



Full wwPDB X-ray Structure Validation Report i

Jun 25, 2024 – 06:08 PM JST

PDB ID : 9IJB
Title : Crystal structure and function analysis of a highly potential drug target 6-phosphogluconate dehydrogenase in *Mycobacterium tuberculosis*
Authors : Wang, Y.Z.; Ren, X.Q.; Li, T.; Zhang, R.D.
Deposited on : 2024-06-22
Resolution : 2.74 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

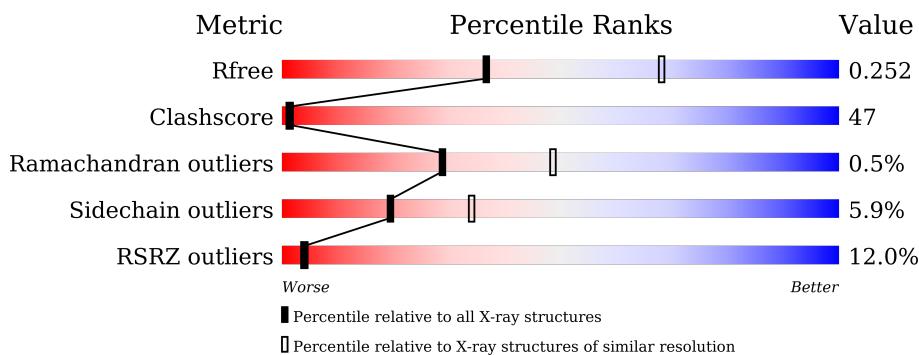
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

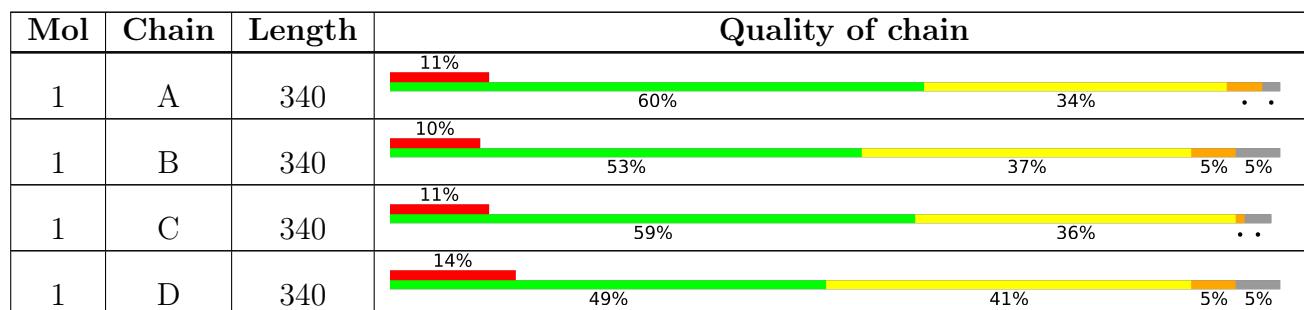
The reported resolution of this entry is 2.74 Å.

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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



2 Entry composition [\(i\)](#)

There are 2 unique types of molecules in this entry. The entry contains 9968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-phosphogluconate dehydrogenase, NAD(+) -dependent, de-carboxylating.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C 2500	N 1558	O 451	S 475	16	0	0
1	B	323	Total	C 2431	N 1518	O 437	S 460	16	0	0
1	C	331	Total	C 2486	N 1551	O 448	S 471	16	0	0
1	D	323	Total	C 2428	N 1517	O 436	S 460	15	0	0

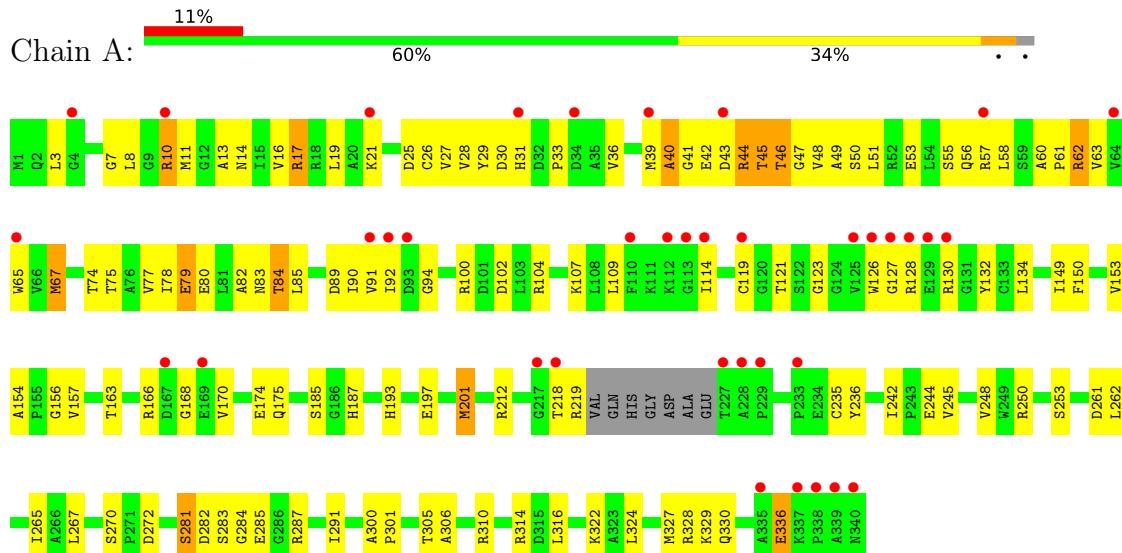
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0
2	B	33	Total O 33 33	0	0
2	C	33	Total O 33 33	0	0
2	D	20	Total O 20 20	0	0

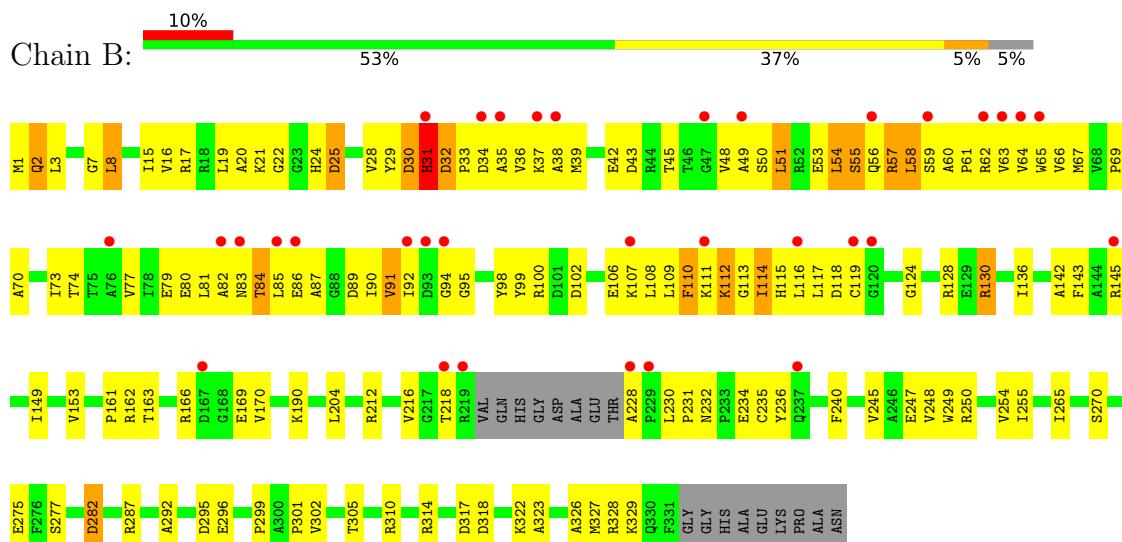
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 6-phosphogluconate dehydrogenase, NAD(+) -dependent, decarboxylating

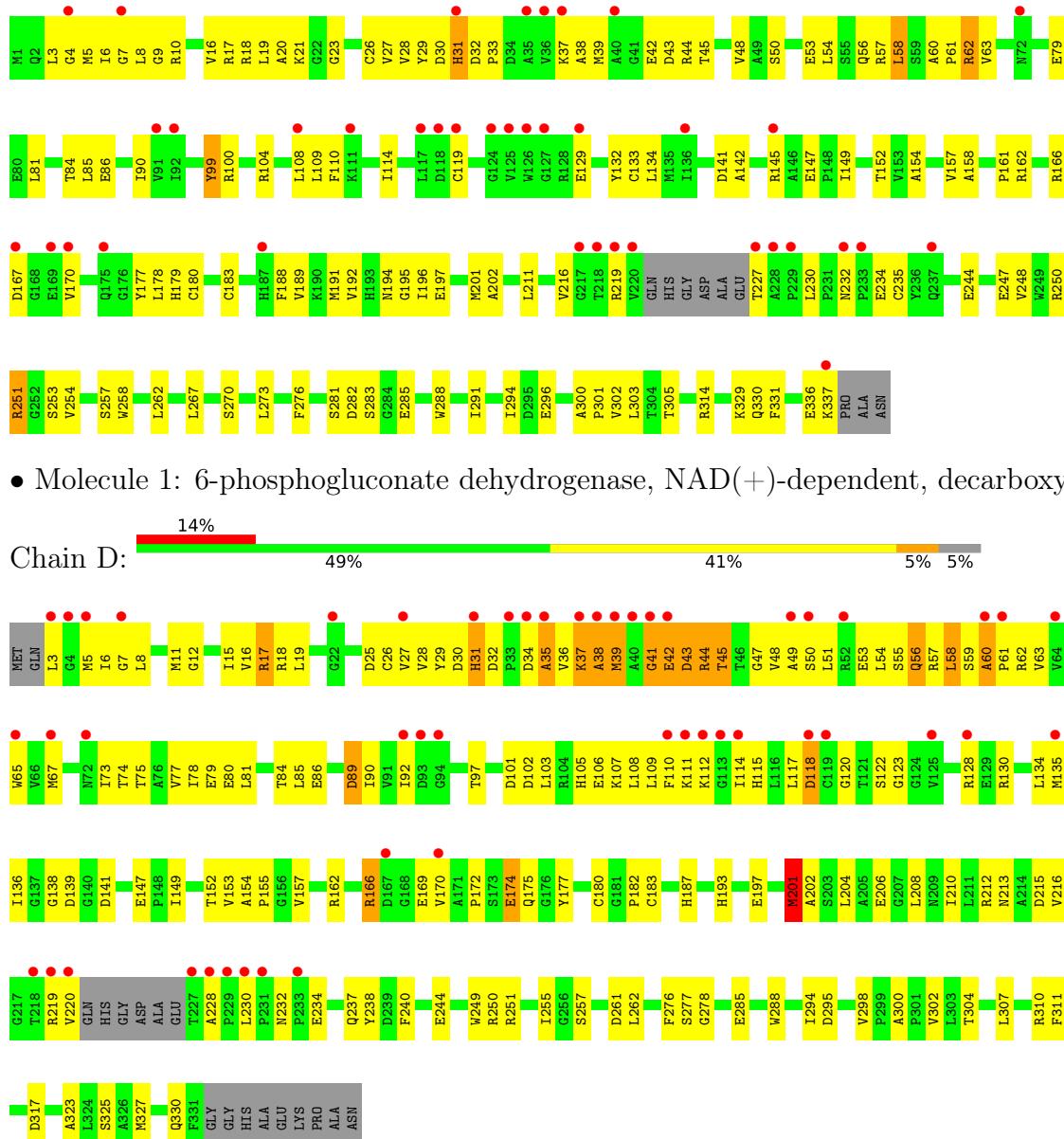


- Molecule 1: 6-phosphogluconate dehydrogenase, NAD(+) -dependent, decarboxylating



- Molecule 1: 6-phosphogluconate dehydrogenase, NAD(+) -dependent, decarboxylating





4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.99 Å 107.25 Å 137.02 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.81 – 2.74 26.81 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.3 (26.81-2.74) 99.3 (26.81-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.95 (at 2.76 Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R , R_{free}	0.198 , 0.251 0.198 , 0.252	Depositor DCC
R_{free} test set	1842 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.8	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9968	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	0.58	0/2550	0.72	1/3454 (0.0%)
1	B	0.59	0/2479	0.79	2/3359 (0.1%)
1	C	0.57	0/2535	0.71	2/3434 (0.1%)
1	D	0.58	0/2476	0.78	5/3357 (0.1%)
All	All	0.58	0/10040	0.75	10/13604 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	LEU	CB-CG-CD2	-6.00	100.79	111.00
1	D	38	ALA	N-CA-C	-5.89	95.11	111.00
1	D	201	MET	O-C-N	-5.73	113.54	122.70
1	D	41	GLY	N-CA-C	-5.66	98.95	113.10
1	C	9	GLY	N-CA-C	-5.29	99.86	113.10
1	C	211	LEU	CA-CB-CG	-5.20	103.34	115.30
1	B	218	THR	C-N-CA	-5.18	108.74	121.70
1	D	298	VAL	C-N-CD	5.15	139.21	128.40
1	D	60	ALA	C-N-CD	5.07	139.04	128.40
1	A	300	ALA	C-N-CD	5.03	138.96	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2500	0	2448	189	0
1	B	2431	0	2385	310	0
1	C	2486	0	2439	157	0
1	D	2428	0	2382	314	0
2	A	37	0	0	7	0
2	B	33	0	0	11	0
2	C	33	0	0	3	0
2	D	20	0	0	12	0
All	All	9968	0	9654	914	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (914) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ARG:HB2	1:D:89:ASP:CB	1.16	1.59
1:B:90:ILE:HG12	1:B:115:HIS:CB	1.18	1.57
1:B:90:ILE:CG1	1:B:115:HIS:HB2	1.29	1.56
1:D:62:ARG:HB2	1:D:89:ASP:CG	1.28	1.52
1:D:62:ARG:CB	1:D:89:ASP:CB	1.77	1.52
1:D:62:ARG:CB	1:D:89:ASP:HB3	1.30	1.48
1:B:90:ILE:CD1	1:B:145:ARG:NH2	1.76	1.48
1:B:90:ILE:HD11	1:B:145:ARG:NH2	1.22	1.45
1:D:27:VAL:CG1	1:D:54:LEU:HD11	1.46	1.43
1:B:63:VAL:CG1	1:B:90:ILE:O	1.66	1.43
1:B:109:LEU:HD23	1:B:114:ILE:CG1	1.37	1.42
1:B:48:VAL:HG13	1:B:53:GLU:CD	1.34	1.41
1:B:63:VAL:HG22	1:B:90:ILE:N	1.28	1.41
1:B:90:ILE:CD1	1:B:142:ALA:HB1	1.49	1.39
1:D:62:ARG:CG	1:D:89:ASP:OD2	1.70	1.39
1:B:67:MET:CE	1:B:94:GLY:C	1.93	1.35
1:B:63:VAL:CG2	1:B:90:ILE:H	1.38	1.33
1:A:40:ALA:O	1:A:45:THR:HG21	1.24	1.31
1:B:55:SER:OG	1:B:84:THR:HG21	1.14	1.29
1:D:62:ARG:HG3	1:D:89:ASP:OD2	1.22	1.28
1:D:122:SER:OG	2:D:401:HOH:O	1.52	1.28
1:B:55:SER:OG	1:B:84:THR:CG2	1.80	1.27
1:D:62:ARG:CA	1:D:89:ASP:HB3	1.65	1.26
1:D:8:LEU:HD23	2:D:404:HOH:O	1.26	1.25
1:A:27:VAL:HG21	1:A:58:LEU:CD1	1.67	1.24
1:D:62:ARG:CB	1:D:89:ASP:OD2	1.83	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:VAL:CG1	1:D:54:LEU:CD1	2.18	1.22
1:D:3:LEU:HD21	1:D:149:ILE:CD1	1.70	1.22
1:B:90:ILE:CD1	1:B:142:ALA:CB	2.17	1.21
1:B:77:VAL:O	1:B:81:LEU:HD12	1.35	1.19
1:B:115:HIS:CD2	1:B:145:ARG:HH22	1.58	1.19
1:A:50:SER:HB3	1:A:53:GLU:CG	1.74	1.18
1:D:27:VAL:HG12	1:D:54:LEU:HD11	1.17	1.17
1:B:45:THR:HG23	2:B:425:HOH:O	1.37	1.17
1:B:67:MET:HE3	1:B:94:GLY:C	1.58	1.17
1:D:86:GLU:O	1:D:89:ASP:OD1	1.62	1.17
1:B:81:LEU:O	1:B:85:LEU:HD23	1.43	1.16
1:D:39:MET:SD	1:D:47:GLY:N	2.19	1.16
1:A:50:SER:HB3	1:A:53:GLU:CB	1.74	1.15
1:D:90:ILE:HG23	1:D:115:HIS:C	1.67	1.15
1:B:67:MET:CE	1:B:94:GLY:O	1.95	1.15
1:C:21:LYS:NZ	1:C:43:ASP:OD1	1.80	1.14
1:D:90:ILE:CG1	1:D:115:HIS:HB2	1.77	1.14
1:D:3:LEU:HD21	1:D:149:ILE:HD12	1.14	1.13
1:D:55:SER:OG	1:D:84:THR:O	1.63	1.13
1:D:152:THR:HG22	2:D:420:HOH:O	1.46	1.13
1:B:48:VAL:HG13	1:B:53:GLU:OE2	1.42	1.13
1:A:305:THR:HG21	1:B:301:PRO:HB2	1.26	1.12
1:B:109:LEU:CD2	1:B:114:ILE:HG13	1.73	1.12
1:B:67:MET:HE1	1:B:94:GLY:O	1.46	1.12
1:A:8:LEU:HD13	1:A:30:ASP:HB2	1.32	1.11
1:B:109:LEU:CD2	1:B:114:ILE:CG1	2.24	1.11
1:D:62:ARG:HB3	1:D:89:ASP:CB	1.79	1.11
1:D:27:VAL:HG12	1:D:54:LEU:CD1	1.78	1.10
1:D:43:ASP:O	1:D:45:THR:HG22	1.50	1.10
1:B:62:ARG:HE	1:B:86:GLU:CD	1.55	1.09
1:A:33:PRO:HA	1:A:36:VAL:CG1	1.81	1.09
1:D:5:MET:CE	1:D:15:ILE:HG21	1.83	1.09
1:B:48:VAL:CG1	1:B:53:GLU:CG	2.31	1.08
1:A:50:SER:HB3	1:A:53:GLU:HB2	1.27	1.08
1:B:45:THR:CG2	2:B:425:HOH:O	1.95	1.08
1:D:5:MET:HE3	1:D:15:ILE:HG21	1.17	1.07
1:B:48:VAL:HG13	1:B:53:GLU:CG	1.84	1.07
1:B:48:VAL:CG1	1:B:53:GLU:OE2	2.00	1.07
1:D:90:ILE:HG23	1:D:115:HIS:CB	1.85	1.07
1:B:90:ILE:CD1	1:B:145:ARG:HH21	1.44	1.07
1:B:111:LYS:O	1:B:112:LYS:NZ	1.87	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ALA:HA	1:A:45:THR:OG1	1.52	1.06
1:B:48:VAL:CG1	1:B:53:GLU:CD	2.23	1.06
1:D:27:VAL:HG11	1:D:54:LEU:CD1	1.82	1.06
1:B:90:ILE:HD13	1:B:142:ALA:CB	1.83	1.05
1:A:27:VAL:HG21	1:A:58:LEU:HD13	1.37	1.05
1:A:33:PRO:CA	1:A:36:VAL:HG12	1.87	1.04
1:C:62:ARG:NH2	1:C:86:GLU:OE2	1.90	1.04
1:D:36:VAL:O	1:D:38:ALA:O	1.76	1.04
1:D:234:GLU:O	1:D:237:GLN:NE2	1.90	1.04
1:C:31:HIS:CD2	1:C:32:ASP:N	2.25	1.03
1:C:234:GLU:OE1	1:C:234:GLU:N	1.91	1.03
1:A:50:SER:HB3	1:A:53:GLU:HG3	1.37	1.03
1:B:115:HIS:CD2	1:B:145:ARG:NH2	2.27	1.03
1:B:33:PRO:O	1:B:37:LYS:N	1.91	1.03
1:D:57:ARG:O	1:D:62:ARG:NH1	1.91	1.02
1:B:90:ILE:HD13	1:B:142:ALA:HB1	1.03	1.01
1:B:2:GLN:OE1	1:B:2:GLN:N	1.93	1.01
1:D:27:VAL:HG11	1:D:54:LEU:HD11	1.33	1.01
1:A:27:VAL:CG2	1:A:58:LEU:CD1	2.39	1.00
1:B:17:ARG:HD2	1:B:128:ARG:HH21	1.23	1.00
1:C:31:HIS:HD2	1:C:32:ASP:N	1.58	1.00
1:D:39:MET:HB2	1:D:42:GLU:N	1.76	1.00
1:D:36:VAL:C	1:D:38:ALA:O	1.98	1.00
1:B:77:VAL:O	1:B:81:LEU:CD1	2.10	0.99
1:D:3:LEU:CD2	1:D:149:ILE:CD1	2.40	0.99
1:B:48:VAL:HG12	1:B:50:SER:H	1.25	0.99
1:B:85:LEU:HB3	1:B:89:ASP:OD1	1.62	0.99
1:B:90:ILE:CG1	1:B:115:HIS:CB	2.06	0.98
1:D:39:MET:HB2	1:D:42:GLU:H	1.28	0.98
1:B:90:ILE:HD11	1:B:145:ARG:HH22	1.15	0.98
1:D:90:ILE:HG12	1:D:115:HIS:HB2	1.45	0.98
1:D:42:GLU:HB3	1:D:45:THR:HG23	1.45	0.98
1:A:40:ALA:C	1:A:45:THR:HG21	1.83	0.97
1:A:50:SER:CB	1:A:53:GLU:HB2	1.93	0.97
1:A:33:PRO:HA	1:A:36:VAL:HG12	0.99	0.97
1:A:109:LEU:O	1:A:114:ILE:HG13	1.65	0.97
1:D:43:ASP:O	1:D:45:THR:CG2	2.12	0.97
1:B:90:ILE:HD12	1:B:145:ARG:NH2	1.78	0.96
1:D:42:GLU:HB3	1:D:45:THR:CG2	1.95	0.96
1:B:91:VAL:CG2	1:B:116:LEU:HD13	1.96	0.96
1:C:6:ILE:HD11	1:C:54:LEU:HD22	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:GLY:O	1:D:15:ILE:HG22	1.66	0.95
1:C:17:ARG:O	1:C:21:LYS:HG2	1.67	0.95
1:B:28:VAL:HG11	2:B:425:HOH:O	1.65	0.94
1:B:109:LEU:HD23	1:B:114:ILE:HG13	0.97	0.94
1:B:1:MET:O	1:B:25:ASP:N	1.98	0.94
1:C:178:LEU:HD23	1:C:179:HIS:N	1.82	0.94
1:B:67:MET:CE	1:B:95:GLY:N	2.30	0.94
1:C:31:HIS:HD2	1:C:32:ASP:H	1.07	0.94
1:D:39:MET:SD	1:D:47:GLY:CA	2.55	0.93
1:D:62:ARG:HB3	1:D:89:ASP:HB2	1.45	0.93
1:B:58:LEU:HD22	1:B:59:SER:H	1.32	0.93
1:D:62:ARG:CB	1:D:89:ASP:CG	2.08	0.93
1:B:84:THR:HG22	1:B:85:LEU:H	1.32	0.93
1:B:115:HIS:HD2	1:B:145:ARG:NH2	1.63	0.93
1:D:90:ILE:CG2	1:D:115:HIS:HB2	1.99	0.93
1:B:109:LEU:HD23	1:B:114:ILE:HG12	1.51	0.92
1:B:48:VAL:HG11	1:B:53:GLU:HG2	1.52	0.92
1:B:50:SER:O	1:B:54:LEU:HB2	1.66	0.92
1:D:42:GLU:HB3	1:D:45:THR:OG1	1.70	0.92
1:D:172:PRO:O	1:D:175:GLN:HB2	1.69	0.92
1:C:194:ASN:ND2	1:C:285:GLU:OE1	2.03	0.92
1:B:83:ASN:O	1:B:84:THR:OG1	1.88	0.92
1:D:51:LEU:HD11	1:D:81:LEU:HD23	1.50	0.92
1:B:90:ILE:HD11	1:B:115:HIS:CD2	2.04	0.92
1:B:48:VAL:CG1	1:B:53:GLU:HG2	1.98	0.91
1:D:7:GLY:C	1:D:8:LEU:HD12	1.90	0.91
1:A:27:VAL:CG2	1:A:58:LEU:HD11	1.99	0.91
1:D:39:MET:SD	1:D:47:GLY:HA3	2.11	0.91
1:B:63:VAL:HG13	1:B:90:ILE:C	1.91	0.91
1:D:62:ARG:CB	1:D:89:ASP:HB2	1.95	0.90
1:A:60:ALA:HA	1:A:62:ARG:HG3	1.52	0.90
1:D:90:ILE:CG2	1:D:115:HIS:CB	2.49	0.90
1:D:39:MET:HB3	1:D:42:GLU:HB2	1.52	0.90
1:B:55:SER:CB	1:B:84:THR:CG2	2.50	0.90
1:C:166:ARG:NH2	1:D:244:GLU:OE2	2.05	0.90
1:C:31:HIS:CD2	1:C:32:ASP:HB2	2.07	0.89
1:D:62:ARG:HB2	1:D:89:ASP:OD2	1.55	0.89
1:A:13:ALA:HA	1:A:39:MET:CE	2.02	0.89
1:D:42:GLU:OE1	1:D:43:ASP:N	2.03	0.89
1:B:17:ARG:CD	1:B:128:ARG:HH21	1.85	0.89
1:C:197:GLU:O	1:C:201:MET:HG2	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:HIS:HD2	1:B:145:ARG:HH22	0.90	0.89
1:B:48:VAL:HG11	1:B:53:GLU:CG	2.03	0.89
1:D:39:MET:CB	1:D:42:GLU:HB2	2.03	0.89
1:B:90:ILE:HD12	1:B:145:ARG:HH21	1.35	0.88
1:A:40:ALA:O	1:A:45:THR:CG2	2.18	0.88
1:B:57:ARG:O	1:B:57:ARG:HD3	1.73	0.88
1:D:42:GLU:HB3	1:D:45:THR:CB	2.02	0.88
1:A:50:SER:CB	1:A:53:GLU:HG3	2.03	0.88
1:D:30:ASP:OD1	1:D:31:HIS:N	2.07	0.88
1:B:63:VAL:HG13	1:B:90:ILE:O	0.70	0.88
1:C:251:ARG:HA	2:C:408:HOH:O	1.74	0.88
1:B:17:ARG:HD2	1:B:128:ARG:NH2	1.89	0.88
1:D:38:ALA:HB1	1:D:42:GLU:HG2	1.53	0.87
1:B:90:ILE:HG12	1:B:115:HIS:CG	2.08	0.87
1:B:63:VAL:HG22	1:B:90:ILE:H	0.73	0.87
1:B:24:HIS:HD2	1:B:149:ILE:HD13	1.38	0.86
1:A:17:ARG:HD2	1:A:128:ARG:NH2	1.91	0.86
1:C:162:ARG:NH1	1:C:170:VAL:HG12	1.90	0.86
1:B:77:VAL:HG12	1:B:81:LEU:HD11	1.58	0.86
1:B:84:THR:HB	1:B:85:LEU:HD22	1.58	0.86
1:D:48:VAL:CG1	1:D:53:GLU:HB2	2.05	0.86
1:D:42:GLU:CB	1:D:45:THR:OG1	2.24	0.85
1:B:67:MET:HE3	1:B:94:GLY:CA	2.07	0.85
1:B:108:LEU:CD2	1:B:109:LEU:HD12	2.06	0.85
1:B:84:THR:HB	1:B:85:LEU:CD2	2.07	0.85
1:A:253:SER:O	1:B:130:ARG:NH2	2.10	0.85
1:A:13:ALA:HA	1:A:39:MET:HE1	1.57	0.84
1:D:103:LEU:HD23	1:D:183:CYS:SG	2.17	0.84
1:D:57:ARG:HB3	1:D:57:ARG:NH2	1.90	0.84
1:A:42:GLU:O	1:A:45:THR:HG22	1.78	0.84
1:A:40:ALA:CA	1:A:45:THR:OG1	2.25	0.84
1:B:90:ILE:HD11	1:B:142:ALA:CB	2.06	0.84
1:B:282:ASP:OD1	1:B:287:ARG:HD2	1.78	0.84
1:D:90:ILE:HG23	1:D:115:HIS:CA	2.06	0.84
1:B:39:MET:HG2	1:B:42:GLU:CD	1.97	0.84
1:B:85:LEU:O	1:B:89:ASP:OD1	1.96	0.83
1:A:8:LEU:CD1	1:A:30:ASP:HB2	2.08	0.83
1:A:100:ARG:HD3	1:B:235:CYS:SG	2.19	0.82
1:B:24:HIS:CD2	1:B:149:ILE:HD13	2.15	0.82
1:B:50:SER:CB	1:B:53:GLU:H	1.93	0.82
1:D:81:LEU:HD23	2:D:403:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASN:HB3	1:A:128:ARG:HB2	1.61	0.81
1:B:35:ALA:O	1:B:38:ALA:HB3	1.80	0.81
1:A:291:ILE:HG23	1:C:291:ILE:HG12	1.62	0.81
1:C:108:LEU:HD23	1:C:109:LEU:HD12	1.61	0.81
1:B:67:MET:HE1	1:B:95:GLY:HA2	1.62	0.81
1:B:90:ILE:CD1	1:B:115:HIS:CB	2.59	0.81
1:C:31:HIS:CD2	1:C:32:ASP:H	1.93	0.81
1:B:58:LEU:CD2	1:B:59:SER:H	1.93	0.80
1:D:90:ILE:HG23	1:D:115:HIS:HB2	1.57	0.80
1:B:33:PRO:O	1:B:37:LYS:CB	2.30	0.79
1:D:56:GLN:C	1:D:57:ARG:HG2	2.01	0.79
1:B:67:MET:HE2	1:B:95:GLY:N	1.97	0.79
1:C:108:LEU:HD23	1:C:108:LEU:O	1.82	0.79
1:D:48:VAL:HG12	1:D:50:SER:H	1.47	0.79
1:A:212:ARG:NH2	1:A:272:ASP:OD1	2.14	0.79
1:D:81:LEU:HA	1:D:84:THR:CG2	2.13	0.79
1:D:110:PHE:HE1	1:D:115:HIS:CE1	2.01	0.78
1:D:81:LEU:CD2	2:D:403:HOH:O	2.30	0.78
1:A:305:THR:HG21	1:B:301:PRO:CB	2.12	0.78
1:D:56:GLN:O	1:D:57:ARG:HG2	1.82	0.78
1:A:27:VAL:HG23	1:A:58:LEU:HD11	1.65	0.78
1:A:197:GLU:O	1:A:201:MET:HG3	1.82	0.78
1:B:90:ILE:HD11	1:B:142:ALA:HB2	1.65	0.78
1:C:6:ILE:HD11	1:C:54:LEU:CD2	2.13	0.77
1:B:90:ILE:CD1	1:B:145:ARG:HH22	1.73	0.77
1:C:251:ARG:CA	2:C:408:HOH:O	2.31	0.77
1:B:84:THR:HG22	1:B:85:LEU:N	1.99	0.76
1:C:10:ARG:NH1	2:C:401:HOH:O	2.18	0.76
1:B:39:MET:HG2	1:B:42:GLU:OE1	1.84	0.76
1:B:142:ALA:CB	1:B:145:ARG:HH21	1.99	0.76
1:D:80:GLU:O	1:D:84:THR:HG22	1.84	0.76
1:B:142:ALA:HA	1:B:145:ARG:HE	1.49	0.75
1:B:42:GLU:O	1:B:45:THR:OG1	2.05	0.75
1:C:244:GLU:OE2	1:D:166:ARG:NH2	2.16	0.75
1:C:84:THR:HG22	1:C:85:LEU:HD23	1.67	0.75
1:C:31:HIS:NE2	1:C:32:ASP:HB2	2.01	0.75
1:C:81:LEU:O	1:C:85:LEU:HG	1.86	0.75
1:B:90:ILE:HD12	1:B:142:ALA:HB1	1.61	0.75
1:D:51:LEU:HD21	1:D:84:THR:HG21	1.67	0.75
1:A:16:VAL:HG11	1:A:39:MET:SD	2.27	0.75
1:D:41:GLY:H	1:D:42:GLU:HA	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ILE:HG12	1:D:115:HIS:CB	2.16	0.74
1:A:53:GLU:HA	1:A:56:GLN:HE21	1.53	0.74
1:D:62:ARG:C	1:D:89:ASP:HB3	2.06	0.74
1:B:108:LEU:HD23	1:B:109:LEU:HD12	1.69	0.74
1:B:328:ARG:NH1	2:B:402:HOH:O	2.20	0.74
1:D:47:GLY:O	1:D:48:VAL:HG23	1.87	0.74
1:D:110:PHE:CE1	1:D:115:HIS:CE1	2.75	0.74
1:B:328:ARG:CZ	2:B:402:HOH:O	2.35	0.74
1:D:5:MET:CE	1:D:15:ILE:CG2	2.66	0.74
1:C:62:ARG:NH2	1:C:86:GLU:CD	2.41	0.74
1:B:91:VAL:CG2	1:B:116:LEU:CD1	2.66	0.74
1:D:32:ASP:OD2	1:D:34:ASP:HB3	1.88	0.73
1:D:90:ILE:CB	1:D:115:HIS:HB2	2.18	0.73
1:B:112:LYS:HZ3	1:B:112:LYS:HB2	1.51	0.73
1:C:108:LEU:CD2	1:C:109:LEU:CD1	2.67	0.73
1:A:16:VAL:HG11	1:A:39:MET:CE	2.18	0.73
1:C:27:VAL:HG11	1:C:58:LEU:HD12	1.70	0.73
1:D:3:LEU:CD2	1:D:149:ILE:HD11	2.19	0.73
1:C:26:CYS:HB2	1:C:45:THR:HG22	1.71	0.73
1:D:79:GLU:HG2	1:D:108:LEU:HD11	1.71	0.73
1:C:57:ARG:HD3	1:C:57:ARG:N	2.03	0.73
1:D:92:ILE:HD13	1:D:117:LEU:HB2	1.71	0.72
1:B:114:ILE:HD13	1:B:114:ILE:O	1.88	0.72
1:C:178:LEU:HD23	1:C:179:HIS:C	2.10	0.72
1:B:57:ARG:HD3	1:B:57:ARG:C	2.08	0.72
1:B:48:VAL:HG12	1:B:53:GLU:OE2	1.88	0.72
1:D:51:LEU:HD11	1:D:81:LEU:CD2	2.20	0.72
1:B:90:ILE:CG1	1:B:145:ARG:NH2	2.52	0.71
1:B:112:LYS:NZ	1:B:112:LYS:HB2	2.05	0.71
1:C:27:VAL:HG11	1:C:58:LEU:CD1	2.20	0.71
1:D:59:SER:HB2	1:D:61:PRO:HD2	1.71	0.71
1:D:42:GLU:CB	1:D:45:THR:HG23	2.20	0.71
1:B:270:SER:HB2	1:B:275:GLU:OE1	1.91	0.71
1:D:90:ILE:HG13	1:D:115:HIS:HB2	1.71	0.71
1:D:53:GLU:O	1:D:57:ARG:CG	2.38	0.71
1:D:90:ILE:CG2	1:D:115:HIS:C	2.53	0.71
1:B:62:ARG:N	1:B:89:ASP:HB3	2.04	0.71
1:A:8:LEU:N	1:A:8:LEU:HD12	2.06	0.70
1:B:62:ARG:NE	1:B:86:GLU:CD	2.38	0.70
1:B:84:THR:CB	1:B:85:LEU:HD22	2.21	0.70
1:C:147:GLU:OE1	1:C:177:TYR:OH	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:MET:HE1	1:B:94:GLY:C	1.84	0.70
1:B:67:MET:HE1	1:B:95:GLY:CA	2.22	0.70
1:C:282:ASP:OD2	1:C:314:ARG:NH2	2.24	0.70
1:D:12:GLY:O	1:D:15:ILE:CG2	2.40	0.70
1:B:67:MET:HE3	1:B:94:GLY:O	1.73	0.70
1:B:108:LEU:HD23	1:B:108:LEU:C	2.12	0.70
1:C:129:GLU:N	1:C:129:GLU:OE1	2.26	0.69
1:A:3:LEU:HD13	1:A:149:ILE:HG12	1.74	0.69
1:B:108:LEU:HD22	1:B:109:LEU:HD12	1.74	0.69
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.56	0.69
1:B:81:LEU:O	1:B:85:LEU:CD2	2.34	0.69
1:C:8:LEU:HD13	1:C:39:MET:CG	2.22	0.69
1:C:132:TYR:O	1:C:134:LEU:HD23	1.93	0.68
1:B:90:ILE:CG1	1:B:145:ARG:HH22	2.06	0.68
1:D:51:LEU:C	1:D:51:LEU:HD23	2.14	0.68
1:A:301:PRO:HB2	1:B:305:THR:CG2	2.23	0.68
1:B:7:GLY:O	1:B:8:LEU:HD22	1.92	0.68
1:D:110:PHE:HE1	1:D:115:HIS:HE1	1.42	0.68
1:C:62:ARG:HH21	1:C:86:GLU:CD	1.94	0.68
1:A:51:LEU:O	1:A:84:THR:HG21	1.94	0.68
1:A:16:VAL:HG23	1:A:26:CYS:SG	2.33	0.68
1:B:1:MET:HG3	1:B:2:GLN:H	1.59	0.68
1:B:24:HIS:HD2	1:B:149:ILE:CD1	2.07	0.68
1:B:62:ARG:NH1	1:B:86:GLU:OE2	2.27	0.68
1:D:102:ASP:OD2	1:D:187:HIS:ND1	2.21	0.68
1:B:42:GLU:O	1:B:43:ASP:C	2.30	0.68
1:D:215:ASP:OD2	1:D:219:ARG:NH1	2.27	0.68
1:A:39:MET:O	1:A:41:GLY:N	2.27	0.67
1:C:99:TYR:CE1	1:C:100:ARG:HG3	2.28	0.67
1:D:250:ARG:HD2	1:D:261:ASP:OD1	1.93	0.67
1:B:90:ILE:HD11	1:B:145:ARG:HH21	1.03	0.67
1:D:172:PRO:HA	1:D:175:GLN:HG3	1.77	0.67
1:A:322:LYS:HE2	1:D:276:PHE:O	1.95	0.67
1:C:31:HIS:CD2	1:C:32:ASP:CB	2.76	0.67
1:A:16:VAL:CG1	1:A:39:MET:CE	2.72	0.67
1:C:108:LEU:HD23	1:C:109:LEU:CD1	2.24	0.67
1:D:48:VAL:HG21	1:D:54:LEU:CD1	2.24	0.67
1:B:326:ALA:O	1:B:329:LYS:HG2	1.95	0.67
1:A:44:ARG:HH11	1:A:44:ARG:CG	2.06	0.67
1:B:63:VAL:HG22	1:B:90:ILE:CA	2.23	0.66
1:B:90:ILE:CG1	1:B:115:HIS:CG	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:HG2	1:D:201:MET:CE	2.25	0.66
1:B:30:ASP:OD1	1:B:31:HIS:HD2	1.79	0.66
1:D:27:VAL:HG12	1:D:54:LEU:HD13	1.74	0.66
1:B:90:ILE:CD1	1:B:142:ALA:HB2	2.16	0.66
1:B:85:LEU:HD22	1:B:85:LEU:N	2.10	0.66
1:D:53:GLU:O	1:D:57:ARG:HG3	1.96	0.66
1:A:60:ALA:CA	1:A:62:ARG:HG3	2.25	0.65
1:A:102:ASP:OD2	1:A:187:HIS:ND1	2.29	0.65
1:B:48:VAL:HG11	1:B:53:GLU:CB	2.27	0.65
1:B:81:LEU:HA	1:B:85:LEU:HD21	1.77	0.65
1:C:161:PRO:O	1:D:250:ARG:NH2	2.30	0.65
1:C:8:LEU:HD13	1:C:39:MET:HG2	1.76	0.65
1:B:67:MET:CE	1:B:95:GLY:CA	2.74	0.65
1:C:21:LYS:HE2	1:C:21:LYS:N	2.11	0.65
1:B:318:ASP:OD2	1:B:322:LYS:NZ	2.24	0.65
1:A:19:LEU:HD21	1:A:149:ILE:HG23	1.79	0.65
1:A:60:ALA:HA	1:A:61:PRO:C	2.18	0.65
1:B:51:LEU:HD22	1:B:80:GLU:HB3	1.79	0.65
1:C:8:LEU:N	1:C:30:ASP:OD2	2.29	0.65
1:A:39:MET:O	1:A:45:THR:HB	1.97	0.65
1:B:55:SER:HG	1:B:84:THR:HG21	1.54	0.65
1:B:62:ARG:H	1:B:89:ASP:HB3	1.61	0.64
1:B:48:VAL:CG1	1:B:53:GLU:CB	2.75	0.64
1:D:15:ILE:HG23	1:D:16:VAL:N	2.12	0.64
1:D:213:ASN:O	1:D:216:VAL:HG13	1.96	0.64
1:C:162:ARG:HH11	1:C:170:VAL:HG12	1.60	0.64
1:C:302:VAL:HG13	1:D:302:VAL:HG13	1.80	0.64
1:D:59:SER:HB3	1:D:61:PRO:HD3	1.79	0.64
1:A:39:MET:O	1:A:40:ALA:C	2.36	0.64
1:B:85:LEU:CB	1:B:89:ASP:OD1	2.41	0.64
1:B:90:ILE:CD1	1:B:115:HIS:CD2	2.81	0.64
1:C:23:GLY:HA2	1:C:44:ARG:NH1	2.13	0.64
1:B:90:ILE:CD1	1:B:115:HIS:CG	2.81	0.64
1:C:108:LEU:HD23	1:C:108:LEU:C	2.18	0.64
1:B:33:PRO:O	1:B:37:LYS:HB2	1.97	0.64
1:B:50:SER:HB2	1:B:53:GLU:H	1.62	0.64
1:B:67:MET:HE3	1:B:94:GLY:HA3	1.80	0.64
1:B:90:ILE:CG1	1:B:115:HIS:HB3	2.21	0.64
1:B:90:ILE:HD11	1:B:115:HIS:CG	2.33	0.64
1:D:35:ALA:O	1:D:36:VAL:HG22	1.97	0.64
1:B:270:SER:CB	1:B:275:GLU:OE1	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ASP:O	1:D:45:THR:N	2.31	0.63
1:D:48:VAL:HG21	1:D:54:LEU:HD13	1.80	0.63
1:B:34:ASP:O	1:B:38:ALA:HB2	1.98	0.63
1:D:42:GLU:N	1:D:45:THR:O	2.31	0.63
1:A:74:THR:HG22	1:A:78:ILE:HD11	1.81	0.63
1:B:91:VAL:HG23	1:B:116:LEU:CD1	2.29	0.63
1:B:108:LEU:HD22	1:B:109:LEU:CD1	2.28	0.62
1:B:48:VAL:CG1	1:B:53:GLU:HB3	2.29	0.62
1:C:6:ILE:CD1	1:C:54:LEU:HD22	2.27	0.62
1:D:3:LEU:HD23	1:D:149:ILE:HD11	1.80	0.62
1:A:301:PRO:HB2	1:B:305:THR:HG21	1.81	0.62
1:B:1:MET:HG3	1:B:2:GLN:OE1	1.99	0.62
1:B:48:VAL:HG11	1:B:53:GLU:HB3	1.82	0.62
1:D:78:ILE:N	1:D:78:ILE:HD12	2.13	0.62
1:D:90:ILE:HG23	1:D:115:HIS:O	1.99	0.62
1:D:56:GLN:OE1	1:D:56:GLN:N	2.33	0.62
1:B:67:MET:CE	1:B:95:GLY:HA2	2.29	0.62
1:A:60:ALA:HB2	1:A:62:ARG:NE	2.14	0.62
1:A:306:ALA:O	2:A:401:HOH:O	2.15	0.62
1:D:48:VAL:HG11	1:D:53:GLU:HB2	1.82	0.62
1:A:53:GLU:O	1:A:56:GLN:HB2	1.99	0.62
1:B:63:VAL:CG2	1:B:90:ILE:N	2.16	0.61
1:C:253:SER:O	1:D:130:ARG:NH2	2.33	0.61
1:B:81:LEU:HD12	1:B:81:LEU:H	1.65	0.61
1:D:54:LEU:O	1:D:57:ARG:HB2	2.00	0.61
1:B:91:VAL:HG22	1:B:116:LEU:HD13	1.78	0.61
1:A:44:ARG:HG2	1:A:44:ARG:NH1	2.15	0.61
1:A:57:ARG:O	1:A:57:ARG:HG3	2.01	0.61
1:A:55:SER:O	1:A:62:ARG:NH1	2.33	0.61
1:B:2:GLN:CG	1:B:58:LEU:HD13	2.30	0.61
1:D:56:GLN:O	1:D:57:ARG:CG	2.47	0.61
1:D:78:ILE:HD12	1:D:78:ILE:H	1.65	0.61
1:C:3:LEU:O	1:C:27:VAL:HG12	2.01	0.61
1:A:33:PRO:CA	1:A:36:VAL:CG1	2.64	0.61
1:A:282:ASP:OD1	1:A:314:ARG:NH2	2.34	0.61
1:D:57:ARG:HH22	1:D:58:LEU:HD23	1.64	0.61
1:B:328:ARG:NH2	2:B:402:HOH:O	2.33	0.60
1:D:59:SER:CB	1:D:61:PRO:HD2	2.31	0.60
1:D:62:ARG:HB2	1:D:89:ASP:HB3	0.99	0.60
1:D:3:LEU:CD2	1:D:149:ILE:HG13	2.32	0.60
1:D:36:VAL:O	1:D:36:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:VAL:HG13	1:D:53:GLU:HB2	1.80	0.60
1:D:57:ARG:HB3	1:D:57:ARG:HH21	1.64	0.60
1:D:197:GLU:HG2	1:D:201:MET:HE3	1.83	0.60
1:C:30:ASP:OD1	1:C:31:HIS:CD2	2.54	0.60
1:C:296:GLU:HG2	1:D:213:ASN:O	2.01	0.60
1:D:27:VAL:HG11	1:D:54:LEU:HD12	1.76	0.60
1:D:53:GLU:O	1:D:57:ARG:HG2	2.01	0.60
1:B:90:ILE:CD1	1:B:115:HIS:HB3	2.31	0.60
1:C:108:LEU:CD2	1:C:109:LEU:HD12	2.29	0.60
1:C:196:ILE:HD13	1:D:204:LEU:HA	1.81	0.60
1:C:251:ARG:NH1	1:D:157:VAL:O	2.34	0.60
1:C:53:GLU:HG3	1:C:57:ARG:NH2	2.17	0.60
1:C:90:ILE:HD13	1:C:142:ALA:HB1	1.83	0.60
1:D:55:SER:CB	1:D:84:THR:OG1	2.49	0.60
1:A:55:SER:HB2	1:A:84:THR:HG22	1.83	0.60
1:B:16:VAL:HG11	2:B:425:HOH:O	2.01	0.60
1:B:55:SER:CB	1:B:84:THR:HG22	2.31	0.60
1:B:90:ILE:HG23	1:B:115:HIS:C	2.21	0.60
1:D:97:THR:HG22	1:D:101:ASP:HB2	1.82	0.60
1:D:3:LEU:CD1	1:D:26:CYS:SG	2.90	0.60
1:B:84:THR:CG2	1:B:85:LEU:H	2.11	0.60
1:B:48:VAL:HG12	1:B:50:SER:N	2.07	0.60
1:B:275:GLU:OE2	1:B:275:GLU:N	2.31	0.60
1:A:250:ARG:NH1	1:A:261:ASP:OD1	2.30	0.59
1:B:142:ALA:HA	1:B:145:ARG:HH21	1.67	0.59
1:C:109:LEU:HB3	1:C:114:ILE:HB	1.83	0.59
1:A:123:GLY:O	1:A:130:ARG:NH2	2.35	0.59
1:B:55:SER:HB3	1:B:84:THR:HG22	1.84	0.59
1:B:62:ARG:NE	1:B:86:GLU:OE2	2.35	0.59
1:A:29:TYR:CD1	1:A:30:ASP:N	2.71	0.59
1:D:3:LEU:CD2	1:D:149:ILE:CG1	2.81	0.59
1:D:50:SER:HB3	1:D:53:GLU:HG3	1.82	0.59
1:B:77:VAL:CG1	1:B:81:LEU:HD11	2.32	0.59
1:A:250:ARG:HD2	1:A:261:ASP:OD1	2.02	0.59
1:B:90:ILE:CB	1:B:115:HIS:HB2	2.23	0.59
1:C:108:LEU:HD22	1:C:109:LEU:CD1	2.31	0.59
1:D:78:ILE:HG22	1:D:108:LEU:HD22	1.85	0.59
1:D:43:ASP:O	1:D:45:THR:HG23	2.01	0.59
1:D:75:THR:HG23	1:D:105:HIS:NE2	2.17	0.59
1:A:8:LEU:HD11	1:A:29:TYR:C	2.24	0.59
1:D:62:ARG:O	1:D:89:ASP:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ASP:OD1	1:D:141:ASP:N	2.36	0.59
1:A:92:ILE:HD13	1:A:150:PHE:CE1	2.38	0.58
1:D:8:LEU:CD1	1:D:29:TYR:O	2.51	0.58
1:B:81:LEU:C	1:B:85:LEU:HD23	2.22	0.58
1:A:235:CYS:SG	1:B:100:ARG:HD3	2.42	0.58
1:B:28:VAL:CG1	2:B:425:HOH:O	2.36	0.58
1:B:50:SER:O	1:B:54:LEU:N	2.33	0.58
1:C:197:GLU:O	1:C:201:MET:CG	2.47	0.58
1:D:27:VAL:CB	1:D:54:LEU:HD11	2.31	0.58
1:D:55:SER:CB	1:D:84:THR:HG1	2.17	0.58
1:D:55:SER:HB2	1:D:84:THR:OG1	2.02	0.58
1:D:73:ILE:O	1:D:77:VAL:HG23	2.03	0.58
1:D:89:ASP:OD1	1:D:89:ASP:N	2.36	0.58
1:C:170:VAL:HG23	1:C:170:VAL:O	2.01	0.58
1:C:178:LEU:HD23	1:C:178:LEU:C	2.23	0.58
1:D:8:LEU:HD21	1:D:28:VAL:CG1	2.32	0.58
1:D:307:LEU:HD11	1:D:311:PHE:CZ	2.38	0.58
1:B:117:LEU:HD11	1:B:143:PHE:HA	1.85	0.58
1:D:63:VAL:HA	1:D:90:ILE:O	2.02	0.58
1:D:307:LEU:HD11	1:D:311:PHE:CE1	2.39	0.58
1:D:57:ARG:C	1:D:62:ARG:HH11	2.01	0.58
1:B:64:VAL:HG22	1:B:65:TRP:H	1.69	0.58
1:B:55:SER:OG	1:B:84:THR:HG23	1.97	0.57
1:D:3:LEU:HD12	1:D:26:CYS:SG	2.44	0.57
1:D:111:LYS:HG3	1:D:112:LYS:HG2	1.85	0.57
1:D:43:ASP:C	1:D:45:THR:N	2.55	0.57
1:C:230:LEU:HD11	1:D:295:ASP:HB3	1.85	0.57
1:B:84:THR:C	1:B:85:LEU:CD2	2.73	0.57
1:A:17:ARG:HD2	1:A:128:ARG:CZ	2.34	0.57
1:A:327:MET:SD	1:D:201:MET:HB3	2.45	0.57
1:B:79:GLU:O	1:B:82:ALA:HB3	2.04	0.57
1:D:25:ASP:OD1	1:D:44:ARG:CG	2.53	0.57
1:A:262:LEU:HD22	1:D:330:GLN:HB3	1.86	0.57
1:D:49:ALA:N	1:D:53:GLU:OE2	2.31	0.57
1:B:142:ALA:CA	1:B:145:ARG:HH21	2.18	0.57
1:B:254:VAL:O	2:B:401:HOH:O	2.18	0.57
1:C:56:GLN:C	1:C:57:ARG:HD3	2.24	0.57
1:B:87:ALA:HB1	1:B:113:GLY:HA3	1.87	0.57
1:D:48:VAL:HG12	1:D:49:ALA:N	2.19	0.56
1:D:19:LEU:HD21	1:D:149:ILE:HG23	1.87	0.56
1:A:17:ARG:O	1:A:21:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LEU:HD21	1:D:84:THR:CG2	2.36	0.56
1:A:51:LEU:O	1:A:84:THR:CG2	2.54	0.56
1:A:156:GLY:HA2	1:A:175:GLN:NE2	2.21	0.56
1:A:48:VAL:CG1	1:A:53:GLU:HB3	2.35	0.56
1:D:8:LEU:HD21	1:D:28:VAL:HG11	1.88	0.56
1:A:328:ARG:NH2	2:A:404:HOH:O	2.30	0.56
1:C:119:CYS:SG	1:C:134:LEU:CD1	2.93	0.56
1:D:48:VAL:HG13	1:D:53:GLU:CB	2.36	0.56
1:A:305:THR:HB	2:A:426:HOH:O	2.05	0.56
1:D:90:ILE:CG2	1:D:115:HIS:HB3	2.32	0.56
2:A:426:HOH:O	1:B:302:VAL:HA	2.05	0.56
1:C:27:VAL:CG1	1:C:58:LEU:CD1	2.83	0.56
1:A:328:ARG:CZ	1:D:310:ARG:HH12	2.19	0.56
1:D:130:ARG:O	1:D:155:PRO:HB3	2.07	0.55
1:D:57:ARG:HB3	1:D:57:ARG:CZ	2.35	0.55
1:A:284:GLY:HA2	1:A:287:ARG:HD2	1.88	0.55
1:D:41:GLY:N	1:D:42:GLU:HA	2.22	0.55
1:D:62:ARG:O	1:D:89:ASP:CA	2.55	0.55
1:B:2:GLN:HG3	1:B:58:LEU:HD13	1.88	0.55
1:D:39:MET:HB2	1:D:42:GLU:HB2	1.88	0.55
1:A:284:GLY:HA3	1:D:228:ALA:HB2	1.88	0.55
1:A:328:ARG:NH1	2:A:404:HOH:O	2.35	0.55
1:B:85:LEU:O	1:B:89:ASP:CG	2.45	0.55
1:B:142:ALA:HA	1:B:145:ARG:NE	2.20	0.55
1:D:59:SER:CB	1:D:61:PRO:CD	2.85	0.55
1:D:62:ARG:N	1:D:89:ASP:HB3	2.20	0.54
1:B:33:PRO:CD	1:B:34:ASP:H	2.21	0.54
1:A:43:ASP:OD1	1:A:44:ARG:HD2	2.07	0.54
1:D:317:ASP:OD1	1:D:317:ASP:N	2.36	0.54
1:A:39:MET:HA	1:A:42:GLU:OE1	2.07	0.54
1:A:324:LEU:HD11	2:D:418:HOH:O	2.08	0.54
1:D:37:LYS:HD3	1:D:37:LYS:C	2.27	0.54
1:B:33:PRO:C	1:B:37:LYS:HB2	2.28	0.54
1:B:91:VAL:HG23	1:B:116:LEU:HD13	1.84	0.54
1:D:152:THR:CG2	2:D:420:HOH:O	2.25	0.54
1:A:58:LEU:O	1:A:62:ARG:NH1	2.40	0.54
1:A:79:GLU:O	1:A:82:ALA:HB3	2.08	0.54
1:D:169:GLU:HG2	1:D:170:VAL:N	2.23	0.54
1:C:188:PHE:O	1:C:191:MET:HG2	2.07	0.54
1:D:7:GLY:O	1:D:8:LEU:HD12	2.07	0.54
1:D:59:SER:HB3	1:D:61:PRO:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:VAL:CG2	1:D:54:LEU:HD13	2.37	0.54
1:C:18:ARG:NH2	1:C:154:ALA:O	2.41	0.54
1:A:156:GLY:HA2	1:A:175:GLN:HE21	1.73	0.53
1:B:228:ALA:N	1:C:283:SER:O	2.41	0.53
1:A:50:SER:CB	1:A:53:GLU:CB	2.61	0.53
1:B:30:ASP:C	1:B:32:ASP:H	2.11	0.53
1:B:42:GLU:O	1:B:45:THR:CB	2.57	0.53
1:C:81:LEU:HD22	1:C:85:LEU:HD21	1.91	0.53
1:D:56:GLN:C	1:D:57:ARG:CG	2.76	0.53
1:D:238:TYR:CB	1:D:240:PHE:CE1	2.91	0.53
1:A:236:TYR:OH	1:B:295:ASP:OD2	2.26	0.53
1:D:6:ILE:CD1	1:D:81:LEU:HD11	2.37	0.53
1:B:50:SER:O	1:B:54:LEU:CB	2.48	0.53
1:B:282:ASP:OD2	1:B:314:ARG:NH2	2.39	0.53
1:D:62:ARG:O	1:D:90:ILE:N	2.41	0.53
1:A:83:ASN:O	1:A:85:LEU:N	2.41	0.53
1:A:327:MET:SD	1:D:201:MET:CB	2.96	0.53
1:B:81:LEU:HA	1:B:85:LEU:CD2	2.38	0.53
1:D:62:ARG:O	1:D:89:ASP:HB3	2.09	0.53
1:B:329:LYS:HD2	1:C:276:PHE:HE1	1.74	0.53
1:D:5:MET:HE3	1:D:15:ILE:CG2	2.12	0.53
1:D:60:ALA:N	1:D:61:PRO:CD	2.72	0.53
1:D:62:ARG:O	1:D:89:ASP:HA	2.09	0.53
1:D:197:GLU:CG	1:D:201:MET:HE2	2.38	0.53
1:B:292:ALA:O	1:B:296:GLU:HG3	2.10	0.52
1:D:51:LEU:HD21	1:D:84:THR:CB	2.38	0.52
1:A:78:ILE:HG23	1:A:109:LEU:HD11	1.91	0.52
1:A:127:GLY:HA3	1:A:132:TYR:CE1	2.43	0.52
1:B:84:THR:C	1:B:85:LEU:HD22	2.30	0.52
1:D:154:ALA:HB1	1:D:155:PRO:HD2	1.91	0.52
1:A:123:GLY:HA2	1:A:130:ARG:NH2	2.24	0.52
1:A:39:MET:O	1:A:42:GLU:N	2.42	0.52
1:A:13:ALA:CA	1:A:39:MET:CE	2.82	0.52
1:A:301:PRO:HB2	1:B:305:THR:HG23	1.89	0.52
1:D:8:LEU:HD12	1:D:8:LEU:N	2.24	0.52
1:D:48:VAL:HG21	1:D:54:LEU:HD12	1.92	0.52
1:D:90:ILE:HG23	1:D:115:HIS:HB3	1.86	0.52
1:A:7:GLY:C	1:A:8:LEU:HD12	2.30	0.52
1:D:41:GLY:N	1:D:42:GLU:CA	2.71	0.52
1:B:30:ASP:H	1:B:36:VAL:CG2	2.23	0.52
1:D:57:ARG:HH21	1:D:57:ARG:CB	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ILE:CG1	1:B:115:HIS:CD2	2.92	0.52
1:C:53:GLU:O	1:C:57:ARG:HG2	2.10	0.52
1:D:43:ASP:N	1:D:43:ASP:OD1	2.42	0.52
1:B:112:LYS:HB3	1:B:114:ILE:HG23	1.92	0.52
1:C:3:LEU:HD12	1:C:3:LEU:C	2.31	0.51
1:B:29:TYR:HB3	1:B:54:LEU:HD11	1.92	0.51
1:B:30:ASP:O	1:B:32:ASP:N	2.43	0.51
1:D:36:VAL:CA	1:D:38:ALA:O	2.57	0.51
1:D:48:VAL:HG13	1:D:53:GLU:OE2	2.10	0.51
1:C:43:ASP:OD1	1:C:43:ASP:O	2.28	0.51
1:D:16:VAL:HA	1:D:19:LEU:HB2	1.91	0.51
1:D:19:LEU:HD13	1:D:26:CYS:SG	2.50	0.51
1:B:33:PRO:HG2	1:B:34:ASP:N	2.26	0.51
1:B:48:VAL:HG12	1:B:49:ALA:N	2.26	0.51
1:C:6:ILE:HD13	1:C:29:TYR:HB3	1.91	0.51
1:B:90:ILE:HD13	1:B:115:HIS:HB3	1.93	0.51
1:C:3:LEU:CD1	1:C:26:CYS:HA	2.41	0.51
1:A:63:VAL:HG22	1:A:90:ILE:HB	1.92	0.51
1:C:33:PRO:O	1:C:37:LYS:HG2	2.10	0.51
1:D:216:VAL:HG23	1:D:230:LEU:HD22	1.93	0.51
1:B:110:PHE:C	1:B:112:LYS:H	2.13	0.51
1:D:39:MET:CB	1:D:42:GLU:CB	2.85	0.51
1:D:51:LEU:CD1	1:D:81:LEU:CD2	2.88	0.51
1:A:29:TYR:CE1	1:A:31:HIS:HA	2.46	0.51
1:A:50:SER:CA	1:A:53:GLU:HB2	2.39	0.51
1:D:39:MET:HE3	1:D:39:MET:H	1.76	0.51
1:B:53:GLU:O	1:B:57:ARG:HB2	2.11	0.51
1:C:267:LEU:HD23	1:C:273:LEU:HD21	1.92	0.51
1:A:13:ALA:HA	1:A:39:MET:HE2	1.92	0.50
1:B:169:GLU:HG2	1:B:170:VAL:N	2.25	0.50
1:D:57:ARG:H	1:D:62:ARG:NH1	2.09	0.50
1:B:69:PRO:HB2	1:B:73:ILE:HD13	1.94	0.50
1:D:43:ASP:C	1:D:45:THR:H	2.15	0.50
1:D:60:ALA:N	1:D:61:PRO:HD3	2.26	0.50
1:B:33:PRO:CG	1:B:34:ASP:N	2.73	0.50
1:B:91:VAL:HG22	1:B:116:LEU:CD1	2.40	0.50
1:B:33:PRO:CG	1:B:34:ASP:H	2.23	0.50
1:C:302:VAL:HG13	1:D:302:VAL:CG1	2.41	0.50
1:D:17:ARG:NH1	2:D:404:HOH:O	2.44	0.50
1:A:27:VAL:C	1:A:28:VAL:CG1	2.80	0.50
1:A:132:TYR:O	1:A:154:ALA:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PRO:O	1:B:37:LYS:CA	2.59	0.50
1:C:251:ARG:NE	1:D:174:GLU:O	2.44	0.50
1:D:48:VAL:CG1	1:D:49:ALA:N	2.75	0.50
1:A:53:GLU:HA	1:A:56:GLN:NE2	2.24	0.50
1:B:33:PRO:HG2	1:B:34:ASP:H	1.76	0.50
1:C:133:CYS:HB2	1:D:251:ARG:O	2.12	0.50
1:D:238:TYR:HB3	1:D:240:PHE:CE1	2.47	0.50
1:A:39:MET:C	1:A:41:GLY:N	2.63	0.49
1:A:163:THR:HG23	1:B:265:ILE:HG12	1.94	0.49
1:C:8:LEU:HD13	1:C:39:MET:HG3	1.91	0.49
1:C:3:LEU:HD11	1:C:26:CYS:SG	2.52	0.49
1:C:141:ASP:O	1:C:145:ARG:N	2.42	0.49
1:A:48:VAL:HG12	1:A:49:ALA:N	2.27	0.49
1:B:247:GLU:HA	1:B:250:ARG:HG3	1.93	0.49
1:C:162:ARG:NH1	1:C:170:VAL:CG1	2.70	0.49
1:D:15:ILE:CG2	1:D:16:VAL:N	2.74	0.49
1:A:16:VAL:HG11	1:A:39:MET:HE1	1.93	0.49
1:A:265:ILE:HG12	1:B:163:THR:HG23	1.93	0.49
1:B:60:ALA:HA	1:B:61:PRO:C	2.32	0.49
1:B:107:LYS:O	1:B:108:LEU:C	2.50	0.49
1:B:77:VAL:HG12	1:B:81:LEU:CD1	2.37	0.49
1:C:20:ALA:O	1:C:44:ARG:HD3	2.12	0.49
1:D:5:MET:HE2	1:D:15:ILE:CG2	2.42	0.49
1:A:8:LEU:HD13	1:A:30:ASP:CB	2.22	0.49
1:B:19:LEU:HD21	1:B:149:ILE:HG23	1.94	0.49
1:A:29:TYR:CE1	1:A:30:ASP:O	2.66	0.49
1:A:242:ILE:HG22	1:A:267:LEU:HD13	1.94	0.48
1:A:270:SER:OG	2:A:403:HOH:O	2.19	0.48
1:D:3:LEU:HD11	1:D:26:CYS:SG	2.52	0.48
1:D:169:GLU:HG2	1:D:170:VAL:H	1.78	0.48
1:A:40:ALA:N	1:A:45:THR:OG1	2.45	0.48
1:B:277:SER:H	1:C:336:GLU:CD	2.17	0.48
1:C:7:GLY:O	1:C:8:LEU:HD23	2.13	0.48
1:C:192:VAL:O	1:C:196:ILE:HG13	2.13	0.48
1:D:39:MET:HB2	1:D:42:GLU:CA	2.41	0.48
1:C:230:LEU:HD13	1:D:295:ASP:O	2.13	0.48
1:D:42:GLU:C	1:D:45:THR:HG23	2.34	0.48
1:B:83:ASN:C	1:B:84:THR:HG1	1.94	0.48
1:B:85:LEU:CD2	1:B:85:LEU:N	2.75	0.48
1:B:216:VAL:HG12	1:B:236:TYR:HB3	1.94	0.48
1:C:219:ARG:HG3	1:C:219:ARG:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:HD11	1:D:29:TYR:O	2.13	0.48
1:D:162:ARG:HH22	1:D:169:GLU:C	2.16	0.48
1:A:11:MET:HB3	1:A:67:MET:HE1	1.94	0.48
1:A:185:SER:HB2	1:B:240:PHE:HE1	1.77	0.48
1:C:202:ALA:HB1	1:D:302:VAL:HG21	1.95	0.48
1:A:91:VAL:HG21	1:A:109:LEU:HD13	1.94	0.48
1:B:70:ALA:HA	1:B:74:THR:OG1	2.13	0.48
1:C:26:CYS:O	1:C:45:THR:HA	2.14	0.48
1:D:48:VAL:CG1	1:D:53:GLU:CB	2.86	0.48
1:C:258:TRP:O	1:C:262:LEU:HG	2.13	0.48
1:A:134:LEU:HD11	1:A:153:VAL:CG2	2.44	0.48
1:B:245:VAL:O	1:B:248:VAL:HG12	2.13	0.48
1:D:43:ASP:O	1:D:44:ARG:C	2.52	0.48
1:D:56:GLN:O	1:D:57:ARG:CD	2.62	0.48
1:A:47:GLY:O	1:A:48:VAL:HG23	2.14	0.48
1:A:305:THR:CG2	1:B:301:PRO:HB2	2.19	0.48
1:B:112:LYS:NZ	1:B:112:LYS:CB	2.73	0.48
1:A:16:VAL:CG1	1:A:39:MET:HE2	2.43	0.47
1:B:329:LYS:HD2	1:C:276:PHE:CE1	2.49	0.47
1:D:3:LEU:HD21	1:D:149:ILE:CG1	2.37	0.47
1:D:18:ARG:NH1	1:D:128:ARG:O	2.47	0.47
1:A:281:SER:O	1:A:310:ARG:NH1	2.46	0.47
1:B:29:TYR:CB	1:B:54:LEU:HD11	2.45	0.47
1:C:247:GLU:O	1:C:250:ARG:HB2	2.14	0.47
1:D:29:TYR:CG	1:D:30:ASP:N	2.83	0.47
1:D:238:TYR:HB2	1:D:240:PHE:CE1	2.48	0.47
1:A:39:MET:O	1:A:45:THR:CB	2.63	0.47
1:A:48:VAL:HG12	1:A:50:SER:H	1.78	0.47
1:C:3:LEU:O	1:C:3:LEU:HD12	2.14	0.47
1:C:232:ASN:HB3	1:C:235:CYS:SG	2.54	0.47
1:D:47:GLY:O	1:D:48:VAL:CG2	2.59	0.47
1:D:123:GLY:N	2:D:401:HOH:O	2.42	0.47
1:D:147:GLU:OE2	1:D:177:TYR:OH	2.27	0.47
1:B:212:ARG:O	1:B:212:ARG:HG3	2.13	0.47
1:D:41:GLY:H	1:D:42:GLU:CA	2.20	0.47
1:D:51:LEU:CD1	2:D:403:HOH:O	2.62	0.47
1:A:104:ARG:O	1:A:107:LYS:HB2	2.15	0.47
1:B:1:MET:HB2	1:B:2:GLN:OE1	2.15	0.47
1:B:17:ARG:CZ	1:B:42:GLU:OE1	2.62	0.47
1:B:84:THR:O	1:B:85:LEU:HB2	2.15	0.47
1:D:197:GLU:HG2	1:D:201:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG23	1:A:26:CYS:CB	2.45	0.47
1:A:27:VAL:C	1:A:28:VAL:HG13	2.35	0.47
1:A:50:SER:CB	1:A:53:GLU:CG	2.64	0.47
1:B:323:ALA:O	1:B:327:MET:HG3	2.13	0.47
1:C:99:TYR:CD1	1:C:100:ARG:N	2.83	0.47
1:B:287:ARG:HB3	1:D:294:ILE:CG2	2.45	0.47
1:A:60:ALA:HB2	1:A:62:ARG:HE	1.78	0.47
1:B:1:MET:CG	1:B:2:GLN:N	2.77	0.47
1:B:65:TRP:HE1	1:B:94:GLY:HA3	1.80	0.47
1:C:38:ALA:O	1:C:42:GLU:OE2	2.33	0.47
1:D:90:ILE:CG2	1:D:115:HIS:O	2.61	0.47
1:A:29:TYR:HE1	1:A:31:HIS:HA	1.79	0.46
1:B:62:ARG:CZ	1:B:86:GLU:OE2	2.63	0.46
1:D:42:GLU:HB2	1:D:45:THR:OG1	2.10	0.46
1:A:65:TRP:HE1	1:A:67:MET:CG	2.28	0.46
1:C:7:GLY:N	1:C:29:TYR:O	2.37	0.46
1:D:85:LEU:HB2	1:D:114:ILE:CD1	2.45	0.46
1:A:283:SER:HB2	1:A:285:GLU:OE1	2.16	0.46
1:D:285:GLU:HG3	1:D:288:TRP:CZ3	2.50	0.46
1:A:250:ARG:NH2	1:B:161:PRO:O	2.45	0.46
1:A:284:GLY:CA	1:D:228:ALA:HB2	2.45	0.46
1:D:215:ASP:OD2	1:D:219:ARG:CZ	2.64	0.46
1:A:27:VAL:CG2	1:A:58:LEU:HD13	2.23	0.46
1:A:245:VAL:O	1:A:248:VAL:HG12	2.14	0.46
1:C:108:LEU:HD22	1:C:109:LEU:HD13	1.97	0.46
1:B:270:SER:OG	1:B:275:GLU:OE2	2.32	0.46
1:D:118:ASP:O	1:D:136:ILE:HA	2.14	0.46
1:B:45:THR:HG21	2:B:425:HOH:O	1.86	0.46
1:B:249:TRP:CD2	1:B:255:ILE:HD11	2.51	0.46
1:C:20:ALA:HB1	1:C:44:ARG:HB2	1.96	0.46
1:C:60:ALA:HA	1:C:62:ARG:HG3	1.96	0.46
1:A:8:LEU:CD1	1:A:29:TYR:C	2.84	0.46
1:B:84:THR:CG2	1:B:85:LEU:HD22	2.46	0.46
1:B:99:TYR:O	1:B:102:ASP:HB2	2.16	0.46
1:C:48:VAL:CG1	1:C:50:SER:H	2.29	0.46
1:D:3:LEU:O	1:D:26:CYS:HA	2.15	0.46
1:D:17:ARG:NH1	1:D:38:ALA:HB2	2.31	0.46
1:D:103:LEU:CD2	1:D:183:CYS:SG	2.98	0.46
1:B:232:ASN:HA	1:B:234:GLU:OE1	2.16	0.45
1:B:299:PRO:HD3	1:D:311:PHE:HB3	1.98	0.45
1:C:5:MET:HG2	1:C:16:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:HG12	1:B:236:TYR:CB	2.46	0.45
1:C:19:LEU:HD21	1:C:149:ILE:HG23	1.98	0.45
1:C:31:HIS:CD2	1:C:32:ASP:CA	2.97	0.45
1:D:59:SER:O	1:D:62:ARG:NH1	2.49	0.45
1:A:8:LEU:CD1	1:A:8:LEU:N	2.76	0.45
1:A:157:VAL:H	1:A:175:GLN:NE2	2.14	0.45
1:B:59:SER:OG	1:B:60:ALA:O	2.35	0.45
1:B:77:VAL:C	1:B:81:LEU:CD1	2.82	0.45
1:C:31:HIS:CD2	1:C:31:HIS:C	2.89	0.45
1:C:189:VAL:HG23	1:D:240:PHE:CE2	2.52	0.45
1:D:117:LEU:HD23	1:D:138:GLY:HA3	1.97	0.45
1:A:29:TYR:CE1	1:A:30:ASP:C	2.90	0.45
1:B:1:MET:CG	1:B:2:GLN:H	2.23	0.45
1:B:90:ILE:HG13	1:B:145:ARG:NH2	2.32	0.45
1:C:244:GLU:O	1:C:248:VAL:HG12	2.17	0.45
1:C:18:ARG:NH2	1:C:152:THR:O	2.49	0.45
1:C:296:GLU:OE1	1:D:210:ILE:O	2.34	0.45
1:C:301:PRO:O	1:C:305:THR:HB	2.17	0.45
1:C:301:PRO:O	1:C:305:THR:HG22	2.16	0.45
1:D:109:LEU:HD22	1:D:114:ILE:HG21	1.99	0.45
1:A:47:GLY:O	1:A:48:VAL:CG2	2.65	0.45
1:A:168:GLY:N	2:A:402:HOH:O	2.17	0.45
1:B:231:PRO:O	1:B:232:ASN:HB2	2.17	0.45
1:C:178:LEU:HD23	1:C:179:HIS:CA	2.47	0.45
1:C:195:GLY:O	1:C:303:LEU:HD22	2.17	0.45
1:A:329:LYS:HD3	1:A:330:GLN:HG3	1.99	0.44
1:D:149:ILE:O	1:D:153:VAL:HG23	2.17	0.44
1:A:92:ILE:HD13	1:A:150:PHE:HE1	1.81	0.44
1:A:92:ILE:CD1	1:A:150:PHE:CZ	3.01	0.44
1:D:8:LEU:HD21	1:D:28:VAL:HG13	1.98	0.44
1:D:54:LEU:HD12	1:D:54:LEU:HA	1.83	0.44
1:A:166:ARG:HA	1:A:166:ARG:HD3	1.78	0.44
1:B:30:ASP:C	1:B:32:ASP:N	2.70	0.44
1:C:281:SER:HA	1:C:314:ARG:HE	1.81	0.44
1:D:25:ASP:OD1	1:D:44:ARG:HG3	2.17	0.44
1:D:79:GLU:HG2	1:D:108:LEU:CD1	2.45	0.44
1:B:85:LEU:CA	1:B:89:ASP:OD1	2.65	0.44
1:D:39:MET:H	1:D:39:MET:CE	2.30	0.44
1:D:55:SER:O	1:D:62:ARG:CZ	2.65	0.44
1:D:238:TYR:HB2	1:D:240:PHE:HE1	1.83	0.44
1:B:33:PRO:O	1:B:37:LYS:HB3	2.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ILE:HD12	1:B:142:ALA:CB	2.29	0.44
1:D:323:ALA:O	1:D:327:MET:HG3	2.18	0.44
1:A:8:LEU:HD21	1:A:28:VAL:HB	1.98	0.44
1:A:109:LEU:HD13	1:A:114:ILE:HD13	1.21	0.44
1:C:8:LEU:CD1	1:C:39:MET:HG3	2.48	0.44
1:D:249:TRP:CD2	1:D:255:ILE:HD11	2.52	0.44
1:D:300:ALA:O	1:D:304:THR:OG1	2.24	0.44
1:C:10:ARG:NH1	1:C:10:ARG:HG2	2.33	0.44
1:C:253:SER:HB2	1:D:193:HIS:NE2	2.33	0.44
1:D:12:GLY:C	1:D:15:ILE:HG22	2.36	0.44
1:D:81:LEU:HA	1:D:84:THR:HG23	1.97	0.44
1:B:317:ASP:OD1	1:B:317:ASP:N	2.41	0.44
1:C:5:MET:HG2	1:C:16:VAL:CG2	2.48	0.44
1:C:189:VAL:HG23	1:D:240:PHE:HE2	1.81	0.43
1:C:329:LYS:HG3	1:C:330:GLN:N	2.32	0.43
1:C:28:VAL:HG21	1:C:39:MET:HB2	2.00	0.43
1:C:119:CYS:SG	1:C:134:LEU:HD13	2.58	0.43
1:B:81:LEU:CA	1:B:85:LEU:HD21	2.46	0.43
1:B:94:GLY:HA2	1:B:119:CYS:O	2.18	0.43
1:C:81:LEU:CD2	1:C:85:LEU:HD21	2.48	0.43
1:D:58:LEU:O	1:D:59:SER:HB2	2.18	0.43
1:A:75:THR:HA	1:A:78:ILE:CD1	2.48	0.43
1:B:142:ALA:HA	1:B:145:ARG:NH2	2.32	0.43
1:B:310:ARG:HD2	2:B:424:HOH:O	2.18	0.43
1:D:55:SER:O	1:D:62:ARG:NH2	2.51	0.43
1:B:20:ALA:C	1:B:22:GLY:H	2.21	0.43
1:C:4:GLY:HA2	1:C:27:VAL:HG13	2.00	0.43
1:C:79:GLU:HG2	1:C:108:LEU:HD11	2.00	0.43
1:D:55:SER:HB3	1:D:56:GLN:OE1	2.17	0.43
1:A:11:MET:HB3	1:A:11:MET:HE2	1.92	0.43
1:A:40:ALA:CA	1:A:45:THR:HG21	2.47	0.43
1:B:2:GLN:HA	1:B:25:ASP:O	2.19	0.43
1:B:81:LEU:CA	1:B:85:LEU:CD2	2.97	0.43
1:C:178:LEU:CD2	1:C:179:HIS:C	2.85	0.43
1:A:74:THR:HG22	1:A:78:ILE:CD1	2.47	0.43
1:A:107:LYS:HB3	1:A:107:LYS:HE2	1.85	0.43
1:A:94:GLY:HA2	1:A:119:CYS:O	2.19	0.43
1:D:65:TRP:HE1	1:D:67:MET:HG3	1.83	0.43
1:D:201:MET:O	1:D:202:ALA:C	2.55	0.43
1:D:204:LEU:HD23	1:D:208:LEU:HG	2.00	0.43
1:A:114:ILE:HG13	1:A:114:ILE:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LEU:HD22	1:C:62:ARG:HB3	2.01	0.43
1:D:31:HIS:ND1	1:D:31:HIS:C	2.72	0.43
1:A:8:LEU:HD11	1:A:29:TYR:O	2.18	0.42
1:A:57:ARG:O	1:A:57:ARG:CG	2.67	0.42
1:B:108:LEU:HD23	1:B:108:LEU:O	2.19	0.42
1:C:3:LEU:HD11	1:C:26:CYS:HA	2.01	0.42
1:C:254:VAL:HG23	2:D:401:HOH:O	2.19	0.42
1:C:270:SER:O	1:C:273:LEU:HD23	2.19	0.42
1:A:25:ASP:OD1	1:A:44:ARG:NH1	2.53	0.42
1:A:126:TRP:CD1	1:A:126:TRP:N	2.87	0.42
1:A:330:GLN:NE2	1:D:262:LEU:O	2.53	0.42
1:B:33:PRO:C	1:B:35:ALA:N	2.72	0.42
1:B:98:TYR:CZ	1:B:100:ARG:HG3	2.54	0.42
1:C:31:HIS:O	1:C:33:PRO:HD3	2.20	0.42
1:D:11:MET:HB3	1:D:67:MET:CE	2.49	0.42
1:A:33:PRO:C	1:A:36:VAL:HG12	2.39	0.42
1:A:74:THR:O	1:A:77:VAL:N	2.52	0.42
1:A:80:GLU:C	1:A:82:ALA:N	2.72	0.42
1:A:327:MET:SD	1:D:201:MET:HB2	2.59	0.42
1:C:216:VAL:HG13	1:C:230:LEU:CD2	2.49	0.42
1:A:244:GLU:OE2	1:B:166:ARG:NH2	2.38	0.42
1:B:17:ARG:O	1:B:21:LYS:HG3	2.18	0.42
1:A:26:CYS:O	1:A:46:THR:HB	2.20	0.42
1:C:201:MET:HG2	1:C:201:MET:H	1.62	0.42
1:B:63:VAL:HG12	1:B:64:VAL:N	2.34	0.42
1:D:32:ASP:OD2	1:D:34:ASP:N	2.49	0.42
1:D:135:MET:HB3	1:D:180:CYS:SG	2.59	0.42
1:A:287:ARG:HG2	1:C:294:ILE:HG23	2.01	0.42
1:A:316:LEU:HA	1:A:316:LEU:HD23	1.72	0.42
1:B:35:ALA:O	1:B:38:ALA:CB	2.61	0.42
1:B:106:GLU:HB2	1:B:116:LEU:HD23	2.01	0.42
1:D:39:MET:CE	1:D:39:MET:N	2.83	0.42
1:D:89:ASP:O	1:D:114:ILE:HG23	2.20	0.42
1:B:3:LEU:HD21	1:B:19:LEU:HD13	2.01	0.42
1:B:67:MET:HE2	1:B:95:GLY:CA	2.45	0.42
1:B:110:PHE:C	1:B:112:LYS:N	2.72	0.42
1:A:39:MET:HA	1:A:42:GLU:CD	2.40	0.42
1:B:39:MET:SD	1:B:42:GLU:OE2	2.78	0.42
1:B:91:VAL:O	1:B:116:LEU:HD12	2.20	0.42
1:B:102:ASP:OD1	1:B:118:ASP:HB3	2.20	0.42
1:C:227:THR:OG1	1:C:337:LYS:NZ	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ASP:OD1	1:D:118:ASP:N	2.51	0.41
1:A:16:VAL:CG1	1:A:39:MET:SD	3.04	0.41
1:B:84:THR:CG2	1:B:85:LEU:N	2.69	0.41
1:D:57:ARG:NH2	1:D:57:ARG:CB	2.71	0.41
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.85	0.41
1:C:63:VAL:HG23	1:C:90:ILE:HB	2.02	0.41
1:C:257:SER:HA	1:D:257:SER:HA	2.02	0.41
1:B:56:GLN:HA	1:B:62:ARG:NH2	2.36	0.41
1:D:39:MET:HB2	1:D:42:GLU:CB	2.51	0.41
1:A:212:ARG:NH1	1:A:272:ASP:OD1	2.53	0.41
1:B:3:LEU:CD2	1:B:149:ILE:HD12	2.51	0.41
1:B:15:ILE:HD11	1:B:153:VAL:HG21	2.01	0.41
1:B:34:ASP:HA	1:B:37:LYS:HB3	2.02	0.41
1:B:117:LEU:CD1	1:B:143:PHE:HA	2.50	0.41
1:C:60:ALA:HA	1:C:61:PRO:C	2.40	0.41
1:D:74:THR:O	1:D:78:ILE:HD12	2.20	0.41
1:A:62:ARG:HD2	1:A:89:ASP:CG	2.41	0.41
1:A:121:THR:HG23	1:A:134:LEU:CD2	2.51	0.41
1:B:65:TRP:CE3	1:B:92:ILE:HG21	2.56	0.41
1:B:111:LYS:O	1:B:112:LYS:HB2	2.20	0.41
1:C:300:ALA:HA	1:D:206:GLU:CD	2.40	0.41
1:B:1:MET:HG3	1:B:2:GLN:N	2.29	0.41
1:B:57:ARG:C	1:B:57:ARG:CD	2.85	0.41
1:B:162:ARG:HH21	1:B:166:ARG:HB3	1.86	0.41
1:B:301:PRO:O	1:B:305:THR:HB	2.20	0.41
1:D:120:GLY:O	1:D:134:LEU:HA	2.21	0.41
1:A:29:TYR:CD1	1:A:30:ASP:O	2.74	0.41
1:A:48:VAL:HG11	1:A:53:GLU:HB3	2.02	0.41
1:A:170:VAL:HG13	1:A:174:GLU:HB2	2.01	0.41
1:B:56:GLN:HA	1:B:62:ARG:HH22	1.86	0.41
1:C:60:ALA:HB2	1:C:62:ARG:CZ	2.51	0.41
1:D:50:SER:HB3	1:D:53:GLU:CG	2.49	0.41
1:D:250:ARG:HH11	1:D:261:ASP:CG	2.22	0.41
1:A:212:ARG:CZ	1:A:272:ASP:OD1	2.69	0.41
1:A:284:GLY:HA3	1:D:228:ALA:CB	2.51	0.41
1:B:73:ILE:O	1:B:77:VAL:HG23	2.21	0.41
1:B:110:PHE:HD1	1:B:110:PHE:HA	1.77	0.41
1:C:178:LEU:HD22	1:C:180:CYS:SG	2.61	0.41
1:C:189:VAL:CG2	1:D:240:PHE:CE2	3.04	0.41
1:D:59:SER:O	1:D:62:ARG:CZ	2.69	0.41
1:D:107:LYS:HE3	1:D:107:LYS:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:CG	1:D:201:MET:CE	2.94	0.41
1:A:336:GLU:OE1	1:D:278:GLY:N	2.36	0.41
1:C:3:LEU:HD22	1:C:19:LEU:HD13	2.02	0.41
1:C:157:VAL:O	1:C:158:ALA:C	2.60	0.41
1:D:62:ARG:C	1:D:89:ASP:CB	2.77	0.41
1:D:147:GLU:HG3	1:D:177:TYR:OH	2.21	0.41
1:D:220:VAL:HG22	2:D:419:HOH:O	2.19	0.41
1:B:3:LEU:HD22	1:B:149:ILE:HD12	2.03	0.40
1:B:118:ASP:O	1:B:136:ILE:HA	2.22	0.40
1:B:124:GLY:HA3	1:C:331:PHE:O	2.20	0.40
1:C:20:ALA:HB3	1:C:21:LYS:CE	2.51	0.40
1:D:197:GLU:O	1:D:201:MET:HG2	2.21	0.40
1:A:10:ARG:O	1:A:14:ASN:OD1	2.40	0.40
1:A:92:ILE:HD13	1:A:150:PHE:CZ	2.56	0.40
1:B:20:ALA:C	1:B:22:GLY:N	2.74	0.40
1:B:216:VAL:HG13	1:B:230:LEU:HD22	2.03	0.40
1:C:58:LEU:CD2	1:C:62:ARG:HB3	2.51	0.40
1:A:40:ALA:HA	1:A:45:THR:CB	2.46	0.40
1:A:218:THR:OG1	1:A:219:ARG:N	2.53	0.40
1:B:29:TYR:CD1	1:B:30:ASP:N	2.89	0.40
1:C:285:GLU:HA	1:C:288:TRP:CE3	2.56	0.40
1:D:11:MET:HB3	1:D:67:MET:HE1	2.02	0.40
1:D:36:VAL:O	1:D:37:LYS:C	2.58	0.40
1:D:147:GLU:CG	1:D:177:TYR:OH	2.68	0.40
1:C:31:HIS:HD2	1:C:32:ASP:CB	2.29	0.40
1:A:92:ILE:CD1	1:A:150:PHE:CE1	3.04	0.40
1:D:39:MET:HA	1:D:42:GLU:HG2	2.03	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	329/340 (97%)	312 (95%)	15 (5%)	2 (1%)	25 44
1	B	319/340 (94%)	298 (93%)	19 (6%)	2 (1%)	25 44
1	C	327/340 (96%)	319 (98%)	8 (2%)	0	100 100
1	D	319/340 (94%)	299 (94%)	17 (5%)	3 (1%)	17 32
All	All	1294/1360 (95%)	1228 (95%)	59 (5%)	7 (0%)	29 48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	THR
1	B	84	THR
1	B	31	HIS
1	D	44	ARG
1	A	40	ALA
1	D	35	ALA
1	D	182	PRO

5.3.2 Protein sidechains [\(i\)](#)

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	254/259 (98%)	242 (95%)	12 (5%)	26 45
1	B	248/259 (96%)	229 (92%)	19 (8%)	13 23
1	C	253/259 (98%)	244 (96%)	9 (4%)	35 55
1	D	248/259 (96%)	229 (92%)	19 (8%)	13 23
All	All	1003/1036 (97%)	944 (94%)	59 (6%)	19 34

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	17	ARG
1	A	44	ARG
1	A	45	THR

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Mol	Chain	Res	Type
1	A	46	THR
1	A	62	ARG
1	A	67	MET
1	A	79	GLU
1	A	193	HIS
1	A	201	MET
1	A	281	SER
1	A	336	GLU
1	B	2	GLN
1	B	8	LEU
1	B	25	ASP
1	B	30	ASP
1	B	31	HIS
1	B	32	ASP
1	B	51	LEU
1	B	54	LEU
1	B	55	SER
1	B	57	ARG
1	B	58	LEU
1	B	66	VAL
1	B	91	VAL
1	B	110	PHE
1	B	112	LYS
1	B	114	ILE
1	B	130	ARG
1	B	190	LYS
1	B	282	ASP
1	C	31	HIS
1	C	58	LEU
1	C	62	ARG
1	C	99	TYR
1	C	104	ARG
1	C	110	PHE
1	C	167	ASP
1	C	183	CYS
1	C	251	ARG
1	D	17	ARG
1	D	31	HIS
1	D	37	LYS
1	D	39	MET
1	D	42	GLU
1	D	43	ASP

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Mol	Chain	Res	Type
1	D	45	THR
1	D	56	GLN
1	D	58	LEU
1	D	89	ASP
1	D	106	GLU
1	D	118	ASP
1	D	166	ARG
1	D	174	GLU
1	D	201	MET
1	D	212	ARG
1	D	232	ASN
1	D	277	SER
1	D	325	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	72	ASN
1	A	175	GLN
1	A	334	HIS
1	B	24	HIS
1	B	31	HIS
1	B	115	HIS
1	C	31	HIS
1	C	213	ASN
1	D	115	HIS
1	D	237	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	333/340 (97%)	0.34	37 (11%) 5 5	27, 73, 135, 156	0
1	B	323/340 (95%)	0.39	33 (10%) 6 6	28, 72, 143, 160	0
1	C	331/340 (97%)	0.47	38 (11%) 4 4	30, 82, 128, 147	0
1	D	323/340 (95%)	0.72	49 (15%) 2 2	32, 93, 167, 189	0
All	All	1310/1360 (96%)	0.48	157 (11%) 4 4	27, 81, 144, 189	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	40	ALA	7.0
1	B	219	ARG	6.4
1	B	62	ARG	6.4
1	D	229	PRO	6.3
1	D	228	ALA	6.0
1	D	219	ARG	5.8
1	D	41	GLY	5.7
1	C	170	VAL	5.7
1	D	220	VAL	5.7
1	D	227	THR	5.6
1	D	110	PHE	5.6
1	C	219	ARG	5.6
1	C	125	VAL	5.5
1	C	218	THR	5.4
1	D	218	THR	5.4
1	C	111	LYS	4.9
1	C	7	GLY	4.9
1	B	111	LYS	4.8
1	B	228	ALA	4.8
1	C	233	PRO	4.7
1	C	92	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	31	HIS	4.6
1	C	232	ASN	4.4
1	A	338	PRO	4.4
1	A	340	ASN	4.3
1	B	145	ARG	4.3
1	B	38	ALA	4.3
1	D	4	GLY	4.2
1	D	113	GLY	4.1
1	B	47	GLY	4.1
1	D	3	LEU	4.1
1	A	39	MET	4.1
1	A	113	GLY	4.1
1	D	65	TRP	4.0
1	A	167	ASP	4.0
1	A	64	VAL	4.0
1	C	4	GLY	4.0
1	D	119	CYS	4.0
1	C	108	LEU	3.9
1	B	35	ALA	3.9
1	A	339	ALA	3.8
1	B	82	ALA	3.8
1	D	61	PRO	3.7
1	C	126	TRP	3.7
1	A	10	ARG	3.7
1	A	112	LYS	3.7
1	D	167	ASP	3.6
1	D	93	ASP	3.6
1	C	169	GLU	3.5
1	D	42	GLU	3.5
1	D	49	ALA	3.5
1	C	36	VAL	3.5
1	C	227	THR	3.5
1	D	231	PRO	3.5
1	A	43	ASP	3.5
1	C	228	ALA	3.4
1	B	63	VAL	3.3
1	B	34	ASP	3.3
1	A	129	GLU	3.3
1	B	83	ASN	3.3
1	D	92	ILE	3.2
1	B	86	GLU	3.2
1	C	217	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	125	VAL	3.2
1	B	94	GLY	3.2
1	D	67	MET	3.2
1	C	136	ILE	3.2
1	A	93	ASP	3.1
1	B	92	ILE	3.1
1	B	76	ALA	3.0
1	B	120	GLY	3.0
1	D	94	GLY	3.0
1	C	91	VAL	3.0
1	D	38	ALA	3.0
1	C	37	LYS	3.0
1	C	129	GLU	3.0
1	C	118	ASP	3.0
1	D	5	MET	2.9
1	B	56	GLN	2.9
1	D	170	VAL	2.9
1	C	127	GLY	2.9
1	B	64	VAL	2.9
1	B	31	HIS	2.9
1	A	92	ILE	2.9
1	D	22	GLY	2.8
1	A	114	ILE	2.8
1	C	220	VAL	2.8
1	A	4	GLY	2.8
1	D	27	VAL	2.8
1	D	35	ALA	2.8
1	A	130	ARG	2.8
1	D	135	MET	2.8
1	D	31	HIS	2.8
1	C	117	LEU	2.8
1	A	229	PRO	2.7
1	D	64	VAL	2.7
1	C	175	GLN	2.7
1	D	7	GLY	2.7
1	A	65	TRP	2.7
1	A	31	HIS	2.7
1	D	112	LYS	2.7
1	A	337	LYS	2.6
1	A	34	ASP	2.6
1	B	218	THR	2.6
1	D	39	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	230	LEU	2.6
1	B	65	TRP	2.6
1	D	33	PRO	2.6
1	C	124	GLY	2.6
1	A	110	PHE	2.5
1	C	72	ASN	2.5
1	A	335	ALA	2.5
1	D	111	LYS	2.5
1	D	34	ASP	2.5
1	C	119	CYS	2.5
1	B	229	PRO	2.4
1	C	237	GLN	2.4
1	D	52	ARG	2.4
1	B	116	LEU	2.4
1	B	59	SER	2.3
1	A	127	GLY	2.3
1	A	227	THR	2.3
1	B	119	CYS	2.3
1	A	57	ARG	2.3
1	B	85	LEU	2.3
1	D	114	ILE	2.3
1	B	37	LYS	2.3
1	A	128	ARG	2.3
1	A	218	THR	2.3
1	A	228	ALA	2.3
1	C	40	ALA	2.3
1	A	169	GLU	2.3
1	D	37	LYS	2.2
1	B	237	GLN	2.2
1	D	50	SER	2.2
1	A	119	CYS	2.2
1	B	167	ASP	2.2
1	D	118	ASP	2.2
1	D	128	ARG	2.2
1	C	229	PRO	2.2
1	D	72	ASN	2.1
1	A	125	VAL	2.1
1	A	217	GLY	2.1
1	B	93	ASP	2.1
1	C	167	ASP	2.1
1	C	35	ALA	2.1
1	D	60	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	126	TRP	2.1
1	C	145	ARG	2.1
1	D	233	PRO	2.1
1	A	21	LYS	2.1
1	A	91	VAL	2.1
1	C	187	HIS	2.1
1	B	49	ALA	2.0
1	B	107	LYS	2.0
1	C	337	LYS	2.0
1	A	233	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.