



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K8Z
Title : Crystal Structure of Gudb1 a decryptified secondary glutamate dehydrogenase from *B. subtilis*
Authors : Gunka, K.; Newman, J.A.; Commichau, F.M.; Herzberg, C.; Rodrigues, C.; Hewitt, L.; Lewis, R.J.; Stulke, J.
Deposited on : 2009-10-15
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

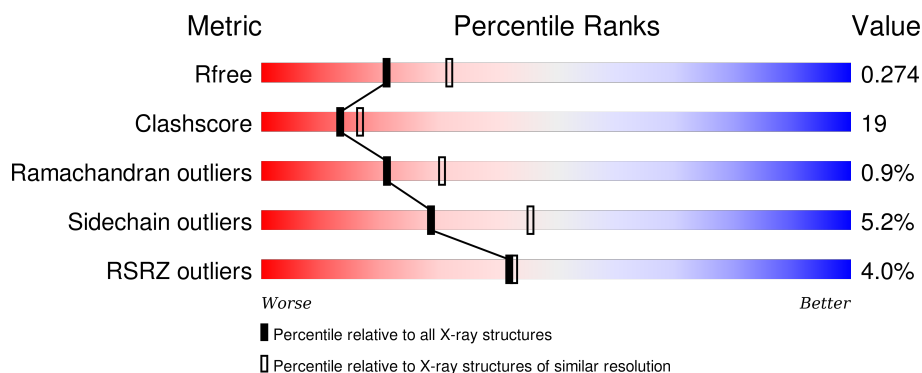
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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. 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.

Mol	Chain	Length	Quality of chain
1	A	423	<div> <div>8%</div> <div> <div></div> <div>60%</div> <div>27%</div> <div>• 11%</div> </div> </div>
1	B	423	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>• 7%</div> </div> </div>
1	C	423	<div> <div>•</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>5% •</div> </div> </div>
1	D	423	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>• 11%</div> </div> </div>
1	E	423	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>• 7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	423	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: green (58%), yellow (33%), and orange (5%). The segments are labeled with their respective percentages: 58%, 33%, and 5%. The bar ends with a small black dot.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18791 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 NAD-specific glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2929	1856	506	549	18			
1	B	392	Total	C	N	O	S	0	0	0
			3049	1932	525	574	18			
1	C	407	Total	C	N	O	S	0	0	0
			3169	2008	545	598	18			
1	D	378	Total	C	N	O	S	0	0	0
			2929	1856	506	549	18			
1	E	392	Total	C	N	O	S	0	0	0
			3049	1932	525	574	18			
1	F	407	Total	C	N	O	S	0	0	0
			3169	2008	545	598	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	SEE REMARK 999	UNP P50735
A	?	-	VAL	SEE REMARK 999	UNP P50735
A	?	-	LYS	SEE REMARK 999	UNP P50735
A	?	-	ALA	SEE REMARK 999	UNP P50735
B	?	-	GLN	SEE REMARK 999	UNP P50735
B	?	-	VAL	SEE REMARK 999	UNP P50735
B	?	-	LYS	SEE REMARK 999	UNP P50735
B	?	-	ALA	SEE REMARK 999	UNP P50735
C	?	-	GLN	SEE REMARK 999	UNP P50735
C	?	-	VAL	SEE REMARK 999	UNP P50735
C	?	-	LYS	SEE REMARK 999	UNP P50735
C	?	-	ALA	SEE REMARK 999	UNP P50735
D	?	-	GLN	SEE REMARK 999	UNP P50735
D	?	-	VAL	SEE REMARK 999	UNP P50735
D	?	-	LYS	SEE REMARK 999	UNP P50735
D	?	-	ALA	SEE REMARK 999	UNP P50735
E	?	-	GLN	SEE REMARK 999	UNP P50735

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	VAL	SEE REMARK 999	UNP P50735
E	?	-	LYS	SEE REMARK 999	UNP P50735
E	?	-	ALA	SEE REMARK 999	UNP P50735
F	?	-	GLN	SEE REMARK 999	UNP P50735
F	?	-	VAL	SEE REMARK 999	UNP P50735
F	?	-	LYS	SEE REMARK 999	UNP P50735
F	?	-	ALA	SEE REMARK 999	UNP P50735

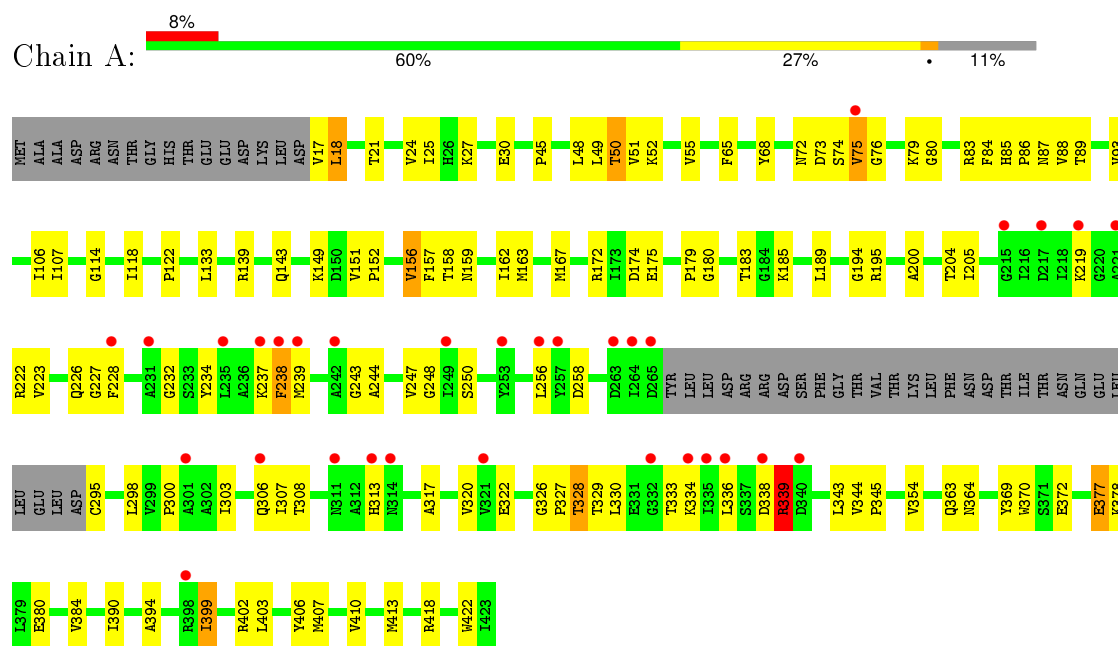
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	85	Total O 85 85	0	0
2	B	66	Total O 66 66	0	0
2	C	88	Total O 88 88	0	0
2	D	73	Total O 73 73	0	0
2	E	84	Total O 84 84	0	0
2	F	101	Total O 101 101	0	0

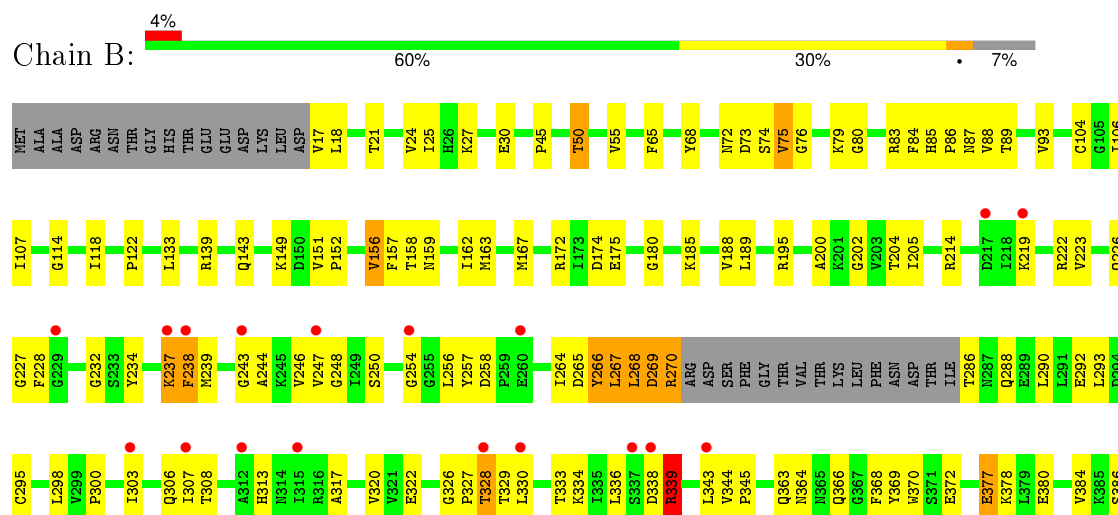
3 Residue-property plots

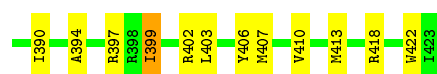
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: NAD-specific glutamate dehydrogenase

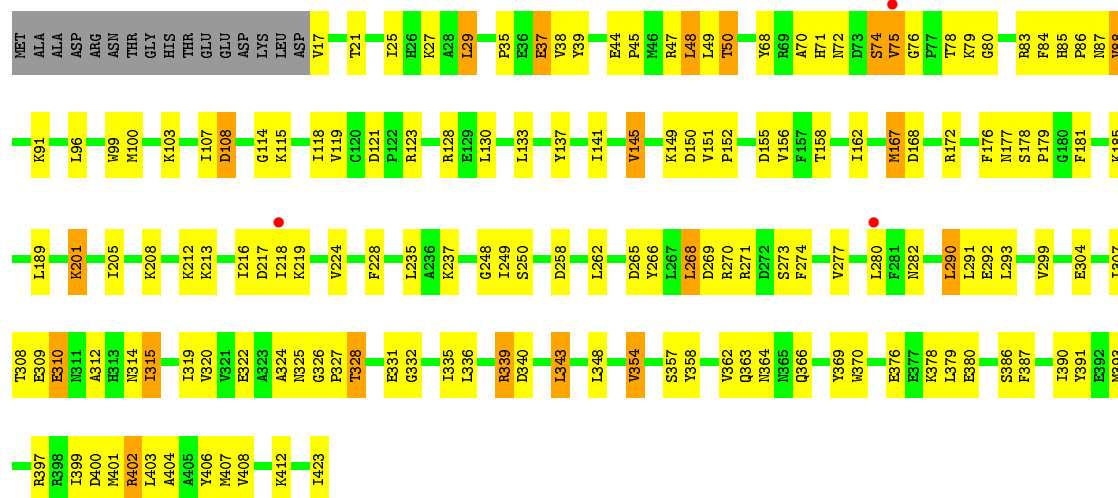


- Molecule 1: NAD-specific glutamate dehydrogenase

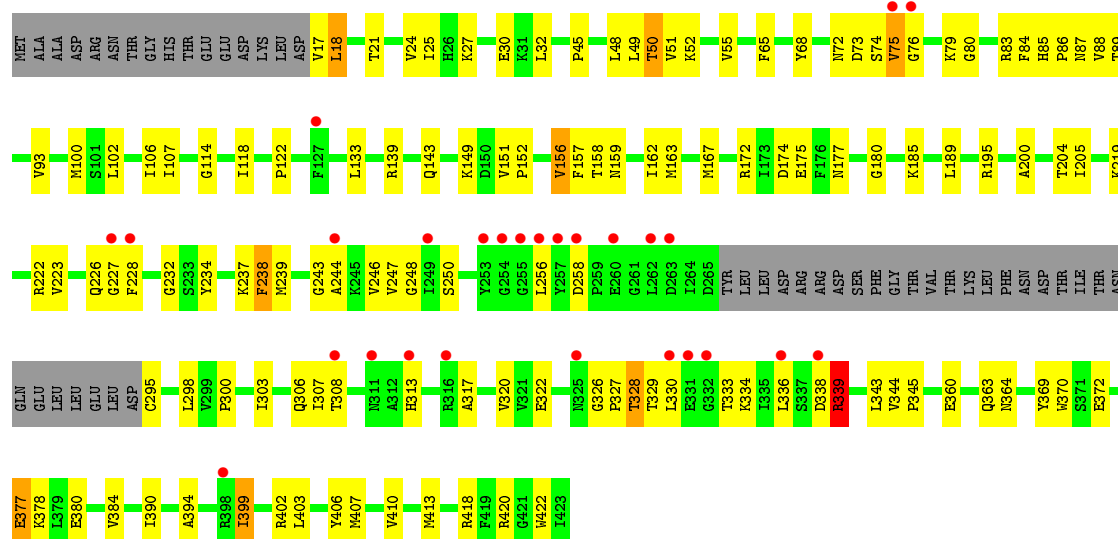




• Molecule 1: NAD-specific glutamate dehydrogenase

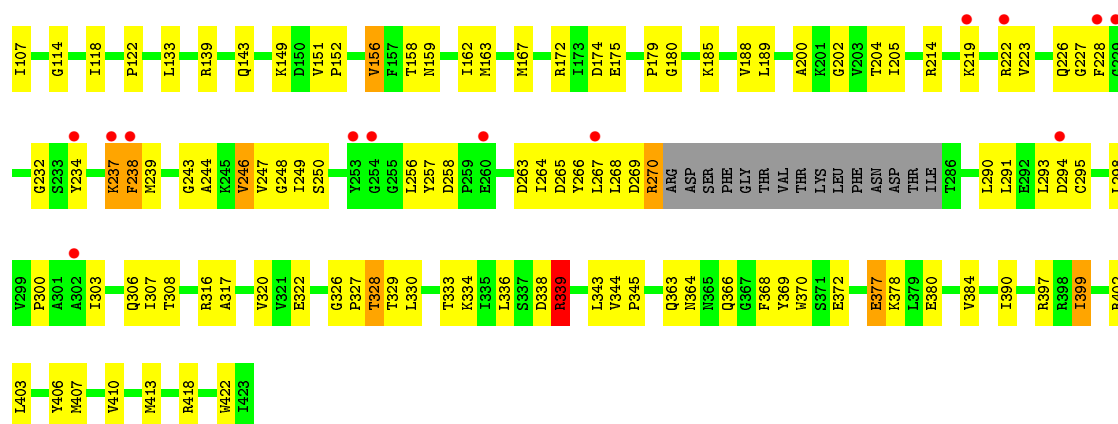


• Molecule 1: NAD-specific glutamate dehydrogenase



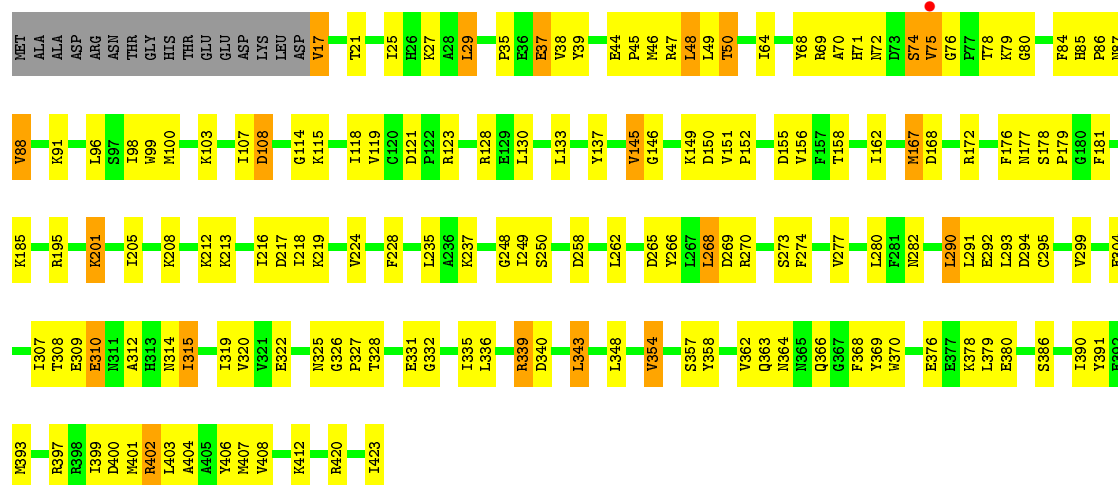
• Molecule 1: NAD-specific glutamate dehydrogenase





• Molecule 1: NAD-specific glutamate dehydrogenase

Chain F: 58% 33% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.22Å 192.49Å 89.39Å 90.00° 118.74° 90.00°	Depositor
Resolution (Å)	19.77 – 2.40 19.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.77-2.40) 96.6 (19.77-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.247 , 0.278 0.246 , 0.274	Depositor DCC
R_{free} test set	4788 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.2	EDS
Estimated twinning fraction	0.367 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 96065 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18791	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/2984	0.47	2/4025 (0.0%)
1	B	0.27	0/3105	0.49	2/4191 (0.0%)
1	C	0.24	0/3228	0.47	0/4359
1	D	0.23	0/2984	0.47	2/4025 (0.0%)
1	E	0.28	0/3105	0.63	3/4191 (0.1%)
1	F	0.24	0/3228	0.47	0/4359
All	All	0.25	0/18634	0.50	9/25150 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	339	ARG	NE-CZ-NH1	-18.95	110.83	120.30
1	E	339	ARG	NE-CZ-NH2	18.04	129.32	120.30
1	E	339	ARG	CD-NE-CZ	8.97	136.16	123.60
1	D	339	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	339	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	339	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	339	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	339	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	339	ARG	NE-CZ-NH1	5.82	123.21	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2929	0	2946	96	0
1	B	3049	0	3064	117	0
1	C	3169	0	3183	152	0
1	D	2929	0	2946	97	0
1	E	3049	0	3064	109	0
1	F	3169	0	3183	158	0
2	A	85	0	0	8	0
2	B	66	0	0	4	0
2	C	88	0	0	10	0
2	D	73	0	0	8	0
2	E	84	0	0	3	0
2	F	101	0	0	9	0
All	All	18791	0	18386	691	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 19.

All (691) 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:B:264:ILE:O	1:B:268:LEU:HB2	1.50	1.11
1:B:270:ARG:HH11	1:B:270:ARG:HG2	0.86	1.03
1:B:270:ARG:HH11	1:B:270:ARG:CG	1.73	0.97
1:B:270:ARG:HG2	1:B:270:ARG:NH1	1.65	0.96
1:F:44:GLU:HG3	1:F:45:PRO:HD2	1.50	0.93
1:C:44:GLU:HG3	1:C:45:PRO:HD2	1.51	0.92
1:F:295:CYS:HB2	2:F:518:HOH:O	1.69	0.91
1:E:250:SER:HB3	1:E:290:LEU:HD13	1.53	0.91
1:D:49:LEU:HD11	1:F:47:ARG:HG2	1.52	0.89
1:A:49:LEU:HD11	1:C:47:ARG:HG2	1.54	0.89
1:D:83:ARG:HA	2:D:485:HOH:O	1.73	0.85
1:E:266:TYR:O	1:E:270:ARG:HG3	1.78	0.84
1:A:83:ARG:HA	2:A:484:HOH:O	1.81	0.81
1:B:264:ILE:O	1:B:268:LEU:N	2.14	0.81
1:C:38:VAL:HG22	1:C:423:ILE:HD12	1.63	0.81
1:B:264:ILE:O	1:B:268:LEU:CB	2.28	0.81
1:F:38:VAL:HG22	1:F:423:ILE:HD12	1.63	0.80
1:B:237:LYS:HE2	1:B:268:LEU:CD1	2.12	0.80
1:B:158:THR:HA	1:B:162:ILE:HD12	1.64	0.79
1:E:158:THR:HA	1:E:162:ILE:HD12	1.64	0.79
1:E:403:LEU:HG	1:E:407:MET:HE3	1.64	0.79
1:C:99:TRP:HZ3	1:C:406:TYR:OH	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:TRP:HZ3	1:F:406:TYR:OH	1.65	0.79
1:D:403:LEU:HG	1:D:407:MET:HE3	1.65	0.79
1:A:403:LEU:HG	1:A:407:MET:HE3	1.65	0.79
1:C:218:ILE:HD11	2:C:504:HOH:O	1.82	0.78
1:B:403:LEU:HG	1:B:407:MET:HE3	1.65	0.78
1:A:158:THR:HA	1:A:162:ILE:HD12	1.64	0.78
1:D:158:THR:HA	1:D:162:ILE:HD12	1.64	0.78
1:E:17:VAL:HG23	1:E:18:LEU:H	1.50	0.77
1:F:99:TRP:HZ3	1:F:406:TYR:HH	1.33	0.77
1:B:17:VAL:HG23	1:B:18:LEU:H	1.50	0.77
1:C:99:TRP:HZ3	1:C:406:TYR:HH	1.32	0.76
1:B:363:GLN:NE2	1:B:370:TRP:H	1.85	0.75
1:A:17:VAL:HG23	1:A:18:LEU:H	1.52	0.74
1:F:290:LEU:HA	1:F:293:LEU:HG	1.70	0.74
1:F:348:LEU:HD22	1:F:390:ILE:HD12	1.70	0.74
1:C:290:LEU:HA	1:C:293:LEU:HG	1.70	0.74
1:C:348:LEU:HD22	1:C:390:ILE:HD12	1.70	0.73
1:E:363:GLN:NE2	1:E:370:TRP:H	1.85	0.73
1:A:363:GLN:NE2	1:A:370:TRP:H	1.85	0.73
1:E:330:LEU:H	1:E:330:LEU:HD12	1.53	0.73
1:F:363:GLN:NE2	1:F:370:TRP:H	1.86	0.73
1:D:363:GLN:NE2	1:D:370:TRP:H	1.86	0.73
1:D:17:VAL:HG23	1:D:18:LEU:H	1.53	0.73
1:D:52:LYS:HE3	1:F:44:GLU:HG2	1.71	0.73
1:C:363:GLN:NE2	1:C:370:TRP:H	1.87	0.72
1:E:223:VAL:HG11	1:E:239:MET:HG3	1.72	0.72
1:A:330:LEU:H	1:A:330:LEU:HD12	1.52	0.72
1:B:330:LEU:HD12	1:B:330:LEU:H	1.54	0.72
1:F:235:LEU:CD2	1:F:299:VAL:HG11	2.20	0.72
1:D:330:LEU:HD12	1:D:330:LEU:H	1.53	0.72
1:A:195:ARG:HD2	2:A:498:HOH:O	1.88	0.72
1:C:168:ASP:O	1:C:172:ARG:HG2	1.90	0.72
1:B:223:VAL:HG11	1:B:239:MET:HG3	1.72	0.72
1:C:235:LEU:CD2	1:C:299:VAL:HG11	2.20	0.72
1:B:237:LYS:HE2	1:B:268:LEU:HD13	1.72	0.71
1:B:269:ASP:O	1:B:270:ARG:C	2.29	0.71
1:F:168:ASP:O	1:F:172:ARG:HG2	1.91	0.71
1:A:223:VAL:HG11	1:A:239:MET:HG3	1.73	0.71
1:B:45:PRO:HA	1:B:72:ASN:HA	1.73	0.70
1:D:223:VAL:HG11	1:D:239:MET:HG3	1.74	0.69
1:F:45:PRO:HA	1:F:72:ASN:HA	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:PRO:HA	1:E:72:ASN:HA	1.73	0.69
1:B:205:ILE:HD13	1:B:380:GLU:HA	1.74	0.69
1:C:85:HIS:HD2	1:C:87:ASN:H	1.40	0.69
1:B:270:ARG:NH1	1:B:270:ARG:CG	2.38	0.69
1:F:85:HIS:HD2	1:F:87:ASN:H	1.40	0.69
1:A:45:PRO:HA	1:A:72:ASN:HA	1.73	0.69
1:F:291:LEU:O	1:F:315:ILE:HG22	1.93	0.69
1:A:205:ILE:HD13	1:A:380:GLU:HA	1.74	0.69
1:E:205:ILE:HD13	1:E:380:GLU:HA	1.75	0.68
1:D:45:PRO:HA	1:D:72:ASN:HA	1.74	0.68
1:D:85:HIS:HD2	1:D:87:ASN:H	1.41	0.68
1:E:85:HIS:HD2	1:E:87:ASN:H	1.41	0.68
1:F:44:GLU:HG3	1:F:45:PRO:CD	2.22	0.68
1:C:44:GLU:HG3	1:C:45:PRO:CD	2.22	0.68
1:C:45:PRO:HA	1:C:72:ASN:HA	1.73	0.68
1:C:291:LEU:O	1:C:315:ILE:HG22	1.93	0.68
1:D:205:ILE:HD13	1:D:380:GLU:HA	1.75	0.68
1:E:17:VAL:HG23	1:E:18:LEU:N	2.08	0.68
1:B:250:SER:HB3	1:B:290:LEU:HG	1.76	0.68
1:A:85:HIS:HD2	1:A:87:ASN:H	1.41	0.68
1:D:204:THR:HG21	1:D:238:PHE:HD2	1.59	0.68
1:B:85:HIS:HD2	1:B:87:ASN:H	1.42	0.68
1:A:17:VAL:HG23	1:A:18:LEU:N	2.09	0.67
1:B:17:VAL:HG23	1:B:18:LEU:N	2.09	0.67
1:C:403:LEU:O	1:C:407:MET:HG3	1.93	0.67
1:D:17:VAL:HG23	1:D:18:LEU:N	2.10	0.67
1:C:96:LEU:HA	1:C:99:TRP:CD1	2.31	0.66
1:F:401:MET:HA	1:F:401:MET:HE2	1.76	0.66
1:F:96:LEU:HA	1:F:99:TRP:CD1	2.31	0.66
1:A:204:THR:HG21	1:A:238:PHE:HD2	1.61	0.66
1:C:401:MET:HE2	1:C:401:MET:HA	1.77	0.66
1:C:74:SER:O	1:C:76:GLY:N	2.29	0.66
1:F:74:SER:O	1:F:76:GLY:N	2.29	0.66
1:B:195:ARG:HD2	2:B:486:HOH:O	1.95	0.66
1:E:204:THR:HG21	1:E:238:PHE:HD2	1.60	0.66
1:F:21:THR:O	1:F:25:ILE:HG13	1.96	0.65
1:E:294:ASP:HB2	1:E:316:ARG:NH1	2.09	0.65
1:F:80:GLY:HA3	1:F:114:GLY:O	1.96	0.65
1:D:139:ARG:HH21	1:E:139:ARG:HH21	1.43	0.65
1:E:17:VAL:CG2	1:E:18:LEU:H	2.09	0.65
1:B:17:VAL:CG2	1:B:18:LEU:H	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:HG21	1:B:238:PHE:HD2	1.61	0.65
1:F:403:LEU:O	1:F:407:MET:HG3	1.96	0.65
1:A:139:ARG:HH21	1:B:139:ARG:HH21	1.42	0.65
1:A:17:VAL:CG2	1:A:18:LEU:H	2.10	0.65
1:B:266:TYR:O	1:B:268:LEU:N	2.29	0.64
1:C:21:THR:O	1:C:25:ILE:HG13	1.98	0.64
1:D:17:VAL:CG2	1:D:18:LEU:H	2.11	0.64
1:F:86:PRO:HG3	1:F:121:ASP:HB2	1.80	0.64
1:D:195:ARG:HD2	2:D:451:HOH:O	1.98	0.64
1:C:80:GLY:HA3	1:C:114:GLY:O	1.97	0.64
1:D:143:GLN:HE21	1:F:149:LYS:NZ	1.95	0.63
1:F:235:LEU:HD21	1:F:299:VAL:HG11	1.79	0.63
1:C:86:PRO:HG3	1:C:121:ASP:HB2	1.81	0.63
1:F:158:THR:HA	1:F:162:ILE:HD12	1.82	0.62
1:C:235:LEU:HD21	1:C:299:VAL:HG11	1.81	0.62
1:E:368:PHE:HA	1:F:358:TYR:OH	1.99	0.62
1:D:85:HIS:CD2	1:D:87:ASN:H	2.18	0.62
1:D:80:GLY:HA3	1:D:114:GLY:O	1.99	0.62
1:F:201:LYS:HE3	1:F:201:LYS:HA	1.82	0.62
1:C:158:THR:HA	1:C:162:ILE:HD12	1.82	0.62
1:D:204:THR:HG21	1:D:238:PHE:CD2	2.34	0.61
1:A:85:HIS:CD2	1:A:87:ASN:H	2.18	0.61
1:C:201:LYS:HA	1:C:201:LYS:HE3	1.82	0.61
1:E:188:VAL:HG12	1:F:412:LYS:HG2	1.82	0.61
1:A:52:LYS:HE3	1:C:44:GLU:HG2	1.82	0.61
1:C:266:TYR:CE2	1:C:270:ARG:HD2	2.36	0.61
1:A:80:GLY:HA3	1:A:114:GLY:O	1.99	0.61
2:C:472:HOH:O	1:F:128:ARG:NH2	2.33	0.61
1:A:333:THR:HG23	1:A:343:LEU:HD23	1.82	0.61
1:B:202:GLY:HA3	2:B:427:HOH:O	2.01	0.61
1:F:266:TYR:CE2	1:F:270:ARG:HD2	2.36	0.61
1:E:333:THR:HG23	1:E:343:LEU:HD23	1.83	0.61
1:C:400:ASP:OD1	1:C:402:ARG:HB2	2.01	0.60
1:B:333:THR:HG23	1:B:343:LEU:HD23	1.83	0.60
1:B:80:GLY:HA3	1:B:114:GLY:O	2.01	0.60
1:E:85:HIS:CD2	1:E:87:ASN:H	2.18	0.60
1:C:80:GLY:O	1:C:152:PRO:HA	2.01	0.60
1:D:100:MET:HG2	2:D:431:HOH:O	2.01	0.60
1:C:402:ARG:HH11	1:C:402:ARG:CG	2.15	0.60
1:F:224:VAL:N	2:F:518:HOH:O	2.34	0.60
1:E:204:THR:HG21	1:E:238:PHE:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:HG21	1:B:238:PHE:CD2	2.36	0.60
1:F:402:ARG:HH11	1:F:402:ARG:CG	2.15	0.60
1:E:246:VAL:HB	1:E:264:ILE:HD11	1.84	0.60
1:F:400:ASP:OD1	1:F:402:ARG:HB2	2.02	0.60
1:E:80:GLY:HA3	1:E:114:GLY:O	2.01	0.60
1:A:204:THR:HG21	1:A:238:PHE:CD2	2.36	0.60
1:B:257:TYR:HD1	1:B:293:LEU:HD13	1.67	0.60
1:D:333:THR:HG23	1:D:343:LEU:HD23	1.83	0.60
1:B:85:HIS:CD2	1:B:87:ASN:H	2.19	0.59
1:F:80:GLY:O	1:F:152:PRO:HA	2.01	0.59
1:A:354:VAL:HG23	2:A:463:HOH:O	2.02	0.59
1:D:51:VAL:HG12	1:F:47:ARG:HG3	1.83	0.59
1:B:368:PHE:HA	1:C:358:TYR:OH	2.02	0.59
1:C:75:VAL:HG23	1:C:75:VAL:O	2.03	0.58
1:C:85:HIS:CD2	1:C:87:ASN:H	2.18	0.58
1:C:213:LYS:HG2	1:C:391:TYR:CE1	2.38	0.58
1:A:143:GLN:HE21	1:C:149:LYS:NZ	2.01	0.58
1:D:307:ILE:HB	1:D:328:THR:HB	1.85	0.58
1:F:85:HIS:CD2	1:F:87:ASN:H	2.18	0.58
1:A:307:ILE:HB	1:A:328:THR:HB	1.86	0.58
1:D:308:THR:HG22	1:D:329:THR:CG2	2.33	0.58
1:F:312:ALA:HA	1:F:315:ILE:HD11	1.86	0.58
1:F:213:LYS:HG2	1:F:391:TYR:CE1	2.39	0.58
1:C:158:THR:HG22	1:C:162:ILE:HD13	1.85	0.58
1:E:202:GLY:HA3	2:E:479:HOH:O	2.03	0.58
1:A:308:THR:HG22	1:A:329:THR:CG2	2.33	0.58
1:A:403:LEU:O	1:A:407:MET:HG3	2.05	0.57
1:C:201:LYS:HD3	1:C:376:GLU:OE1	2.03	0.57
1:A:80:GLY:O	1:A:152:PRO:HA	2.04	0.57
1:C:47:ARG:NH1	1:C:71:HIS:ND1	2.52	0.57
1:C:312:ALA:HA	1:C:315:ILE:HD11	1.86	0.57
1:F:201:LYS:HD3	1:F:376:GLU:OE1	2.03	0.57
1:F:47:ARG:NH1	1:F:71:HIS:ND1	2.52	0.57
1:D:403:LEU:O	1:D:407:MET:HG3	2.05	0.57
1:E:307:ILE:HB	1:E:328:THR:HB	1.86	0.57
2:A:449:HOH:O	1:C:50:THR:HG21	2.05	0.57
1:D:80:GLY:O	1:D:152:PRO:HA	2.04	0.57
1:F:158:THR:HG22	1:F:162:ILE:HD13	1.86	0.57
1:B:143:GLN:HE21	1:E:149:LYS:NZ	2.02	0.57
1:B:307:ILE:HB	1:B:328:THR:HB	1.86	0.57
1:C:363:GLN:HE21	1:C:369:TYR:HA	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLN:HE21	1:B:370:TRP:H	1.51	0.57
1:F:75:VAL:HG23	1:F:75:VAL:O	2.05	0.57
1:C:29:LEU:HD23	1:C:39:TYR:HA	1.87	0.57
1:E:403:LEU:O	1:E:407:MET:HG3	2.04	0.57
1:B:403:LEU:O	1:B:407:MET:HG3	2.05	0.57
1:E:80:GLY:O	1:E:152:PRO:HA	2.05	0.56
1:B:308:THR:HG22	1:B:329:THR:CG2	2.34	0.56
1:B:188:VAL:HG12	1:C:412:LYS:HG2	1.86	0.56
1:F:402:ARG:HG3	1:F:402:ARG:HH11	1.69	0.56
1:F:363:GLN:HE21	1:F:369:TYR:HA	1.71	0.56
1:F:29:LEU:HD23	1:F:39:TYR:HA	1.87	0.56
1:E:308:THR:HG22	1:E:329:THR:CG2	2.34	0.56
1:D:200:ALA:HB1	1:D:234:TYR:CD2	2.40	0.56
1:E:200:ALA:HB1	1:E:234:TYR:CD2	2.41	0.56
1:E:266:TYR:HD2	1:E:267:LEU:HD23	1.70	0.56
1:B:200:ALA:HB1	1:B:234:TYR:CD2	2.41	0.56
1:E:326:GLY:N	1:E:327:PRO:HD3	2.21	0.56
1:B:80:GLY:O	1:B:152:PRO:HA	2.05	0.56
1:A:185:LYS:HZ1	1:A:364:ASN:HD21	1.54	0.56
1:D:185:LYS:HZ1	1:D:364:ASN:HD21	1.54	0.56
1:D:377:GLU:HG3	1:D:378:LYS:N	2.21	0.56
1:E:363:GLN:HE21	1:E:370:TRP:H	1.51	0.55
1:C:402:ARG:HH11	1:C:402:ARG:HG3	1.70	0.55
1:B:149:LYS:NZ	1:E:143:GLN:HE21	2.05	0.55
1:A:200:ALA:HB1	1:A:234:TYR:CD2	2.41	0.55
1:F:295:CYS:CB	2:F:518:HOH:O	2.39	0.55
1:D:326:GLY:N	1:D:327:PRO:HD3	2.22	0.55
1:B:326:GLY:N	1:B:327:PRO:HD3	2.22	0.55
1:D:360:GLU:HB2	2:D:453:HOH:O	2.06	0.55
1:C:397:ARG:HB2	1:C:399:ILE:HG12	1.89	0.55
1:E:17:VAL:CG2	1:E:18:LEU:N	2.70	0.55
1:C:79:LYS:HD2	1:C:151:VAL:O	2.06	0.55
1:A:326:GLY:N	1:A:327:PRO:HD3	2.22	0.55
1:B:17:VAL:CG2	1:B:18:LEU:N	2.70	0.55
1:F:397:ARG:HB2	1:F:399:ILE:HG12	1.89	0.54
1:C:322:GLU:OE1	1:C:402:ARG:NH2	2.40	0.54
1:A:157:PHE:N	2:A:484:HOH:O	2.39	0.54
1:A:377:GLU:HG3	1:A:378:LYS:N	2.23	0.54
1:B:74:SER:O	1:B:76:GLY:N	2.38	0.54
1:F:294:ASP:HB2	2:F:457:HOH:O	2.07	0.54
1:B:288:GLN:O	1:B:292:GLU:OE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:LYS:HZ1	1:F:364:ASN:HD21	1.56	0.54
1:F:185:LYS:NZ	1:F:364:ASN:HD21	2.05	0.54
1:C:118:ILE:HG21	1:C:133:LEU:HD21	1.90	0.54
1:C:185:LYS:NZ	1:C:364:ASN:HD21	2.05	0.54
1:F:270:ARG:NH2	1:F:280:LEU:HD22	2.23	0.54
1:F:322:GLU:OE1	1:F:402:ARG:NH2	2.41	0.54
1:D:185:LYS:NZ	1:D:364:ASN:HD21	2.06	0.54
1:A:363:GLN:HE21	1:A:370:TRP:H	1.52	0.53
1:C:270:ARG:NH2	1:C:280:LEU:HD22	2.23	0.53
1:F:308:THR:OG1	1:F:310:GLU:HG2	2.08	0.53
1:B:75:VAL:HG21	1:B:413:MET:HA	1.90	0.53
1:D:363:GLN:HE21	1:D:370:TRP:H	1.52	0.53
1:E:226:GLN:HE22	1:E:306:GLN:HG3	1.73	0.53
1:E:377:GLU:HG3	1:E:378:LYS:N	2.23	0.53
1:E:75:VAL:HG21	1:E:413:MET:HA	1.90	0.53
1:F:208:LYS:O	1:F:212:LYS:HG3	2.09	0.53
1:C:185:LYS:HZ1	1:C:364:ASN:HD21	1.57	0.53
1:F:79:LYS:HD2	1:F:151:VAL:O	2.08	0.53
1:D:75:VAL:HG21	1:D:413:MET:HA	1.91	0.53
1:F:312:ALA:HA	1:F:315:ILE:CD1	2.38	0.53
1:C:308:THR:OG1	1:C:310:GLU:HG2	2.08	0.53
1:F:118:ILE:HG21	1:F:133:LEU:HD21	1.91	0.53
1:A:185:LYS:NZ	1:A:364:ASN:HD21	2.07	0.53
1:A:75:VAL:HG21	1:A:413:MET:HA	1.91	0.53
1:E:74:SER:O	1:E:76:GLY:N	2.38	0.53
1:C:145:VAL:HG13	1:C:181:PHE:CE1	2.44	0.53
1:B:226:GLN:HE22	1:B:306:GLN:HG3	1.74	0.53
1:E:185:LYS:NZ	1:E:364:ASN:HD21	2.07	0.53
1:A:179:PRO:HD2	2:A:477:HOH:O	2.08	0.53
1:E:18:LEU:O	1:E:18:LEU:HD12	2.10	0.52
1:C:258:ASP:HB2	1:C:262:LEU:HD23	1.90	0.52
1:F:258:ASP:HB2	1:F:262:LEU:HD23	1.90	0.52
1:B:18:LEU:HD12	1:B:18:LEU:O	2.10	0.52
1:B:185:LYS:NZ	1:B:364:ASN:HD21	2.07	0.52
1:D:79:LYS:HZ2	1:D:151:VAL:HG12	1.75	0.52
1:C:85:HIS:CD2	1:C:86:PRO:HD2	2.44	0.52
1:F:228:PHE:CE1	1:F:249:ILE:HD13	2.44	0.52
1:F:85:HIS:CD2	1:F:86:PRO:HD2	2.44	0.52
1:C:228:PHE:CE1	1:C:249:ILE:HD13	2.44	0.52
1:A:51:VAL:HG12	1:C:47:ARG:HG3	1.90	0.52
1:C:208:LYS:O	1:C:212:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:TYR:CZ	1:C:270:ARG:HD2	2.44	0.52
1:A:403:LEU:HG	1:A:407:MET:CE	2.37	0.52
1:C:312:ALA:HA	1:C:315:ILE:CD1	2.39	0.52
1:B:377:GLU:HG3	1:B:378:LYS:N	2.24	0.52
1:C:292:GLU:HG2	1:C:314:ASN:O	2.10	0.52
1:D:403:LEU:HG	1:D:407:MET:CE	2.37	0.52
1:F:74:SER:HB2	2:F:436:HOH:O	2.09	0.51
1:F:292:GLU:HG2	1:F:314:ASN:O	2.10	0.51
1:C:265:ASP:HA	1:C:268:LEU:HD11	1.91	0.51
1:F:145:VAL:HG13	1:F:181:PHE:CE1	2.45	0.51
1:F:118:ILE:HD11	1:F:137:TYR:CD1	2.46	0.51
1:B:79:LYS:HZ2	1:B:151:VAL:HG12	1.73	0.51
1:F:266:TYR:CZ	1:F:270:ARG:HD2	2.45	0.51
1:D:226:GLN:HE22	1:D:306:GLN:HG3	1.74	0.51
1:E:294:ASP:HB2	1:E:316:ARG:HH12	1.75	0.51
1:C:386:SER:O	1:C:390:ILE:HG13	2.11	0.51
1:B:174:ASP:O	1:B:175:GLU:HB2	2.11	0.51
1:D:174:ASP:O	1:D:175:GLU:HB2	2.11	0.51
1:A:226:GLN:HE22	1:A:306:GLN:HG3	1.74	0.51
1:E:403:LEU:HG	1:E:407:MET:CE	2.37	0.51
1:B:403:LEU:HG	1:B:407:MET:CE	2.37	0.51
1:F:386:SER:O	1:F:390:ILE:HG13	2.11	0.51
1:F:121:ASP:OD1	1:F:123:ARG:HB2	2.10	0.51
1:E:322:GLU:CD	1:E:402:ARG:HH22	2.14	0.51
1:D:157:PHE:N	2:D:485:HOH:O	2.39	0.50
1:A:308:THR:HG22	1:A:329:THR:HG23	1.94	0.50
1:F:265:ASP:HA	1:F:268:LEU:HD11	1.92	0.50
1:D:167:MET:CE	1:D:189:LEU:HD13	2.42	0.50
1:C:315:ILE:O	1:C:339:ARG:NH2	2.42	0.50
1:D:308:THR:HG22	1:D:329:THR:HG23	1.94	0.50
1:B:268:LEU:O	1:B:269:ASP:O	2.30	0.50
1:B:322:GLU:CD	1:B:402:ARG:HH22	2.15	0.50
1:E:50:THR:HB	1:E:68:TYR:CD1	2.47	0.50
1:B:50:THR:HB	1:B:68:TYR:CD1	2.47	0.50
1:F:123:ARG:HG2	1:F:274:PHE:CE2	2.47	0.50
1:A:167:MET:CE	1:A:189:LEU:HD13	2.42	0.50
1:C:103:LYS:HZ1	1:C:325:ASN:HD21	1.60	0.50
1:E:79:LYS:HZ2	1:E:151:VAL:HG12	1.74	0.50
1:D:322:GLU:CD	1:D:402:ARG:HH22	2.14	0.50
1:D:50:THR:HB	1:D:68:TYR:CD1	2.47	0.50
1:D:73:ASP:OD1	1:D:75:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:OD1	1:A:75:VAL:HG13	2.11	0.50
1:A:174:ASP:O	1:A:175:GLU:HB2	2.12	0.50
1:C:324:ALA:HB1	2:C:507:HOH:O	2.11	0.50
1:A:50:THR:HB	1:A:68:TYR:CD1	2.47	0.50
1:E:174:ASP:O	1:E:175:GLU:HB2	2.11	0.50
1:C:123:ARG:HG2	1:C:274:PHE:CE2	2.47	0.50
1:F:315:ILE:O	1:F:339:ARG:NH2	2.43	0.50
1:C:402:ARG:NH2	2:C:448:HOH:O	2.44	0.50
1:A:27:LYS:O	1:A:30:GLU:HB3	2.12	0.50
1:C:96:LEU:HD22	1:C:115:LYS:HE2	1.94	0.50
1:C:121:ASP:OD1	1:C:123:ARG:HB2	2.11	0.50
1:F:96:LEU:HD22	1:F:115:LYS:HE2	1.94	0.49
1:C:391:TYR:HA	1:C:401:MET:CE	2.42	0.49
1:C:118:ILE:HD11	1:C:137:TYR:CD1	2.47	0.49
1:F:17:VAL:N	2:F:508:HOH:O	2.44	0.49
1:F:84:PHE:CE1	1:F:118:ILE:HD12	2.47	0.49
1:D:27:LYS:O	1:D:30:GLU:HB3	2.12	0.49
1:B:27:LYS:O	1:B:30:GLU:HB3	2.12	0.49
1:E:27:LYS:O	1:E:30:GLU:HB3	2.12	0.49
1:B:265:ASP:O	1:B:266:TYR:O	2.30	0.49
1:A:322:GLU:CD	1:A:402:ARG:HH22	2.14	0.49
1:F:391:TYR:HA	1:F:401:MET:CE	2.43	0.49
1:B:257:TYR:CD1	1:B:293:LEU:HD13	2.47	0.49
1:B:257:TYR:CD1	1:B:293:LEU:HD22	2.48	0.49
1:F:402:ARG:CG	1:F:402:ARG:NH1	2.75	0.49
1:E:257:TYR:CE1	1:E:293:LEU:HD22	2.48	0.49
1:B:254:GLY:HA2	1:B:286:THR:HA	1.94	0.49
1:A:84:PHE:HB3	1:A:122:PRO:HG3	1.95	0.49
1:E:247:VAL:HG23	1:E:258:ASP:O	2.13	0.49
1:F:103:LYS:HZ1	1:F:325:ASN:HD21	1.61	0.49
1:E:266:TYR:CD2	1:E:266:TYR:O	2.66	0.49
1:C:84:PHE:CE1	1:C:118:ILE:HD12	2.48	0.49
1:F:100:MET:HE1	1:F:354:VAL:HG13	1.94	0.49
1:B:167:MET:CE	1:B:189:LEU:HD13	2.42	0.49
1:C:100:MET:HE1	1:C:354:VAL:HG13	1.94	0.49
1:D:204:THR:CG2	1:D:238:PHE:HD2	2.25	0.48
1:D:84:PHE:HB3	1:D:122:PRO:HG3	1.95	0.48
1:C:265:ASP:O	1:C:268:LEU:HD12	2.13	0.48
1:F:265:ASP:O	1:F:268:LEU:HD12	2.13	0.48
1:C:128:ARG:HA	2:C:445:HOH:O	2.14	0.48
1:D:48:LEU:O	1:F:49:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:THR:HG22	1:B:329:THR:HG23	1.95	0.48
1:E:308:THR:HG22	1:E:329:THR:HG23	1.95	0.48
1:E:257:TYR:HD1	1:E:293:LEU:HD13	1.78	0.48
1:B:73:ASP:OD1	1:B:75:VAL:HG13	2.12	0.48
2:D:466:HOH:O	1:F:64:ILE:HG21	2.13	0.48
1:C:177:ASN:C	1:C:179:PRO:HD3	2.34	0.48
1:C:79:LYS:HD2	1:C:151:VAL:HB	1.96	0.48
1:E:73:ASP:OD1	1:E:75:VAL:HG13	2.12	0.48
1:F:79:LYS:HD2	1:F:151:VAL:HB	1.96	0.48
1:E:180:GLY:HA2	1:E:364:ASN:HD22	1.78	0.48
1:A:79:LYS:HZ2	1:A:151:VAL:HG12	1.78	0.48
1:A:247:VAL:HG23	1:A:258:ASP:O	2.14	0.48
1:D:247:VAL:HG23	1:D:258:ASP:O	2.14	0.48
1:F:88:VAL:HG12	1:F:119:VAL:HG22	1.95	0.48
1:E:167:MET:CE	1:E:189:LEU:HD13	2.43	0.48
1:C:391:TYR:HA	1:C:401:MET:HE1	1.94	0.48
1:E:185:LYS:HZ1	1:E:364:ASN:HD21	1.61	0.48
1:C:331:GLU:O	1:C:335:ILE:HG13	2.14	0.48
1:B:247:VAL:HG23	1:B:258:ASP:O	2.14	0.48
1:A:106:ILE:HG23	1:A:390:ILE:HD11	1.95	0.48
1:C:315:ILE:HD11	1:C:336:LEU:HD21	1.95	0.48
1:A:180:GLY:HA2	1:A:364:ASN:HD22	1.78	0.48
1:D:106:ILE:HG23	1:D:390:ILE:HD11	1.95	0.48
1:E:106:ILE:HG23	1:E:390:ILE:HD11	1.95	0.48
1:A:378:LYS:HD2	1:F:368:PHE:CZ	2.48	0.48
1:B:106:ILE:HG23	1:B:390:ILE:HD11	1.95	0.48
1:B:84:PHE:HB3	1:B:122:PRO:HG3	1.95	0.48
1:F:315:ILE:HD11	1:F:336:LEU:HD21	1.95	0.47
1:F:25:ILE:HG22	1:F:29:LEU:HD22	1.96	0.47
1:C:25:ILE:HG22	1:C:29:LEU:HD22	1.96	0.47
1:C:217:ASP:OD1	1:C:219:LYS:HG2	2.14	0.47
1:B:159:ASN:O	1:B:163:MET:HG2	2.14	0.47
1:C:88:VAL:HG12	1:C:119:VAL:HG22	1.96	0.47
1:B:264:ILE:O	1:B:268:LEU:CA	2.61	0.47
1:E:257:TYR:CD1	1:E:293:LEU:HD22	2.49	0.47
1:E:84:PHE:HB3	1:E:122:PRO:HG3	1.95	0.47
1:A:204:THR:CG2	1:A:238:PHE:HD2	2.27	0.47
1:C:258:ASP:CB	1:C:262:LEU:HD23	2.43	0.47
1:F:217:ASP:OD1	1:F:219:LYS:HG2	2.14	0.47
1:F:393:MET:HE1	1:F:407:MET:HB2	1.96	0.47
1:D:159:ASN:O	1:D:163:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ARG:NH1	1:C:402:ARG:CG	2.75	0.47
1:F:208:LYS:HG2	1:F:218:ILE:HD13	1.97	0.47
1:F:258:ASP:CB	1:F:262:LEU:HD23	2.44	0.47
1:B:180:GLY:HA2	1:B:364:ASN:HD22	1.78	0.47
1:C:393:MET:HE1	1:C:407:MET:HB2	1.96	0.47
1:D:180:GLY:HA2	1:D:364:ASN:HD22	1.79	0.47
1:E:189:LEU:HD22	1:F:420:ARG:HD2	1.96	0.47
1:D:74:SER:HB3	1:D:422:TRP:HH2	1.80	0.47
1:F:307:ILE:HD12	1:F:328:THR:HG22	1.95	0.47
1:F:250:SER:HB3	1:F:290:LEU:HD13	1.96	0.47
1:B:380:GLU:O	1:B:384:VAL:HG23	2.15	0.47
1:A:139:ARG:NH1	1:B:172:ARG:HG2	2.29	0.47
1:C:201:LYS:HB2	2:C:474:HOH:O	2.15	0.47
1:F:177:ASN:C	1:F:179:PRO:HD3	2.34	0.47
1:A:159:ASN:O	1:A:163:MET:HG2	2.15	0.47
1:F:331:GLU:O	1:F:335:ILE:HG13	2.15	0.47
1:B:308:THR:HG22	1:B:329:THR:HG21	1.97	0.47
1:F:294:ASP:CB	2:F:457:HOH:O	2.63	0.47
1:C:145:VAL:CG1	1:C:181:PHE:CE1	2.98	0.47
1:C:307:ILE:HD12	1:C:328:THR:HG22	1.96	0.47
1:B:334:LYS:HE3	1:B:338:ASP:OD2	2.15	0.47
1:E:334:LYS:HE3	1:E:338:ASP:OD2	2.15	0.47
1:C:250:SER:HB3	1:C:290:LEU:HD13	1.96	0.47
1:E:74:SER:HB3	1:E:422:TRP:HH2	1.80	0.47
1:E:159:ASN:O	1:E:163:MET:HG2	2.15	0.47
1:F:343:LEU:O	1:F:401:MET:HG3	2.15	0.46
1:C:266:TYR:O	1:C:269:ASP:HB3	2.14	0.46
1:B:366:GLN:HG2	1:C:366:GLN:HE21	1.80	0.46
1:B:266:TYR:O	1:B:267:LEU:C	2.51	0.46
1:A:380:GLU:O	1:A:384:VAL:HG23	2.14	0.46
1:A:378:LYS:HD2	1:F:368:PHE:HZ	1.80	0.46
1:B:74:SER:HB3	1:B:422:TRP:HH2	1.80	0.46
1:E:89:THR:O	1:E:93:VAL:HG13	2.15	0.46
1:F:205:ILE:HD13	1:F:380:GLU:HA	1.97	0.46
1:F:78:THR:O	1:F:150:ASP:HA	2.15	0.46
1:E:269:ASP:C	1:E:270:ARG:HG2	2.36	0.46
1:F:96:LEU:HD23	1:F:99:TRP:HD1	1.80	0.46
1:D:334:LYS:HE3	1:D:338:ASP:OD2	2.15	0.46
1:E:308:THR:HG22	1:E:329:THR:HG21	1.98	0.46
1:A:228:PHE:N	1:A:250:SER:O	2.49	0.46
1:C:96:LEU:HB3	1:C:115:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:GLU:O	1:D:384:VAL:HG23	2.15	0.46
1:A:74:SER:HB3	1:A:422:TRP:HH2	1.81	0.46
1:C:205:ILE:HD13	1:C:380:GLU:HA	1.97	0.46
1:C:96:LEU:HD23	1:C:99:TRP:HD1	1.80	0.46
1:C:362:VAL:O	1:C:366:GLN:HG3	2.16	0.46
1:D:107:ILE:O	1:D:107:ILE:HG22	2.15	0.46
1:E:380:GLU:O	1:E:384:VAL:HG23	2.16	0.46
1:D:74:SER:O	1:D:76:GLY:N	2.39	0.46
1:A:334:LYS:HE3	1:A:338:ASP:OD2	2.15	0.46
1:D:89:THR:O	1:D:93:VAL:HG13	2.16	0.46
1:E:228:PHE:N	1:E:250:SER:O	2.49	0.46
1:F:96:LEU:HB3	1:F:115:LYS:HE2	1.98	0.46
1:E:291:LEU:HD23	1:E:298:LEU:HD11	1.97	0.46
1:D:228:PHE:N	1:D:250:SER:O	2.49	0.46
1:F:145:VAL:CG1	1:F:181:PHE:CE1	2.99	0.45
1:E:204:THR:HG23	1:E:239:MET:HE3	1.98	0.45
1:B:204:THR:HG23	1:B:239:MET:HE3	1.98	0.45
1:F:213:LYS:HE2	1:F:391:TYR:CD2	2.52	0.45
1:F:266:TYR:O	1:F:269:ASP:HB3	2.15	0.45
1:B:89:THR:O	1:B:93:VAL:HG13	2.16	0.45
1:F:391:TYR:HA	1:F:401:MET:HE1	1.97	0.45
1:E:368:PHE:HA	1:F:358:TYR:HH	1.81	0.45
1:D:308:THR:HG22	1:D:329:THR:HG21	1.97	0.45
1:E:265:ASP:HA	1:E:268:LEU:HD12	1.98	0.45
1:B:204:THR:CG2	1:B:238:PHE:HD2	2.27	0.45
1:C:213:LYS:HE2	1:C:391:TYR:CD2	2.52	0.45
1:C:29:LEU:HD23	1:C:39:TYR:CA	2.47	0.45
1:B:248:GLY:HA2	1:B:256:LEU:O	2.17	0.45
1:B:107:ILE:O	1:B:107:ILE:HG22	2.16	0.45
1:F:115:LYS:HE3	1:F:155:ASP:OD2	2.16	0.45
1:C:208:LYS:HG2	1:C:218:ILE:HD13	1.98	0.45
1:E:204:THR:CG2	1:E:238:PHE:HD2	2.26	0.45
1:E:246:VAL:CB	1:E:264:ILE:HD11	2.45	0.45
1:C:78:THR:O	1:C:150:ASP:HA	2.17	0.45
1:D:219:LYS:O	1:D:243:GLY:O	2.35	0.45
1:D:204:THR:HG23	1:D:239:MET:HE3	1.99	0.45
1:B:228:PHE:N	1:B:250:SER:O	2.49	0.45
1:A:74:SER:O	1:A:76:GLY:N	2.39	0.45
1:E:248:GLY:HA2	1:E:256:LEU:O	2.17	0.45
1:A:107:ILE:HG22	1:A:107:ILE:O	2.16	0.45
1:C:115:LYS:HE3	1:C:155:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:HG23	1:A:239:MET:HE3	1.99	0.45
1:F:29:LEU:HD23	1:F:39:TYR:CA	2.47	0.45
1:C:145:VAL:HG13	1:C:181:PHE:HE1	1.82	0.45
1:F:362:VAL:O	1:F:366:GLN:HG3	2.17	0.45
1:A:89:THR:O	1:A:93:VAL:HG13	2.17	0.45
1:B:269:ASP:O	1:B:270:ARG:O	2.34	0.45
1:D:143:GLN:HE21	1:F:149:LYS:HZ3	1.65	0.45
1:C:103:LYS:NZ	1:C:325:ASN:HD21	2.13	0.45
1:C:216:ILE:HD12	1:C:319:ILE:CD1	2.47	0.45
1:F:123:ARG:HG2	1:F:274:PHE:CD2	2.52	0.45
1:E:298:LEU:HB3	1:E:320:VAL:HG22	1.99	0.45
1:B:313:HIS:HA	1:B:339:ARG:HH11	1.82	0.45
1:E:227:GLY:O	1:E:232:GLY:HA3	2.16	0.45
1:C:123:ARG:HG2	1:C:274:PHE:CD2	2.52	0.45
1:B:397:ARG:NH1	2:B:455:HOH:O	2.49	0.45
1:F:216:ILE:HD12	1:F:319:ILE:CD1	2.47	0.45
1:F:103:LYS:NZ	1:F:325:ASN:HD21	2.14	0.44
1:C:248:GLY:HA3	1:C:293:LEU:HD12	1.99	0.44
1:B:227:GLY:O	1:B:232:GLY:HA3	2.17	0.44
1:D:227:GLY:O	1:D:232:GLY:HA3	2.17	0.44
1:C:224:VAL:HG21	1:C:293:LEU:HB2	2.00	0.44
1:E:107:ILE:HG22	1:E:107:ILE:O	2.17	0.44
1:F:224:VAL:HG21	1:F:293:LEU:HB2	2.00	0.44
1:C:343:LEU:O	1:C:401:MET:HG3	2.17	0.44
1:F:201:LYS:HG2	1:F:379:LEU:HD23	2.00	0.44
1:A:248:GLY:HA2	1:A:256:LEU:O	2.17	0.44
1:E:55:VAL:HB	1:E:65:PHE:HE2	1.83	0.44
1:B:55:VAL:HB	1:B:65:PHE:HE2	1.83	0.44
1:F:404:ALA:O	1:F:408:VAL:HG23	2.17	0.44
1:A:227:GLY:O	1:A:232:GLY:HA3	2.17	0.44
1:D:143:GLN:HE21	1:F:149:LYS:HZ2	1.65	0.44
1:E:246:VAL:CG1	1:E:264:ILE:HD11	2.48	0.44
1:B:298:LEU:HB3	1:B:320:VAL:HG22	1.99	0.44
1:D:248:GLY:HA2	1:D:256:LEU:O	2.17	0.44
1:A:308:THR:HG22	1:A:329:THR:HG21	1.97	0.44
1:E:322:GLU:OE2	1:E:402:ARG:NH2	2.51	0.44
1:D:298:LEU:O	1:D:300:PRO:HD3	2.18	0.44
1:F:79:LYS:HE3	1:F:357:SER:HB3	1.99	0.44
1:B:322:GLU:OE2	1:B:402:ARG:NH2	2.51	0.44
1:E:298:LEU:O	1:E:300:PRO:HD3	2.18	0.44
1:D:139:ARG:NH1	1:E:172:ARG:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:GLU:OE2	1:D:402:ARG:NH2	2.51	0.43
1:D:55:VAL:HB	1:D:65:PHE:HE2	1.82	0.43
1:D:313:HIS:HA	1:D:339:ARG:HH11	1.82	0.43
1:D:85:HIS:CD2	1:D:86:PRO:HD2	2.53	0.43
1:A:55:VAL:HB	1:A:65:PHE:HE2	1.82	0.43
1:F:315:ILE:CD1	1:F:336:LEU:HD21	2.48	0.43
1:C:201:LYS:HG2	1:C:379:LEU:HD23	2.01	0.43
1:F:145:VAL:HG13	1:F:181:PHE:HE1	1.83	0.43
1:D:344:VAL:HA	1:D:345:PRO:HD3	1.75	0.43
1:F:248:GLY:HA3	1:F:293:LEU:HD12	2.00	0.43
1:F:336:LEU:HD12	1:F:343:LEU:HD13	1.99	0.43
1:D:85:HIS:O	1:D:88:VAL:HG12	2.18	0.43
1:C:315:ILE:CD1	1:C:336:LEU:HD21	2.49	0.43
1:C:76:GLY:HA3	2:C:456:HOH:O	2.18	0.43
1:E:291:LEU:HD22	1:E:298:LEU:HD21	2.01	0.43
1:A:313:HIS:HA	1:A:339:ARG:HH11	1.82	0.43
1:A:298:LEU:HB3	1:A:320:VAL:HG22	1.99	0.43
1:A:298:LEU:O	1:A:300:PRO:HD3	2.18	0.43
1:B:266:TYR:O	1:B:269:ASP:N	2.52	0.43
1:F:45:PRO:CA	1:F:72:ASN:HA	2.44	0.43
1:B:363:GLN:HE21	1:B:369:TYR:HA	1.82	0.43
1:C:167:MET:HE2	1:C:167:MET:HB3	1.83	0.43
1:E:85:HIS:O	1:E:88:VAL:HG12	2.19	0.43
1:E:399:ILE:HA	2:E:471:HOH:O	2.17	0.43
1:A:219:LYS:O	1:A:243:GLY:O	2.37	0.43
1:F:91:LYS:NZ	1:F:91:LYS:HB2	2.33	0.43
1:A:363:GLN:HE21	1:A:369:TYR:HA	1.82	0.43
1:C:336:LEU:HD12	1:C:343:LEU:HD13	1.99	0.43
1:C:265:ASP:HB2	2:C:438:HOH:O	2.18	0.43
1:D:50:THR:HB	1:D:68:TYR:HD1	1.83	0.43
1:E:118:ILE:HG21	1:E:133:LEU:HD21	2.01	0.43
1:A:322:GLU:OE2	1:A:402:ARG:NH2	2.52	0.43
1:B:336:LEU:O	1:B:339:ARG:O	2.37	0.43
1:D:298:LEU:HB3	1:D:320:VAL:HG22	1.99	0.43
1:C:35:PRO:HB2	1:C:37:GLU:HG3	2.00	0.43
1:C:340:ASP:O	1:C:340:ASP:CG	2.57	0.43
1:B:118:ILE:HG21	1:B:133:LEU:HD21	2.01	0.43
1:C:212:LYS:HG3	2:C:504:HOH:O	2.18	0.43
1:E:363:GLN:HE21	1:E:369:TYR:HA	1.83	0.43
1:F:340:ASP:O	1:F:340:ASP:CG	2.57	0.43
1:D:363:GLN:HE21	1:D:369:TYR:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:HIS:O	1:B:88:VAL:HG12	2.19	0.43
1:C:404:ALA:O	1:C:408:VAL:HG23	2.19	0.43
1:B:303:ILE:HG13	1:B:306:GLN:NE2	2.34	0.43
1:B:298:LEU:O	1:B:300:PRO:HD3	2.19	0.43
1:B:214:ARG:HA	1:B:214:ARG:HD3	1.90	0.43
1:C:91:LYS:HB2	1:C:91:LYS:NZ	2.34	0.43
1:C:45:PRO:CA	1:C:72:ASN:HA	2.44	0.43
1:A:85:HIS:CD2	1:A:86:PRO:HD2	2.54	0.43
1:C:178:SER:N	1:C:179:PRO:HD3	2.33	0.43
1:A:344:VAL:HA	1:A:345:PRO:HD3	1.74	0.43
1:C:96:LEU:HA	1:C:99:TRP:HD1	1.83	0.42
1:F:96:LEU:HA	1:F:99:TRP:HD1	1.83	0.42
1:F:167:MET:HE3	1:F:168:ASP:HA	2.01	0.42
1:A:85:HIS:O	1:A:88:VAL:HG12	2.18	0.42
1:C:158:THR:HG22	1:C:162:ILE:CD1	2.47	0.42
1:E:303:ILE:HG13	1:E:306:GLN:NE2	2.34	0.42
1:E:85:HIS:CD2	1:E:86:PRO:HD2	2.54	0.42
1:C:145:VAL:CG1	1:C:181:PHE:HE1	2.32	0.42
1:A:303:ILE:HG13	1:A:306:GLN:NE2	2.34	0.42
1:A:50:THR:HB	1:A:68:TYR:HD1	1.84	0.42
1:D:295:CYS:O	1:D:317:ALA:HA	2.19	0.42
1:B:266:TYR:C	1:B:268:LEU:N	2.73	0.42
1:E:249:ILE:HD11	1:E:267:LEU:HD13	2.00	0.42
1:B:85:HIS:CD2	1:B:86:PRO:HD2	2.54	0.42
1:A:295:CYS:O	1:A:317:ALA:HA	2.19	0.42
1:D:303:ILE:HG13	1:D:306:GLN:NE2	2.35	0.42
1:A:74:SER:HB2	2:A:504:HOH:O	2.19	0.42
1:D:295:CYS:N	2:D:478:HOH:O	2.52	0.42
1:C:79:LYS:HE3	1:C:357:SER:HB3	2.00	0.42
1:A:223:VAL:HG23	1:A:244:ALA:HB1	2.01	0.42
1:F:178:SER:N	1:F:179:PRO:HD3	2.34	0.42
1:F:48:LEU:HD12	1:F:70:ALA:HB2	2.01	0.42
1:B:50:THR:HB	1:B:68:TYR:HD1	1.83	0.42
1:F:35:PRO:HB2	1:F:37:GLU:HG3	2.02	0.42
1:A:194:GLY:HA2	2:A:441:HOH:O	2.19	0.42
1:E:219:LYS:O	1:E:243:GLY:O	2.37	0.42
1:F:155:ASP:OD1	1:F:156:VAL:N	2.52	0.42
1:C:167:MET:HE3	1:C:168:ASP:HA	2.02	0.42
1:D:223:VAL:HG23	1:D:244:ALA:HB1	2.02	0.42
1:D:172:ARG:HG2	1:E:139:ARG:NH1	2.35	0.42
1:B:219:LYS:O	1:B:243:GLY:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:O	1:C:49:LEU:HD12	2.20	0.42
1:F:107:ILE:O	1:F:108:ASP:HB3	2.19	0.42
1:D:51:VAL:HA	1:F:46:MET:O	2.19	0.42
1:C:393:MET:HE1	1:C:404:ALA:O	2.20	0.42
1:C:76:GLY:CA	2:C:456:HOH:O	2.67	0.42
1:A:143:GLN:HE21	1:C:149:LYS:HZ2	1.68	0.42
1:F:219:LYS:HB3	1:F:219:LYS:HZ2	1.85	0.42
1:C:107:ILE:O	1:C:108:ASP:HB3	2.19	0.42
1:C:155:ASP:OD1	1:C:156:VAL:N	2.53	0.42
1:F:332:GLY:O	1:F:336:LEU:HG	2.19	0.42
1:C:332:GLY:O	1:C:336:LEU:HG	2.19	0.42
1:F:29:LEU:HD12	1:F:29:LEU:HA	1.73	0.42
1:F:393:MET:HE1	1:F:404:ALA:O	2.20	0.42
1:F:158:THR:HG22	1:F:162:ILE:CD1	2.48	0.42
1:C:268:LEU:HA	1:C:271:ARG:HB2	2.02	0.42
1:E:336:LEU:O	1:E:339:ARG:O	2.38	0.42
1:B:76:GLY:C	1:D:177:ASN:ND2	2.73	0.41
1:E:50:THR:HB	1:E:68:TYR:HD1	1.84	0.41
1:C:189:LEU:HD22	1:D:420:ARG:HD2	2.01	0.41
1:C:27:LYS:HD2	1:C:27:LYS:HA	1.85	0.41
1:A:156:VAL:HG12	1:A:157:PHE:N	2.36	0.41
1:C:213:LYS:HG2	1:C:391:TYR:CZ	2.54	0.41
1:E:366:GLN:HG2	1:F:366:GLN:HE21	1.85	0.41
1:C:48:LEU:HD12	1:C:70:ALA:HB2	2.02	0.41
1:F:370:TRP:HZ2	2:F:495:HOH:O	2.04	0.41
1:A:149:LYS:HG2	1:F:176:PHE:HB3	2.01	0.41
1:B:24:VAL:HG13	1:B:406:TYR:CD2	2.56	0.41
1:A:118:ILE:HG21	1:A:133:LEU:HD21	2.01	0.41
1:D:226:GLN:NE2	2:D:494:HOH:O	2.53	0.41
1:E:237:LYS:HE2	1:E:268:LEU:HD13	2.01	0.41
1:D:394:ALA:HB1	1:D:399:ILE:O	2.21	0.41
1:B:344:VAL:HA	1:B:345:PRO:HD3	1.74	0.41
1:A:24:VAL:HG13	1:A:406:TYR:CD2	2.55	0.41
1:B:266:TYR:HB3	1:B:267:LEU:H	1.53	0.41
1:C:315:ILE:HG12	1:C:315:ILE:H	1.57	0.41
1:E:344:VAL:HA	1:E:345:PRO:HD3	1.75	0.41
1:F:27:LYS:HA	1:F:27:LYS:HD2	1.86	0.41
1:E:214:ARG:HD3	1:E:214:ARG:HA	1.92	0.41
1:E:24:VAL:HG13	1:E:406:TYR:CD2	2.56	0.41
1:B:104:CYS:HB3	2:B:431:HOH:O	2.21	0.41
1:E:223:VAL:HG23	1:E:244:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLN:HE22	1:F:149:LYS:HD3	1.85	0.41
1:F:402:ARG:NH2	2:F:430:HOH:O	2.54	0.41
1:F:145:VAL:HG13	1:F:146:GLY:N	2.35	0.41
1:D:118:ILE:HG21	1:D:133:LEU:HD21	2.01	0.41
1:A:394:ALA:HB1	1:A:399:ILE:O	2.21	0.41
1:F:237:LYS:HE2	1:F:237:LYS:HB3	1.85	0.41
1:E:179:PRO:HD2	2:E:485:HOH:O	2.20	0.41
1:A:143:GLN:HE22	1:C:149:LYS:HD3	1.86	0.41
1:D:336:LEU:O	1:D:339:ARG:O	2.38	0.41
1:B:21:THR:O	1:B:25:ILE:HG12	2.20	0.41
1:E:21:THR:O	1:E:25:ILE:HG12	2.20	0.41
1:F:167:MET:HE2	1:F:167:MET:HB3	1.85	0.41
1:F:315:ILE:HG12	1:F:315:ILE:H	1.57	0.41
1:A:172:ARG:HG2	1:B:139:ARG:NH1	2.36	0.41
1:C:29:LEU:HD12	1:C:29:LEU:HA	1.73	0.41
1:F:145:VAL:CG1	1:F:181:PHE:HE1	2.33	0.41
1:F:326:GLY:N	1:F:327:PRO:HD3	2.36	0.41
1:A:21:THR:O	1:A:25:ILE:HG12	2.21	0.41
1:E:295:CYS:O	1:E:317:ALA:HA	2.20	0.41
1:B:83:ARG:HB2	1:B:156:VAL:HB	2.03	0.41
1:D:24:VAL:HG13	1:D:406:TYR:CD2	2.55	0.41
1:E:83:ARG:HB2	1:E:156:VAL:HB	2.02	0.41
1:B:295:CYS:O	1:B:317:ALA:HA	2.20	0.41
1:C:83:ARG:HB2	1:C:156:VAL:HB	2.02	0.40
1:F:213:LYS:HG2	1:F:391:TYR:CZ	2.55	0.40
1:F:213:LYS:HE2	1:F:391:TYR:CE2	2.56	0.40
1:B:247:VAL:HG22	1:B:247:VAL:O	2.21	0.40
1:A:336:LEU:O	1:A:339:ARG:O	2.39	0.40
1:C:387:PHE:CD2	1:C:387:PHE:C	2.95	0.40
1:D:21:THR:O	1:D:25:ILE:HG12	2.21	0.40
1:B:223:VAL:HG23	1:B:244:ALA:HB1	2.02	0.40
1:E:397:ARG:O	1:E:399:ILE:HG23	2.21	0.40
1:C:49:LEU:HD23	1:C:141:ILE:HG22	2.03	0.40
1:C:237:LYS:HE2	1:C:237:LYS:HB3	1.85	0.40
1:D:156:VAL:HG12	1:D:157:PHE:N	2.37	0.40
1:F:69:ARG:HD2	1:F:115:LYS:O	2.21	0.40
1:C:85:HIS:CD2	1:C:87:ASN:HB2	2.56	0.40
1:C:50:THR:HB	1:C:68:TYR:CD1	2.57	0.40
1:E:247:VAL:O	1:E:247:VAL:HG22	2.21	0.40
1:B:156:VAL:HG12	1:B:157:PHE:N	2.35	0.40
1:F:195:ARG:HA	1:F:195:ARG:HD2	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ASP:OD2	1:E:266:TYR:HB2	2.21	0.40
1:A:83:ARG:HB2	1:A:156:VAL:HB	2.03	0.40
1:F:85:HIS:CD2	1:F:87:ASN:HB2	2.56	0.40
1:F:25:ILE:HD11	1:F:98:ILE:CG2	2.51	0.40
1:C:219:LYS:HB3	1:C:219:LYS:HZ2	1.87	0.40
1:B:107:ILE:HA	1:B:386:SER:OG	2.22	0.40
1:C:326:GLY:N	1:C:327:PRO:HD3	2.36	0.40
1:C:213:LYS:HE2	1:C:391:TYR:CE2	2.56	0.40
1:A:79:LYS:NZ	1:A:183:THR:OG1	2.49	0.40
1:D:247:VAL:O	1:D:247:VAL:HG22	2.21	0.40
1:F:50:THR:HB	1:F:68:TYR:CD1	2.57	0.40
1:B:394:ALA:HB1	1:B:399:ILE:O	2.20	0.40
1:C:176:PHE:HB3	1:D:149:LYS:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	374/423 (88%)	353 (94%)	19 (5%)	2 (0%)	34	48
1	B	388/423 (92%)	365 (94%)	17 (4%)	6 (2%)	13	17
1	C	405/423 (96%)	376 (93%)	25 (6%)	4 (1%)	19	28
1	D	374/423 (88%)	353 (94%)	18 (5%)	3 (1%)	24	35
1	E	388/423 (92%)	366 (94%)	19 (5%)	3 (1%)	24	35
1	F	405/423 (96%)	376 (93%)	25 (6%)	4 (1%)	19	28
All	All	2334/2538 (92%)	2189 (94%)	123 (5%)	22 (1%)	21	30

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	VAL
1	B	156	VAL
1	B	266	TYR
1	B	267	LEU
1	B	269	ASP
1	D	156	VAL
1	E	156	VAL
1	A	75	VAL
1	B	75	VAL
1	C	75	VAL
1	C	273	SER
1	C	277	VAL
1	D	75	VAL
1	E	75	VAL
1	F	75	VAL
1	F	273	SER
1	F	277	VAL
1	C	108	ASP
1	F	108	ASP
1	B	246	VAL
1	E	246	VAL
1	D	246	VAL

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	312/353 (88%)	300 (96%)	12 (4%)	40	60
1	B	326/353 (92%)	313 (96%)	13 (4%)	38	58
1	C	340/353 (96%)	315 (93%)	25 (7%)	17	26
1	D	312/353 (88%)	298 (96%)	14 (4%)	34	52
1	E	326/353 (92%)	313 (96%)	13 (4%)	38	58
1	F	340/353 (96%)	316 (93%)	24 (7%)	18	28
All	All	1956/2118 (92%)	1855 (95%)	101 (5%)	29	45

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	50	THR
1	A	222	ARG
1	A	237	LYS
1	A	238	PHE
1	A	328	THR
1	A	339	ARG
1	A	372	GLU
1	A	377	GLU
1	A	399	ILE
1	A	410	VAL
1	A	418	ARG
1	B	50	THR
1	B	222	ARG
1	B	237	LYS
1	B	238	PHE
1	B	268	LEU
1	B	270	ARG
1	B	328	THR
1	B	339	ARG
1	B	372	GLU
1	B	377	GLU
1	B	399	ILE
1	B	410	VAL
1	B	418	ARG
1	C	17	VAL
1	C	29	LEU
1	C	37	GLU
1	C	48	LEU
1	C	50	THR
1	C	74	SER
1	C	88	VAL
1	C	130	LEU
1	C	145	VAL
1	C	167	MET
1	C	201	LYS
1	C	268	LEU
1	C	282	ASN
1	C	290	LEU
1	C	304	GLU
1	C	309	GLU
1	C	310	GLU

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Mol	Chain	Res	Type
1	C	315	ILE
1	C	320	VAL
1	C	328	THR
1	C	339	ARG
1	C	343	LEU
1	C	354	VAL
1	C	378	LYS
1	C	402	ARG
1	D	18	LEU
1	D	32	LEU
1	D	50	THR
1	D	102	LEU
1	D	222	ARG
1	D	237	LYS
1	D	238	PHE
1	D	328	THR
1	D	339	ARG
1	D	372	GLU
1	D	377	GLU
1	D	399	ILE
1	D	410	VAL
1	D	418	ARG
1	E	32	LEU
1	E	50	THR
1	E	222	ARG
1	E	237	LYS
1	E	238	PHE
1	E	270	ARG
1	E	328	THR
1	E	339	ARG
1	E	372	GLU
1	E	377	GLU
1	E	399	ILE
1	E	410	VAL
1	E	418	ARG
1	F	17	VAL
1	F	29	LEU
1	F	37	GLU
1	F	48	LEU
1	F	50	THR
1	F	74	SER
1	F	88	VAL

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Mol	Chain	Res	Type
1	F	130	LEU
1	F	145	VAL
1	F	167	MET
1	F	201	LYS
1	F	268	LEU
1	F	282	ASN
1	F	290	LEU
1	F	304	GLU
1	F	309	GLU
1	F	310	GLU
1	F	315	ILE
1	F	320	VAL
1	F	339	ARG
1	F	343	LEU
1	F	354	VAL
1	F	378	LYS
1	F	402	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	143	GLN
1	A	193	HIS
1	A	226	GLN
1	A	305	ASN
1	A	363	GLN
1	A	364	ASN
1	B	72	ASN
1	B	85	HIS
1	B	143	GLN
1	B	193	HIS
1	B	226	GLN
1	B	305	ASN
1	B	363	GLN
1	B	364	ASN
1	C	85	HIS
1	C	87	ASN
1	C	161	GLN
1	C	226	GLN
1	C	325	ASN
1	C	363	GLN

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Mol	Chain	Res	Type
1	C	364	ASN
1	C	366	GLN
1	D	85	HIS
1	D	143	GLN
1	D	193	HIS
1	D	226	GLN
1	D	305	ASN
1	D	363	GLN
1	D	364	ASN
1	E	85	HIS
1	E	143	GLN
1	E	193	HIS
1	E	226	GLN
1	E	287	ASN
1	E	305	ASN
1	E	363	GLN
1	E	364	ASN
1	F	85	HIS
1	F	87	ASN
1	F	161	GLN
1	F	226	GLN
1	F	325	ASN
1	F	363	GLN
1	F	364	ASN
1	F	366	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	378/423 (89%)	0.35	32 (8%)	13 13	26, 43, 77, 92	0
1	B	392/423 (92%)	0.28	18 (4%)	36 37	27, 43, 77, 92	0
1	C	407/423 (96%)	-0.13	3 (0%)	89 88	24, 39, 59, 74	0
1	D	378/423 (89%)	0.39	27 (7%)	19 19	27, 43, 77, 93	0
1	E	392/423 (92%)	0.18	14 (3%)	46 47	26, 43, 77, 92	0
1	F	407/423 (96%)	-0.04	1 (0%)	95 95	23, 39, 59, 74	0
All	All	2354/2538 (92%)	0.17	95 (4%)	42 43	23, 42, 75, 93	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	253	TYR	8.9
1	D	257	TYR	5.8
1	A	253	TYR	5.7
1	A	264	ILE	5.2
1	B	254	GLY	5.2
1	A	256	LEU	4.8
1	A	332	GLY	4.7
1	A	263	ASP	4.6
1	D	338	ASP	4.5
1	A	338	ASP	4.3
1	A	231	ALA	4.3
1	D	256	LEU	4.3
1	D	228	PHE	4.3
1	E	260	GLU	4.2
1	D	249	ILE	4.1
1	E	229	GLY	4.1
1	A	235	LEU	4.0
1	A	257	TYR	4.0
1	D	332	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	334	LYS	3.7
1	D	398	ARG	3.7
1	B	338	ASP	3.7
1	D	263	ASP	3.6
1	B	315	ILE	3.6
1	A	219	LYS	3.5
1	B	219	LYS	3.5
1	A	242	ALA	3.4
1	D	330	LEU	3.3
1	B	229	GLY	3.2
1	A	228	PHE	3.2
1	A	238	PHE	3.1
1	B	260	GLU	3.1
1	D	316	ARG	3.1
1	B	307	ILE	3.1
1	A	340	ASP	3.0
1	B	330	LEU	3.0
1	E	228	PHE	3.0
1	A	265	ASP	3.0
1	D	75	VAL	3.0
1	D	260	GLU	2.9
1	D	255	GLY	2.9
1	A	313	HIS	2.8
1	E	234	TYR	2.8
1	C	218	ILE	2.8
1	A	398	ARG	2.8
1	A	336	LEU	2.7
1	C	75	VAL	2.7
1	A	311	ASN	2.7
1	B	237	LYS	2.6
1	E	294	ASP	2.6
1	A	239	MET	2.6
1	D	311	ASN	2.6
1	B	238	PHE	2.6
1	B	243	GLY	2.6
1	D	227	GLY	2.6
1	A	314	ASN	2.6
1	A	75	VAL	2.6
1	E	254	GLY	2.6
1	D	127	PHE	2.6
1	A	321	VAL	2.5
1	D	76	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	303	ILE	2.5
1	B	312	ALA	2.5
1	B	337	SER	2.5
1	D	331	GLU	2.5
1	C	280	LEU	2.4
1	A	301	ALA	2.4
1	B	217	ASP	2.4
1	D	313	HIS	2.4
1	D	308	THR	2.4
1	E	253	TYR	2.4
1	D	254	GLY	2.3
1	E	237	LYS	2.3
1	E	219	LYS	2.3
1	A	237	LYS	2.3
1	E	222	ARG	2.3
1	D	262	LEU	2.3
1	D	336	LEU	2.3
1	D	325	ASN	2.3
1	A	215	GLY	2.3
1	A	217	ASP	2.3
1	B	343	LEU	2.2
1	A	335	ILE	2.2
1	B	328	THR	2.2
1	A	221	ALA	2.2
1	A	249	ILE	2.2
1	E	267	LEU	2.1
1	E	238	PHE	2.1
1	F	75	VAL	2.1
1	D	244	ALA	2.1
1	E	302	ALA	2.1
1	B	247	VAL	2.0
1	E	75	VAL	2.0
1	A	306	GLN	2.0
1	D	258	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.