR:HG23	2.13	0.49
1:B:15:ARG:CG	1:B:16:ILE:N	2.75	0.49
1:C:168:LYS:HG2	1:C:168:LYS:O	2.13	0.49
1:A:82:ARG:HD3	1:B:112:TYR:OH	2.12	0.49
1:D:230:LYS:HD2	1:D:231:VAL:H	1.75	0.49
1:B:13:LYS:HG2	3:B:311:HOH:O	2.13	0.48
3:A:329:HOH:O	1:B:130:LEU:HD12	2.12	0.48
1:D:207:PHE:CD2	1:D:228:PHE:HB2	2.48	0.48
1:B:26:PHE:HD2	3:B:257:HOH:O	1.95	0.48
1:A:151:THR:HG22	1:A:153:PHE:HB3	1.94	0.48
1:B:176:VAL:HG13	1:B:195:ILE:HG12	1.95	0.48
1:C:41:TYR:CE2	1:C:228:PHE:CZ	3.01	0.48
1:C:96:GLN:HB2	3:C:253:HOH:O	2.13	0.48
1:C:29:ALA:O	1:C:32:PHE:HB2	2.14	0.48
1:C:202:GLY:O	1:C:205:TYR:HB2	2.14	0.48
1:A:23:ASP:OD1	1:A:196:GLU:HB3	2.13	0.48
1:C:114:ARG:CG	1:C:115:LEU:N	2.77	0.48
1:C:93:ALA:O	1:C:96:GLN:HB2	2.14	0.48
1:D:172:ILE:HG12	1:D:188:GLY:CA	2.35	0.48
1:C:11:LYS:NZ	1:C:13:LYS:HD3	2.28	0.48
1:A:142:VAL:HG12	3:A:296:HOH:O	2.13	0.48
1:A:172:ILE:O	1:A:189:ASP:N	2.39	0.48
1:B:112:TYR:CD1	1:B:112:TYR:N	2.80	0.48
1:A:68:PHE:HZ	1:A:102:GLU:O	1.97	0.48
1:C:130:LEU:C	1:C:130:LEU:HD13	2.34	0.48
1:B:59:LEU:O	1:B:63:ILE:HG23	2.14	0.48
1:A:182:ARG:HG2	1:A:183:SER:N	2.29	0.48
1:D:24:ASN:HA	1:D:26:PHE:CE1	2.47	0.48
1:D:225:ARG:O	1:D:229:GLU:HB2	2.13	0.48
1:A:74:ILE:HG23	1:A:143:LEU:HD23	1.96	0.48
1:C:114:ARG:HH22	1:D:114:ARG:HE	1.60	0.47
1:A:37:HIS:CD2	1:B:106:PRO:HA	2.48	0.47
1:B:70:GLU:O	3:B:287:HOH:O	2.20	0.47
1:A:33:LEU:N	1:C:58:LYS:HG2	2.29	0.47
1:D:129:VAL:CG2	1:D:158:PHE:CD1	2.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:78:LEU:CD2	1:B:78:LEU:HD11	2.40	0.47
1:B:127:LEU:O	1:B:154:THR:HB	2.14	0.47
1:C:187:LYS:HG2	3:C:263:HOH:O	2.12	0.47
1:D:230:LYS:HD3	1:D:230:LYS:HA	1.73	0.47
1:B:155:LEU:HB3	1:B:186:LEU:HD13	1.96	0.47
1:C:89:ILE:HA	1:C:92:LEU:HB2	1.96	0.47
1:A:173:ALA:HA	1:A:190:PHE:O	2.13	0.47
1:C:85:PHE:HE2	1:C:112:TYR:OH	1.97	0.47
1:A:65:ARG:HA	1:A:65:ARG:HD3	1.51	0.47
1:C:115:LEU:CB	1:C:130:LEU:H	2.26	0.47
1:A:114:ARG:HG3	1:A:130:LEU:HG	1.96	0.47
1:C:155:LEU:CB	1:C:186:LEU:HD12	2.40	0.47
1:C:150:ASP:OD1	1:C:150:ASP:N	2.48	0.47
1:D:41:TYR:O	1:D:221:SER:HB2	2.14	0.47
1:D:136:ILE:HG23	1:D:137:PHE:CD1	2.50	0.47
1:B:96:GLN:HB3	1:B:96:GLN:HE21	1.51	0.47
1:A:126:GLN:HA	1:A:153:PHE:HE2	1.79	0.47
1:D:52:VAL:O	1:D:56:VAL:HG23	2.15	0.47
1:D:144:ILE:HD13	1:D:158:PHE:HE2	1.79	0.46
1:D:19:MET:CE	1:D:193:PHE:CE1	2.98	0.46
1:B:222:ASP:O	1:B:226:LYS:HB2	2.15	0.46
1:C:57:GLU:HB2	1:C:91:TYR:CZ	2.50	0.46
1:B:207:PHE:CE2	1:B:228:PHE:HB2	2.49	0.46
1:B:40:PRO:HG2	1:B:41:TYR:CD2	2.49	0.46
1:A:49:GLY:HA2	1:A:52:VAL:HG13	1.97	0.46
1:A:87:LEU:HA	1:A:87:LEU:HD12	1.62	0.46
1:B:34:VAL:HA	1:B:35:PRO:HD3	1.69	0.46
1:A:142:VAL:CG1	3:A:296:HOH:O	2.64	0.46
1:A:126:GLN:O	1:A:126:GLN:HG3	2.15	0.46
1:C:41:TYR:CE2	1:C:228:PHE:CE2	3.03	0.46
1:A:104:SER:OG	1:A:104:SER:O	2.30	0.46
1:C:158:PHE:CE2	1:C:162:LEU:CD2	2.96	0.46
1:A:140:LYS:O	1:A:168:LYS:N	2.48	0.46
1:D:39:LYS:CB	1:D:40:PRO:HD3	2.32	0.46
1:C:187:LYS:HD2	1:C:187:LYS:HA	1.74	0.46
1:D:63:ILE:O	1:D:66:THR:HB	2.15	0.46
1:C:158:PHE:HD1	1:C:161:ARG:HH12	1.64	0.46
1:D:130:LEU:C	1:D:130:LEU:CD1	2.84	0.46
1:D:136:ILE:HG23	1:D:137:PHE:CE1	2.51	0.46
1:C:89:ILE:CG2	1:C:108:PHE:CE2	2.99	0.46
1:B:202:GLY:HA2	1:B:211:PHE:O	2.16	0.46
1:D:108:PHE:N	1:D:108:PHE:CD1	2.83	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:206:ASP:OD1	1:C:209:GLU:HA	2.16	0.46
1:C:198:VAL:CG1	1:C:199:TRP:N	2.79	0.46
1:D:69:GLY:O	1:D:70:GLU:HG2	2.16	0.46
1:C:163:LYS:HB2	1:C:163:LYS:HZ2	1.77	0.45
1:A:196:GLU:O	1:A:198:VAL:HG12	2.16	0.45
1:C:138:ARG:O	1:C:139:ASP:HB2	2.15	0.45
1:D:176:VAL:CG1	1:D:177:GLU:N	2.79	0.45
1:D:6:ILE:CG2	1:D:163:LYS:CD	2.93	0.45
1:C:61:TYR:CE2	1:C:65:ARG:HD2	2.52	0.45
1:C:200:ILE:HG13	1:C:200:ILE:O	2.16	0.45
1:A:144:ILE:CD1	1:A:155:LEU:HD11	2.37	0.45
1:B:220:LEU:HD22	1:B:221:SER:N	2.32	0.45
1:D:43:ASP:HA	3:D:280:HOH:O	2.15	0.45
1:C:131:SER:HB2	1:C:132:ASP:H	1.43	0.45
1:C:171:ARG:HA	1:C:189:ASP:OD2	2.17	0.45
1:A:77:ILE:HD11	1:A:144:ILE:HD11	1.98	0.45
1:C:148:ILE:CG1	1:C:149:VAL:N	2.78	0.45
1:C:59:LEU:O	1:C:63:ILE:HD12	2.15	0.45
1:A:52:VAL:HA	1:A:193:PHE:HZ	1.82	0.45
1:D:39:LYS:N	1:D:40:PRO:CD	2.79	0.45
1:D:77:ILE:HG13	1:D:146:GLU:HG2	1.98	0.45
1:A:96:GLN:CG	1:A:107:PRO:HG3	2.47	0.45
1:D:34:VAL:HG12	1:D:39:LYS:HA	1.99	0.45
1:C:202:GLY:O	1:C:205:TYR:HD2	1.99	0.45
1:B:134:LEU:CD2	1:B:137:PHE:CE2	2.99	0.45
1:B:141:HIS:CD2	1:B:168:LYS:HD2	2.52	0.45
1:B:230:LYS:HG3	1:B:230:LYS:O	2.16	0.45
1:B:148:ILE:HD13	1:B:148:ILE:HG21	1.67	0.45
1:C:170:MET:O	1:C:171:ARG:HG2	2.17	0.45
1:B:207:PHE:O	1:B:210:MET:HB2	2.17	0.45
1:A:142:VAL:CB	3:A:296:HOH:O	2.61	0.45
1:C:179:ARG:HH21	1:C:196:GLU:HB2	1.82	0.45
1:B:4:LYS:HD2	1:B:4:LYS:HA	1.39	0.45
1:D:78:LEU:HD12	1:D:112:TYR:CD2	2.50	0.45
1:D:224:ALA:O	1:D:228:PHE:HB2	2.17	0.45
1:D:22:PRO:HB2	1:D:25:THR:HG21	1.98	0.45
1:A:22:PRO:HG2	1:A:25:THR:OG1	2.17	0.45
1:D:39:LYS:HB3	1:D:40:PRO:CD	2.42	0.45
1:B:134:LEU:HD13	1:B:162:LEU:HD13	1.99	0.45
1:B:200:ILE:HA	1:B:218:ALA:O	2.17	0.45
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.69	0.45
1:C:39:LYS:N	1:C:40:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:180:THR:CG2	1:D:181:ASP:N	2.77	0.44
1:A:108:PHE:CD1	1:A:108:PHE:N	2.85	0.44
1:B:208:ASN:O	1:B:209:GLU:HB2	2.17	0.44
1:D:74:ILE:HG22	1:D:85:PHE:CE1	2.50	0.44
1:C:139:ASP:OD1	1:C:139:ASP:O	2.36	0.44
1:D:19:MET:HE3	1:D:21:ILE:CD1	2.35	0.44
1:A:151:THR:C	1:A:153:PHE:N	2.70	0.44
1:D:129:VAL:O	1:D:161:ARG:NH2	2.50	0.44
1:A:6:ILE:HG21	1:A:170:MET:CG	2.47	0.44
1:C:216:HIS:ND1	1:C:216:HIS:N	2.49	0.44
1:B:55:ARG:HD2	1:B:55:ARG:HA	1.70	0.44
1:C:138:ARG:HH11	1:C:138:ARG:CG	2.30	0.44
1:D:51:LEU:HD23	1:D:51:LEU:HA	1.67	0.44
1:D:79:LYS:HE2	1:D:212:ARG:NH2	2.33	0.44
1:B:106:PRO:HG2	1:B:109:PHE:CZ	2.53	0.44
1:C:207:PHE:CE2	1:C:225:ARG:HA	2.51	0.44
1:A:63:ILE:CD1	1:A:190:PHE:CG	3.00	0.44
1:A:100:GLY:CA	1:D:65:ARG:HH21	2.30	0.44
1:C:77:ILE:HD13	1:C:113:VAL:CG2	2.47	0.44
1:C:72:LEU:HD13	1:C:74:ILE:HG12	1.98	0.44
1:B:227:LYS:CD	1:B:227:LYS:O	2.65	0.44
1:B:66:THR:HG21	1:B:190:PHE:HZ	1.83	0.44
1:B:136:ILE:O	1:B:140:LYS:HE3	2.18	0.44
1:B:61:TYR:O	1:B:64:HIS:HB3	2.17	0.44
1:D:23:ASP:O	1:D:25:THR:HG23	2.18	0.44
1:B:75:ILE:C	1:B:75:ILE:HD13	2.38	0.44
1:C:18:PRO:CB	1:C:191:VAL:HG13	2.47	0.44
1:C:11:LYS:HZ1	1:C:13:LYS:HD3	1.82	0.44
1:B:155:LEU:HB2	3:B:315:HOH:O	2.18	0.43
1:D:207:PHE:HE2	1:D:225:ARG:HA	1.78	0.43
1:C:148:ILE:HG22	1:C:205:TYR:HE1	1.84	0.43
1:A:15:ARG:HH12	1:A:191:VAL:HG11	1.78	0.43
1:C:35:PRO:CB	1:C:36:PRO:HD2	2.45	0.43
1:B:134:LEU:HD23	1:B:137:PHE:CE2	2.51	0.43
1:C:220:LEU:HD23	1:C:220:LEU:H	1.82	0.43
1:D:151:THR:HG22	1:D:152:GLY:N	2.33	0.43
1:C:56:VAL:HG22	1:C:84:PHE:CE1	2.48	0.43
1:C:175:LEU:O	1:C:192:GLY:HA3	2.18	0.43
1:A:51:LEU:HD22	1:A:51:LEU:O	2.18	0.43
1:A:182:ARG:HB2	1:A:182:ARG:NH1	2.33	0.43
1:C:47:LEU:O	1:C:216:HIS:HB3	2.18	0.43
1:A:148:ILE:HD12	1:A:176:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:79:LYS:HE3	3:B:261:HOH:O	2.18	0.43
1:C:16:ILE:HG13	1:C:17:GLU:N	2.32	0.43
1:D:202:GLY:O	1:D:205:TYR:HD2	2.01	0.43
1:A:35:PRO:HA	1:A:36:PRO:HD3	1.78	0.43
1:A:89:ILE:HB	1:A:108:PHE:CZ	2.54	0.43
1:D:143:LEU:HD11	1:D:173:ALA:HB2	2.01	0.43
1:D:114:ARG:O	1:D:130:LEU:HB3	2.18	0.43
1:D:151:THR:CG2	1:D:153:PHE:HB3	2.48	0.43
1:C:29:ALA:CA	1:C:45:ILE:CD1	2.97	0.43
1:C:29:ALA:HB2	1:C:45:ILE:CD1	2.48	0.43
1:C:9:TYR:CD1	1:C:170:MET:HE2	2.54	0.43
1:C:148:ILE:HG12	1:C:149:VAL:N	2.34	0.43
1:B:142:VAL:CG1	1:B:170:MET:HG3	2.49	0.43
1:B:220:LEU:HD11	1:B:225:ARG:HB2	2.00	0.43
1:B:130:LEU:HA	1:B:130:LEU:HD23	1.47	0.43
1:C:6:ILE:HD13	1:C:6:ILE:C	2.38	0.43
1:C:97:LYS:NZ	1:D:215:ASP:OD2	2.48	0.43
1:A:33:LEU:HD23	1:A:33:LEU:C	2.39	0.42
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.50	0.42
1:B:42:ILE:CD1	1:B:218:ALA:CB	2.97	0.42
1:D:140:LYS:N	1:D:168:LYS:H	2.17	0.42
1:D:15:ARG:NH1	1:D:191:VAL:HG21	2.34	0.42
1:A:56:VAL:HG23	1:A:91:TYR:CD2	2.54	0.42
1:D:230:LYS:HD3	1:D:231:VAL:H	1.78	0.42
1:A:157:GLU:HG3	1:A:158:PHE:N	2.34	0.42
1:C:68:PHE:CZ	1:C:101:ARG:CG	3.02	0.42
1:B:137:PHE:O	1:B:140:LYS:HB2	2.19	0.42
1:B:227:LYS:HG3	1:B:228:PHE:CD2	2.55	0.42
1:C:48:PRO:O	1:C:52:VAL:HG13	2.19	0.42
1:A:210:MET:O	1:A:211:PHE:HB2	2.19	0.42
1:B:129:VAL:HG21	1:B:158:PHE:CE1	2.55	0.42
1:C:21:ILE:HG23	1:C:21:ILE:HD12	1.71	0.42
1:C:79:LYS:HG2	1:C:79:LYS:HZ2	1.75	0.42
1:D:129:VAL:CG1	1:D:158:PHE:CB	2.93	0.42
1:B:187:LYS:HD3	1:B:187:LYS:HA	1.08	0.42
1:D:64:HIS:O	1:D:68:PHE:HB2	2.20	0.42
1:B:155:LEU:CB	1:B:186:LEU:CD1	2.98	0.42
1:A:182:ARG:CZ	1:A:182:ARG:CB	2.98	0.42
1:D:189:ASP:HB3	3:D:294:HOH:O	2.18	0.42
1:A:119:GLN:HB3	1:A:124:THR:C	2.40	0.42
1:D:172:ILE:HG21	1:D:172:ILE:HD12	1.86	0.42
1:A:182:ARG:HG2	1:A:183:SER:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:ILE:CD1	1:A:190:PHE:CD2	3.03	0.42
1:D:56:VAL:HG11	1:D:87:LEU:HB3	2.00	0.42
1:D:207:PHE:CD2	1:D:228:PHE:CB	3.03	0.42
1:D:178:LYS:HD3	1:D:195:ILE:CG1	2.49	0.42
1:A:113:VAL:HG12	1:A:131:SER:CB	2.42	0.42
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.87	0.42
1:D:183:SER:HB3	1:D:185:SER:H	1.85	0.42
1:C:172:ILE:HG22	1:C:173:ALA:N	2.35	0.42
1:C:163:LYS:HB2	1:C:163:LYS:HZ3	1.83	0.42
1:A:202:GLY:O	1:A:205:TYR:HB2	2.20	0.41
1:A:143:LEU:HD11	1:A:173:ALA:HB2	2.01	0.41
1:B:58:LYS:NZ	1:D:30:ASP:O	2.53	0.41
1:A:123:SER:HB2	1:A:124:THR:H	1.57	0.41
1:C:130:LEU:HA	1:C:130:LEU:HD22	1.27	0.41
1:A:78:LEU:HD13	1:A:112:TYR:HD1	1.85	0.41
1:B:59:LEU:O	1:B:63:ILE:CG2	2.69	0.41
1:B:105:VAL:HG23	1:B:106:PRO:CD	2.31	0.41
1:D:19:MET:CE	1:D:193:PHE:CD1	3.04	0.41
1:C:159:GLY:O	1:C:170:MET:HE1	2.19	0.41
1:C:82:ARG:CD	1:C:86:ASN:ND2	2.83	0.41
1:A:151:THR:CG2	1:A:153:PHE:HB3	2.50	0.41
1:A:174:THR:O	1:A:191:VAL:HA	2.21	0.41
1:A:202:GLY:HA2	1:A:211:PHE:O	2.20	0.41
1:D:187:LYS:HB3	1:D:187:LYS:HE3	1.74	0.41
1:D:79:LYS:HD2	1:D:79:LYS:HA	1.22	0.41
1:A:56:VAL:HG21	1:A:87:LEU:HB3	2.03	0.41
1:B:155:LEU:HB2	1:B:186:LEU:HD12	2.03	0.41
1:C:174:THR:O	1:C:191:VAL:HA	2.20	0.41
1:C:114:ARG:HG2	1:C:115:LEU:N	2.33	0.41
1:A:100:GLY:HA3	1:D:65:ARG:HH21	1.85	0.41
1:C:44:LYS:HG3	1:C:219:VAL:CB	2.51	0.41
1:B:138:ARG:O	1:B:139:ASP:HB2	2.21	0.41
1:A:114:ARG:CG	1:A:130:LEU:HD11	2.51	0.41
1:A:45:ILE:HD13	1:A:216:HIS:HB2	2.03	0.41
1:A:6:ILE:HG21	1:A:170:MET:HG3	2.03	0.41
1:C:6:ILE:HG23	1:C:7:GLU:OE2	2.21	0.41
1:D:51:LEU:C	1:D:51:LEU:HD22	2.41	0.41
1:C:136:ILE:CD1	1:C:136:ILE:C	2.88	0.41
1:B:206:ASP:HA	1:B:210:MET:O	2.20	0.41
1:B:220:LEU:CD1	1:B:225:ARG:HB2	2.51	0.41
1:D:82:ARG:HD2	1:D:86:ASN:HD22	1.85	0.41
1:A:198:VAL:HG22	1:A:199:TRP:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:GLY:CA	1:D:65:ARG:NH2	2.83	0.41
1:C:77:ILE:CD1	1:C:113:VAL:CG2	2.98	0.41
1:B:58:LYS:HG3	1:B:58:LYS:O	2.21	0.41
1:D:84:PHE:O	1:D:88:LEU:HB2	2.21	0.41
1:C:155:LEU:HD12	1:C:155:LEU:HA	1.11	0.41
1:B:193:PHE:N	1:B:193:PHE:CD1	2.89	0.41
1:C:82:ARG:O	1:C:86:ASN:HB2	2.21	0.40
1:A:107:PRO:HB2	1:A:108:PHE:CD1	2.56	0.40
1:B:36:PRO:HG2	1:B:37:HIS:H	1.86	0.40
1:D:178:LYS:CD	1:D:197:ASP:HA	2.38	0.40
1:B:156:THR:CG2	1:B:186:LEU:HD11	2.51	0.40
1:A:78:LEU:HA	1:A:78:LEU:HD12	1.61	0.40
1:D:44:LYS:HE2	1:D:219:VAL:HG11	2.03	0.40
1:B:105:VAL:CG2	1:B:106:PRO:CD	2.95	0.40
1:A:6:ILE:HD12	1:A:170:MET:CG	2.38	0.40
1:D:207:PHE:HD2	1:D:228:PHE:HB2	1.87	0.40
1:D:107:PRO:CB	1:D:108:PHE:CD1	3.01	0.40
1:B:207:PHE:HE2	1:B:228:PHE:HB2	1.86	0.40
1:A:172:ILE:O	1:A:172:ILE:HG13	2.18	0.40
1:D:166:GLY:N	1:D:167:PRO:HD3	2.35	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	223/231 (96%)	184 (82%)	28 (13%)	11 (5%)	3	2
1	B	215/231 (93%)	189 (88%)	18 (8%)	8 (4%)	5	4
1	C	211/231 (91%)	171 (81%)	27 (13%)	13 (6%)	2	1
1	D	211/231 (91%)	186 (88%)	20 (10%)	5 (2%)	9	9
All	All	860/924 (93%)	730 (85%)	93 (11%)	37 (4%)	4	3

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	79	LYS
1	A	121	ASP
1	A	230	LYS
1	B	182	ARG
1	B	183	SER
1	B	229	GLU
1	B	230	LYS
1	C	15	ARG
1	C	131	SER
1	C	139	ASP
1	C	154	THR
1	D	79	LYS
1	A	122	ASN
1	A	182	ARG
1	C	128	THR
1	C	207	PHE
1	C	208	ASN
1	D	13	LYS
1	D	132	ASP
1	D	183	SER
1	A	102	GLU
1	A	120	ASN
1	A	132	ASP
1	B	5	PRO
1	C	79	LYS
1	C	228	PHE
1	A	13	LYS
1	B	79	LYS
1	C	152	GLY
1	C	223	ALA
1	C	184	ASN
1	D	148	ILE
1	A	148	ILE
1	B	136	ILE
1	C	192	GLY
1	B	4	LYS

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	202/206 (98%)	147 (73%)	55 (27%)	0	0
1	B	195/206 (95%)	138 (71%)	57 (29%)	0	0
1	C	191/206 (93%)	126 (66%)	65 (34%)	0	0
1	D	192/206 (93%)	130 (68%)	62 (32%)	0	0
All	All	780/824 (95%)	541 (69%)	239 (31%)	0	0

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	ILE
1	A	8	ASP
1	A	11	LYS
1	A	13	LYS
1	A	39	LYS
1	A	41	TYR
1	A	43	ASP
1	A	51	LEU
1	A	52	VAL
1	A	65	ARG
1	A	66	THR
1	A	72	LEU
1	A	78	LEU
1	A	79	LYS
1	A	87	LEU
1	A	89	ILE
1	A	92	LEU
1	A	101	ARG
1	A	104	SER
1	A	107	PRO
1	A	119	GLN
1	A	120	ASN
1	A	123	SER
1	A	127	LEU
1	A	128	THR
1	A	129	VAL
1	A	136	ILE
1	A	140	LYS
1	A	144	ILE
1	A	145	VAL

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Mol	Chain	Res	Type
1	A	149	VAL
1	A	150	ASP
1	A	154	THR
1	A	155	LEU
1	A	157	GLU
1	A	160	GLU
1	A	162	LEU
1	A	172	ILE
1	A	180	THR
1	A	181	ASP
1	A	182	ARG
1	A	186	LEU
1	A	187	LYS
1	A	191	VAL
1	A	199	TRP
1	A	200	ILE
1	A	204	CYS
1	A	213	ASP
1	A	215	ASP
1	A	225	ARG
1	A	226	LYS
1	A	227	LYS
1	A	229	GLU
1	A	230	LYS
1	B	3	SER
1	B	4	LYS
1	B	6	ILE
1	B	13	LYS
1	B	15	ARG
1	B	21	ILE
1	B	30	ASP
1	B	44	LYS
1	B	46	LEU
1	B	47	LEU
1	B	51	LEU
1	B	53	LYS
1	B	55	ARG
1	B	63	ILE
1	B	65	ARG
1	B	66	THR
1	B	70	GLU
1	B	72	LEU

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Mol	Chain	Res	Type
1	B	74	ILE
1	B	75	ILE
1	B	79	LYS
1	B	82	ARG
1	B	87	LEU
1	B	92	LEU
1	B	94	THR
1	B	96	GLN
1	B	102	GLU
1	B	115	LEU
1	B	127	LEU
1	B	129	VAL
1	B	130	LEU
1	B	132	ASP
1	B	135	SER
1	B	138	ARG
1	B	145	VAL
1	B	147	ASP
1	B	149	VAL
1	B	150	ASP
1	B	154	THR
1	B	155	LEU
1	B	156	THR
1	B	157	GLU
1	B	161	ARG
1	B	162	LEU
1	B	168	LYS
1	B	180	THR
1	B	182	ARG
1	B	184	ASN
1	B	187	LYS
1	B	191	VAL
1	B	204	CYS
1	B	212	ARG
1	B	220	LEU
1	B	225	ARG
1	B	226	LYS
1	B	227	LYS
1	B	231	VAL
1	C	6	ILE
1	C	8	ASP
1	C	11	LYS

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Mol	Chain	Res	Type
1	C	16	ILE
1	C	17	GLU
1	C	28	ASN
1	C	30	ASP
1	C	41	TYR
1	C	42	ILE
1	C	43	ASP
1	C	44	LYS
1	C	46	LEU
1	C	47	LEU
1	C	51	LEU
1	C	65	ARG
1	C	66	THR
1	C	72	LEU
1	C	74	ILE
1	C	78	LEU
1	C	79	LYS
1	C	87	LEU
1	C	88	LEU
1	C	89	ILE
1	C	92	LEU
1	C	101	ARG
1	C	102	GLU
1	C	103	SER
1	C	104	SER
1	C	105	VAL
1	C	114	ARG
1	C	115	LEU
1	C	127	LEU
1	C	133	ASP
1	C	135	SER
1	C	136	ILE
1	C	138	ARG
1	C	144	ILE
1	C	153	PHE
1	C	154	THR
1	C	155	LEU
1	C	161	ARG
1	C	162	LEU
1	C	163	LYS
1	C	168	LYS
1	C	169	SER

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Mol	Chain	Res	Type
1	C	170	MET
1	C	171	ARG
1	C	174	THR
1	C	176	VAL
1	C	177	GLU
1	C	178	LYS
1	C	187	LYS
1	C	193	PHE
1	C	194	SER
1	C	196	GLU
1	C	198	VAL
1	C	203	CYS
1	C	204	CYS
1	C	209	GLU
1	C	216	HIS
1	C	217	VAL
1	C	220	LEU
1	C	227	LYS
1	C	229	GLU
1	C	230	LYS
1	D	6	ILE
1	D	11	LYS
1	D	21	ILE
1	D	26	PHE
1	D	30	ASP
1	D	38	CYS
1	D	42	ILE
1	D	45	ILE
1	D	47	LEU
1	D	51	LEU
1	D	53	LYS
1	D	58	LYS
1	D	72	LEU
1	D	78	LEU
1	D	79	LYS
1	D	87	LEU
1	D	88	LEU
1	D	90	ASP
1	D	94	THR
1	D	99	SER
1	D	102	GLU
1	D	104	SER

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Mol	Chain	Res	Type
1	D	105	VAL
1	D	110	GLU
1	D	115	LEU
1	D	128	THR
1	D	129	VAL
1	D	130	LEU
1	D	132	ASP
1	D	139	ASP
1	D	145	VAL
1	D	148	ILE
1	D	149	VAL
1	D	153	PHE
1	D	154	THR
1	D	160	GLU
1	D	162	LEU
1	D	165	VAL
1	D	168	LYS
1	D	172	ILE
1	D	181	ASP
1	D	182	ARG
1	D	183	SER
1	D	184	ASN
1	D	185	SER
1	D	187	LYS
1	D	194	SER
1	D	199	TRP
1	D	201	VAL
1	D	203	CYS
1	D	204	CYS
1	D	209	GLU
1	D	210	MET
1	D	215	ASP
1	D	220	LEU
1	D	221	SER
1	D	222	ASP
1	D	225	ARG
1	D	226	LYS
1	D	227	LYS
1	D	229	GLU
1	D	230	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	216	HIS
1	B	96	GLN
1	B	184	ASN
1	C	28	ASN
1	C	86	ASN
1	C	184	ASN
1	D	24	ASN
1	D	64	HIS
1	D	96	GLN
1	D	184	ASN
1	D	208	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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