Full wwPDB X-ray Structure Validation Report ⓘ

Jul 24, 2024 – 04:19 pm BST

PDB ID	:	8QWB
Title	:	Crystal structure of citrate synthase from Methylophaga sulfidovorans
Authors	:	Mais, C.-N.; Bange, G.; Sendker, F.L.; Hochberg, G.
Deposited on	:	2023-10-19
Resolution	:	3.20 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 ⓘ 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 ⓘ) were used in the production of this report:

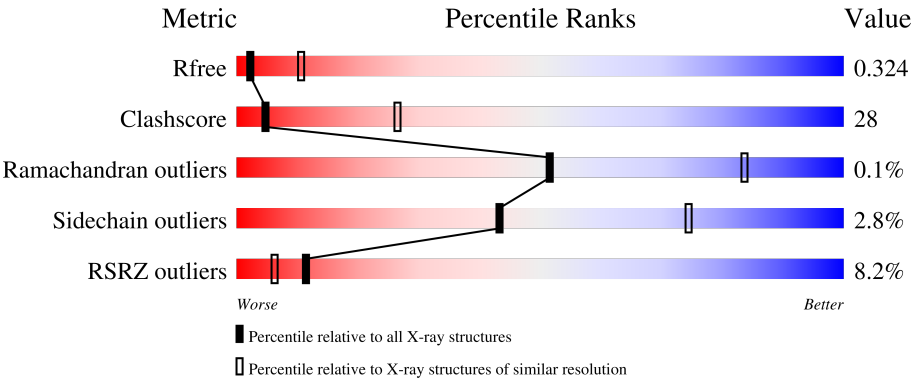
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	397	4% 43% 37% · 18%
1	B	397	8% 43% 38% · 18%
1	C	397	7% 46% 32% · 22%
1	D	397	5% 48% 32% · 18%
1	E	397	5% 43% 36% · 19%

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Mol	Chain	Length	Quality of chain
1	F	397	5% 43% 36% 20%
1	G	397	9% 38% 39% 21%
1	H	397	8% 40% 38% 21%
1	I	397	6% 41% 35% 22%
1	J	397	4% 42% 37% 18%
1	K	397	9% 41% 36% 22%
1	L	397	9% 37% 40% 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 30057 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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2555	1628	434	475	18			
1	B	327	Total	C	N	O	S	0	0	0
			2580	1642	437	482	19			
1	C	311	Total	C	N	O	S	0	0	0
			2441	1552	409	463	17			
1	D	324	Total	C	N	O	S	0	0	0
			2552	1623	434	477	18			
1	E	321	Total	C	N	O	S	0	0	0
			2533	1611	431	473	18			
1	F	318	Total	C	N	O	S	0	0	0
			2509	1597	427	468	17			
1	G	313	Total	C	N	O	S	0	0	0
			2457	1564	414	462	17			
1	H	315	Total	C	N	O	S	0	0	0
			2484	1581	421	465	17			
1	I	311	Total	C	N	O	S	0	0	0
			2446	1555	416	458	17			
1	J	326	Total	C	N	O	S	0	0	0
			2563	1632	433	480	18			
1	K	309	Total	C	N	O	S	0	0	0
			2433	1552	409	456	16			
1	L	317	Total	C	N	O	S	0	0	0
			2504	1594	423	469	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	expression tag	UNP A0A1I4B681
A	387	VAL	-	expression tag	UNP A0A1I4B681
A	388	PRO	-	expression tag	UNP A0A1I4B681
A	389	ARG	-	expression tag	UNP A0A1I4B681
A	390	LEU	-	expression tag	UNP A0A1I4B681

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Chain	Residue	Modelled	Actual	Comment	Reference
A	391	GLU	-	expression tag	UNP A0A1I4B681
A	392	HIS	-	expression tag	UNP A0A1I4B681
A	393	HIS	-	expression tag	UNP A0A1I4B681
A	394	HIS	-	expression tag	UNP A0A1I4B681
A	395	HIS	-	expression tag	UNP A0A1I4B681
A	396	HIS	-	expression tag	UNP A0A1I4B681
A	397	HIS	-	expression tag	UNP A0A1I4B681
B	386	LEU	-	expression tag	UNP A0A1I4B681
B	387	VAL	-	expression tag	UNP A0A1I4B681
B	388	PRO	-	expression tag	UNP A0A1I4B681
B	389	ARG	-	expression tag	UNP A0A1I4B681
B	390	LEU	-	expression tag	UNP A0A1I4B681
B	391	GLU	-	expression tag	UNP A0A1I4B681
B	392	HIS	-	expression tag	UNP A0A1I4B681
B	393	HIS	-	expression tag	UNP A0A1I4B681
B	394	HIS	-	expression tag	UNP A0A1I4B681
B	395	HIS	-	expression tag	UNP A0A1I4B681
B	396	HIS	-	expression tag	UNP A0A1I4B681
B	397	HIS	-	expression tag	UNP A0A1I4B681
C	386	LEU	-	expression tag	UNP A0A1I4B681
C	387	VAL	-	expression tag	UNP A0A1I4B681
C	388	PRO	-	expression tag	UNP A0A1I4B681
C	389	ARG	-	expression tag	UNP A0A1I4B681
C	390	LEU	-	expression tag	UNP A0A1I4B681
C	391	GLU	-	expression tag	UNP A0A1I4B681
C	392	HIS	-	expression tag	UNP A0A1I4B681
C	393	HIS	-	expression tag	UNP A0A1I4B681
C	394	HIS	-	expression tag	UNP A0A1I4B681
C	395	HIS	-	expression tag	UNP A0A1I4B681
C	396	HIS	-	expression tag	UNP A0A1I4B681
C	397	HIS	-	expression tag	UNP A0A1I4B681
D	386	LEU	-	expression tag	UNP A0A1I4B681
D	387	VAL	-	expression tag	UNP A0A1I4B681
D	388	PRO	-	expression tag	UNP A0A1I4B681
D	389	ARG	-	expression tag	UNP A0A1I4B681
D	390	LEU	-	expression tag	UNP A0A1I4B681
D	391	GLU	-	expression tag	UNP A0A1I4B681
D	392	HIS	-	expression tag	UNP A0A1I4B681
D	393	HIS	-	expression tag	UNP A0A1I4B681
D	394	HIS	-	expression tag	UNP A0A1I4B681
D	395	HIS	-	expression tag	UNP A0A1I4B681
D	396	HIS	-	expression tag	UNP A0A1I4B681

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Chain	Residue	Modelled	Actual	Comment	Reference
D	397	HIS	-	expression tag	UNP A0A1I4B681
E	386	LEU	-	expression tag	UNP A0A1I4B681
E	387	VAL	-	expression tag	UNP A0A1I4B681
E	388	PRO	-	expression tag	UNP A0A1I4B681
E	389	ARG	-	expression tag	UNP A0A1I4B681
E	390	LEU	-	expression tag	UNP A0A1I4B681
E	391	GLU	-	expression tag	UNP A0A1I4B681
E	392	HIS	-	expression tag	UNP A0A1I4B681
E	393	HIS	-	expression tag	UNP A0A1I4B681
E	394	HIS	-	expression tag	UNP A0A1I4B681
E	395	HIS	-	expression tag	UNP A0A1I4B681
E	396	HIS	-	expression tag	UNP A0A1I4B681
E	397	HIS	-	expression tag	UNP A0A1I4B681
F	386	LEU	-	expression tag	UNP A0A1I4B681
F	387	VAL	-	expression tag	UNP A0A1I4B681
F	388	PRO	-	expression tag	UNP A0A1I4B681
F	389	ARG	-	expression tag	UNP A0A1I4B681
F	390	LEU	-	expression tag	UNP A0A1I4B681
F	391	GLU	-	expression tag	UNP A0A1I4B681
F	392	HIS	-	expression tag	UNP A0A1I4B681
F	393	HIS	-	expression tag	UNP A0A1I4B681
F	394	HIS	-	expression tag	UNP A0A1I4B681
F	395	HIS	-	expression tag	UNP A0A1I4B681
F	396	HIS	-	expression tag	UNP A0A1I4B681
F	397	HIS	-	expression tag	UNP A0A1I4B681
G	386	LEU	-	expression tag	UNP A0A1I4B681
G	387	VAL	-	expression tag	UNP A0A1I4B681
G	388	PRO	-	expression tag	UNP A0A1I4B681
G	389	ARG	-	expression tag	UNP A0A1I4B681
G	390	LEU	-	expression tag	UNP A0A1I4B681
G	391	GLU	-	expression tag	UNP A0A1I4B681
G	392	HIS	-	expression tag	UNP A0A1I4B681
G	393	HIS	-	expression tag	UNP A0A1I4B681
G	394	HIS	-	expression tag	UNP A0A1I4B681
G	395	HIS	-	expression tag	UNP A0A1I4B681
G	396	HIS	-	expression tag	UNP A0A1I4B681
G	397	HIS	-	expression tag	UNP A0A1I4B681
H	386	LEU	-	expression tag	UNP A0A1I4B681
H	387	VAL	-	expression tag	UNP A0A1I4B681
H	388	PRO	-	expression tag	UNP A0A1I4B681
H	389	ARG	-	expression tag	UNP A0A1I4B681
H	390	LEU	-	expression tag	UNP A0A1I4B681

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Chain	Residue	Modelled	Actual	Comment	Reference
H	391	GLU	-	expression tag	UNP A0A1I4B681
H	392	HIS	-	expression tag	UNP A0A1I4B681
H	393	HIS	-	expression tag	UNP A0A1I4B681
H	394	HIS	-	expression tag	UNP A0A1I4B681
H	395	HIS	-	expression tag	UNP A0A1I4B681
H	396	HIS	-	expression tag	UNP A0A1I4B681
H	397	HIS	-	expression tag	UNP A0A1I4B681
I	386	LEU	-	expression tag	UNP A0A1I4B681
I	387	VAL	-	expression tag	UNP A0A1I4B681
I	388	PRO	-	expression tag	UNP A0A1I4B681
I	389	ARG	-	expression tag	UNP A0A1I4B681
I	390	LEU	-	expression tag	UNP A0A1I4B681
I	391	GLU	-	expression tag	UNP A0A1I4B681
I	392	HIS	-	expression tag	UNP A0A1I4B681
I	393	HIS	-	expression tag	UNP A0A1I4B681
I	394	HIS	-	expression tag	UNP A0A1I4B681
I	395	HIS	-	expression tag	UNP A0A1I4B681
I	396	HIS	-	expression tag	UNP A0A1I4B681
I	397	HIS	-	expression tag	UNP A0A1I4B681
J	386	LEU	-	expression tag	UNP A0A1I4B681
J	387	VAL	-	expression tag	UNP A0A1I4B681
J	388	PRO	-	expression tag	UNP A0A1I4B681
J	389	ARG	-	expression tag	UNP A0A1I4B681
J	390	LEU	-	expression tag	UNP A0A1I4B681
J	391	GLU	-	expression tag	UNP A0A1I4B681
J	392	HIS	-	expression tag	UNP A0A1I4B681
J	393	HIS	-	expression tag	UNP A0A1I4B681
J	394	HIS	-	expression tag	UNP A0A1I4B681
J	395	HIS	-	expression tag	UNP A0A1I4B681
J	396	HIS	-	expression tag	UNP A0A1I4B681
J	397	HIS	-	expression tag	UNP A0A1I4B681
K	386	LEU	-	expression tag	UNP A0A1I4B681
K	387	VAL	-	expression tag	UNP A0A1I4B681
K	388	PRO	-	expression tag	UNP A0A1I4B681
K	389	ARG	-	expression tag	UNP A0A1I4B681
K	390	LEU	-	expression tag	UNP A0A1I4B681
K	391	GLU	-	expression tag	UNP A0A1I4B681
K	392	HIS	-	expression tag	UNP A0A1I4B681
K	393	HIS	-	expression tag	UNP A0A1I4B681
K	394	HIS	-	expression tag	UNP A0A1I4B681
K	395	HIS	-	expression tag	UNP A0A1I4B681
K	396	HIS	-	expression tag	UNP A0A1I4B681

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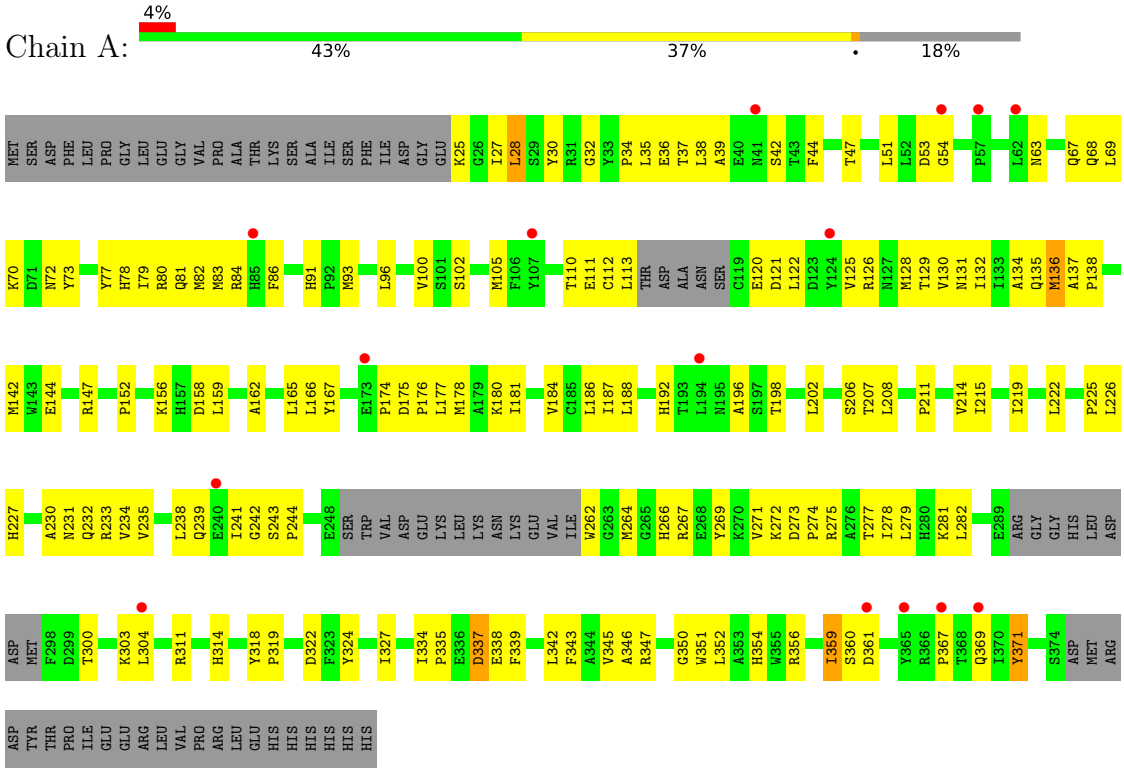
Chain	Residue	Modelled	Actual	Comment	Reference
K	397	HIS	-	expression tag	UNP A0A1I4B681
L	386	LEU	-	expression tag	UNP A0A1I4B681
L	387	VAL	-	expression tag	UNP A0A1I4B681
L	388	PRO	-	expression tag	UNP A0A1I4B681
L	389	ARG	-	expression tag	UNP A0A1I4B681
L	390	LEU	-	expression tag	UNP A0A1I4B681
L	391	GLU	-	expression tag	UNP A0A1I4B681
L	392	HIS	-	expression tag	UNP A0A1I4B681
L	393	HIS	-	expression tag	UNP A0A1I4B681
L	394	HIS	-	expression tag	UNP A0A1I4B681
L	395	HIS	-	expression tag	UNP A0A1I4B681
L	396	HIS	-	expression tag	UNP A0A1I4B681
L	397	HIS	-	expression tag	UNP A0A1I4B681

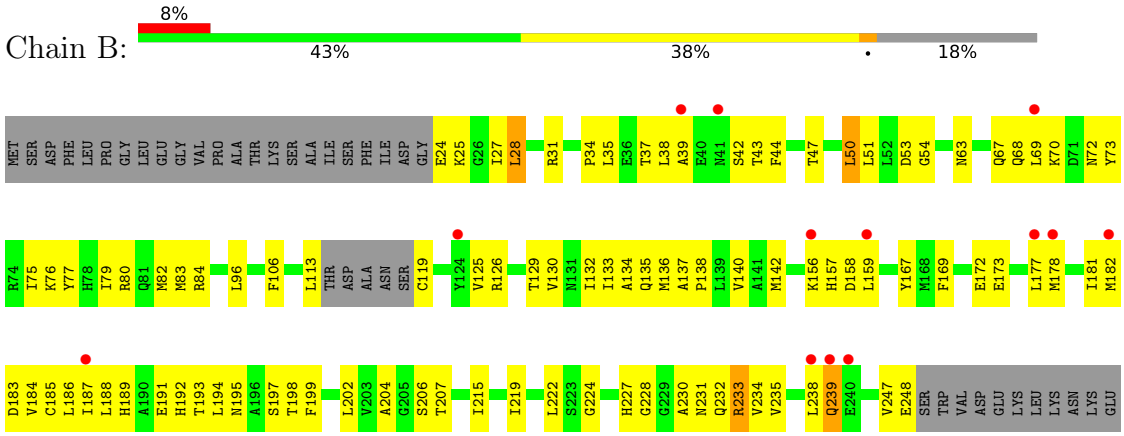
3 Residue-property plots (i)

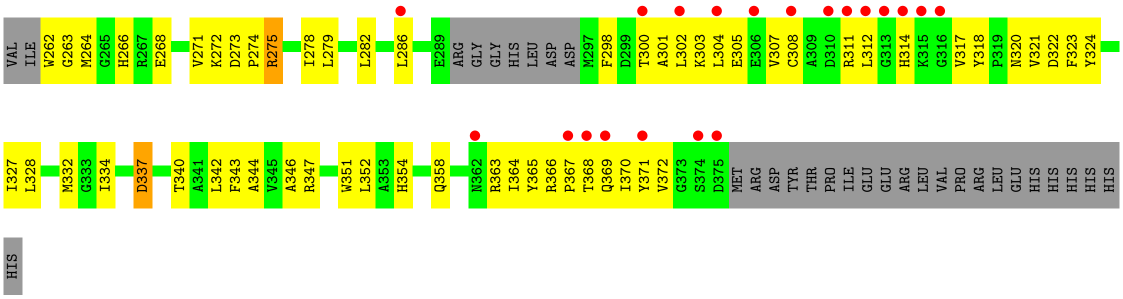
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Citrate synthase



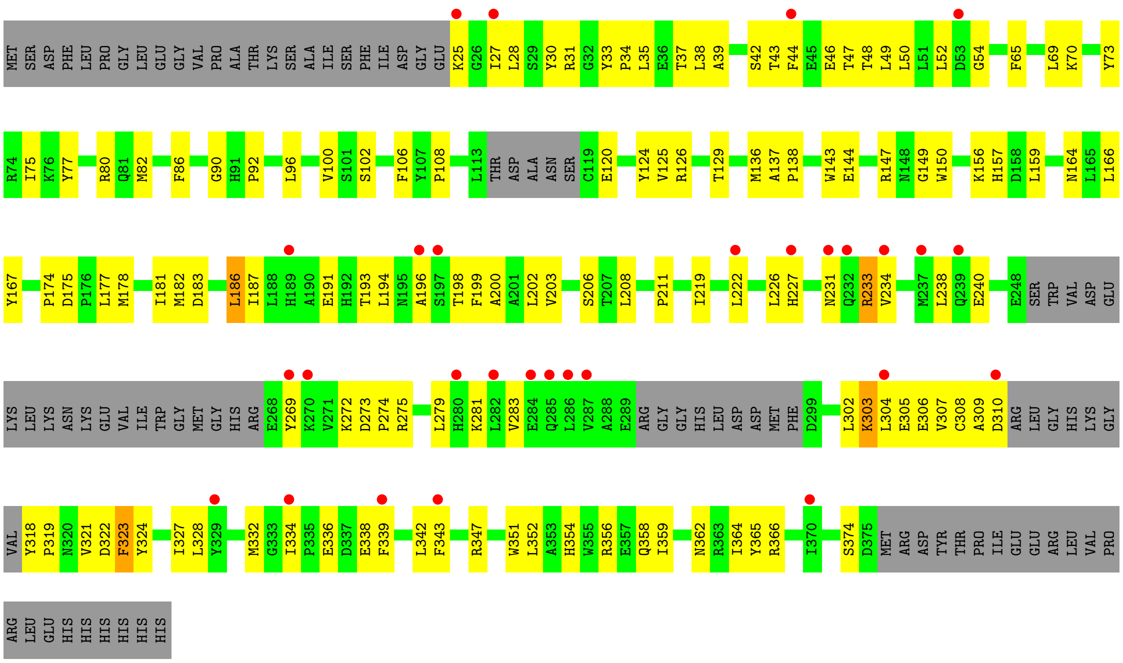
• Molecule 1: Citrate synthase





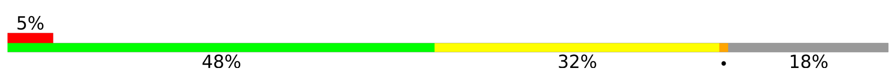
• Molecule 1: Citrate synthase

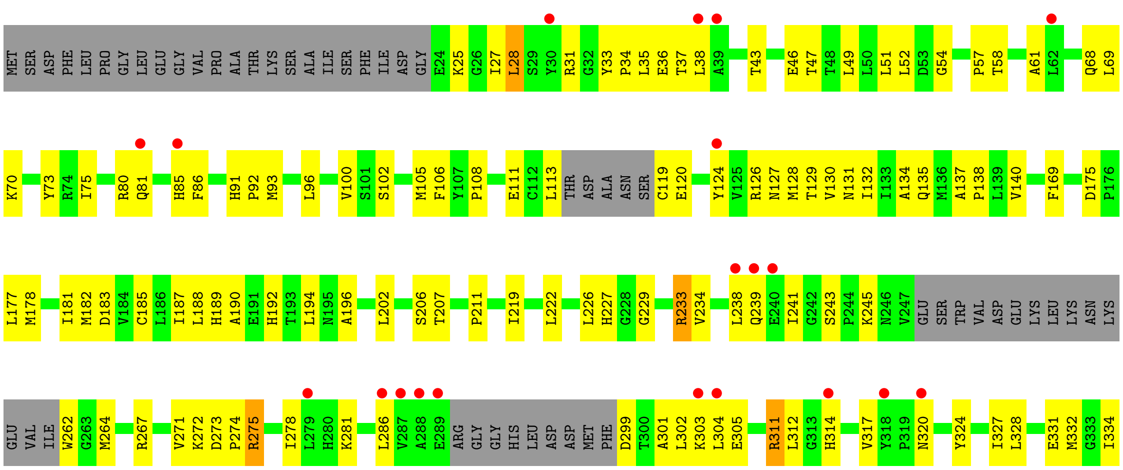
Chain C:

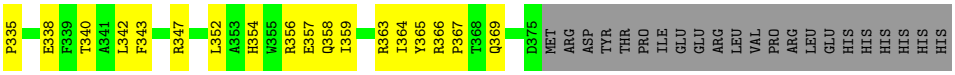


• Molecule 1: Citrate synthase

Chain D:

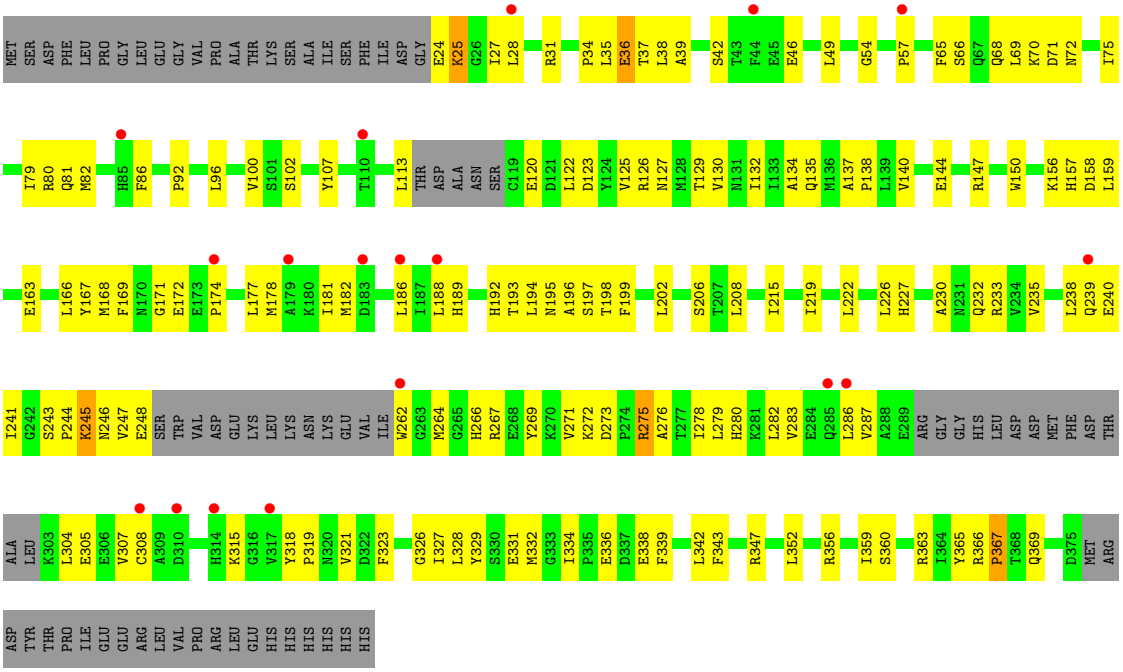






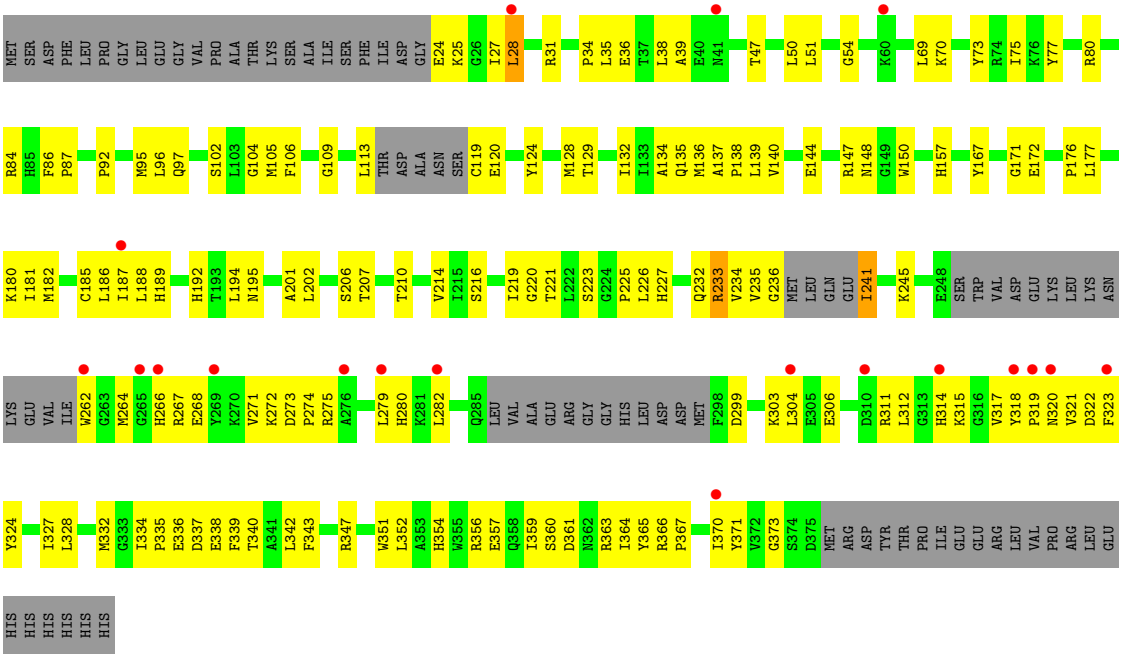
• Molecule 1: Citrate synthase

Chain E:



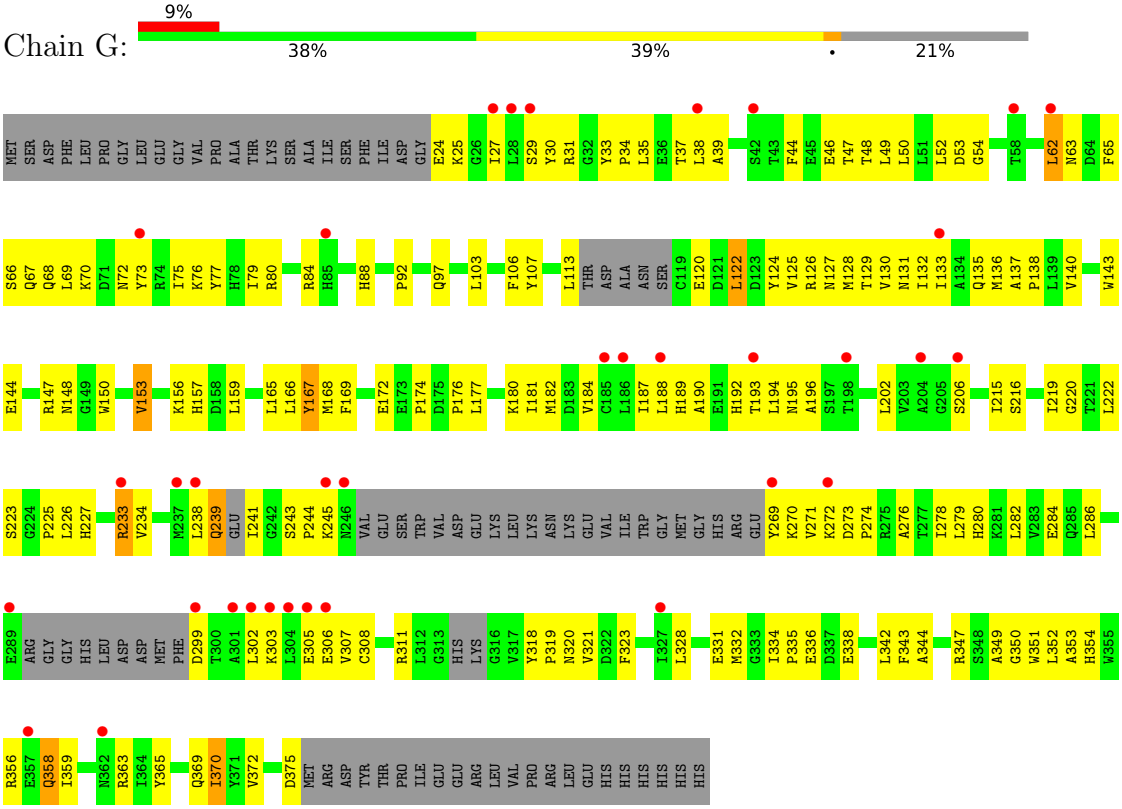
• Molecule 1: Citrate synthase

Chain F:



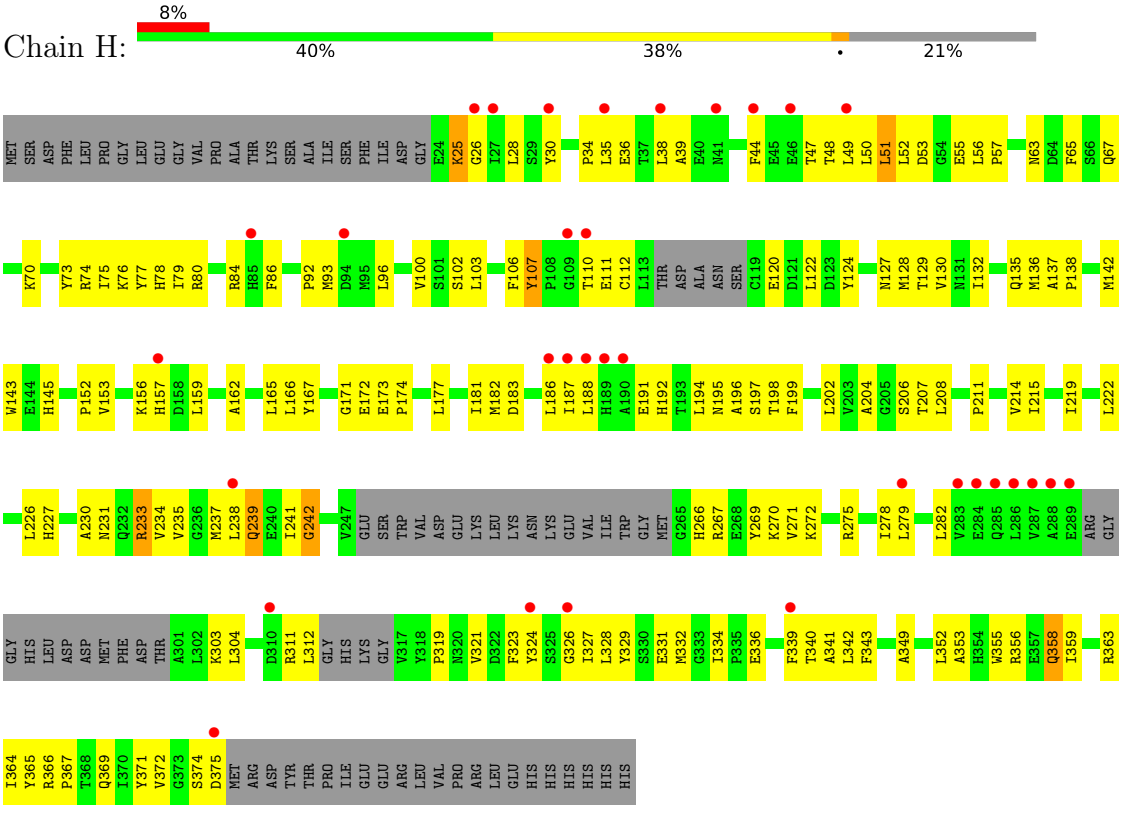
• Molecule 1: Citrate synthase

Chain G:



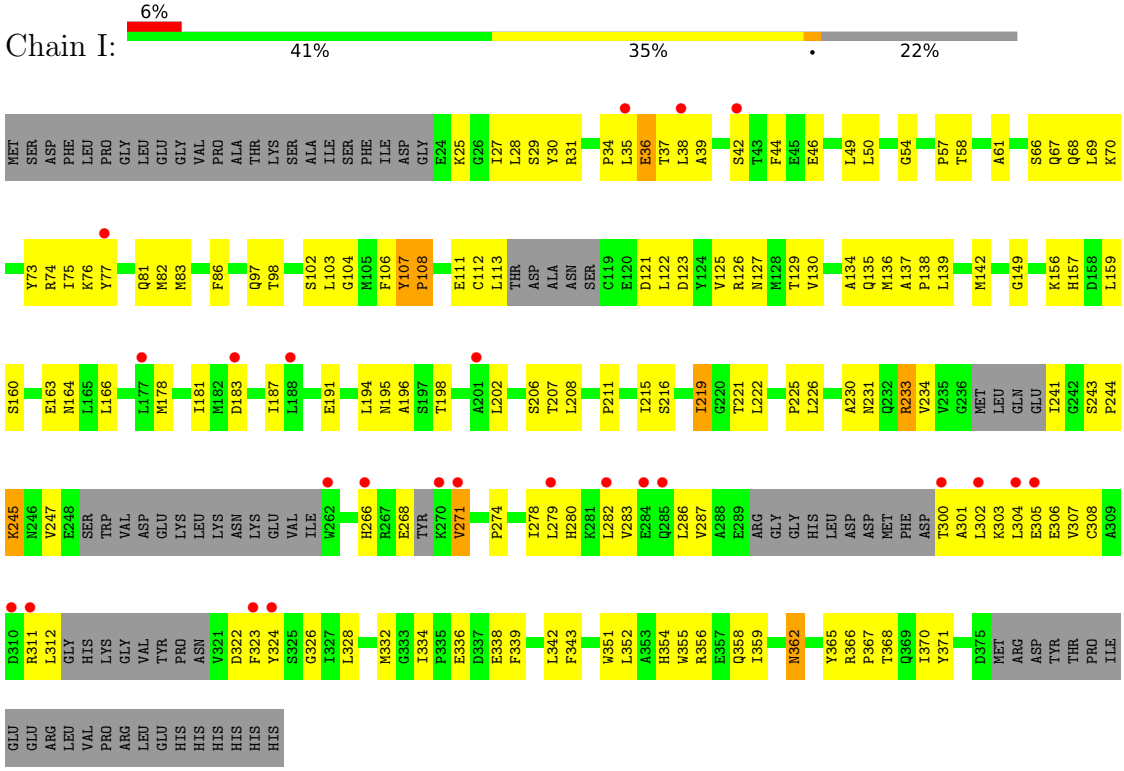
• Molecule 1: Citrate synthase

Chain H:



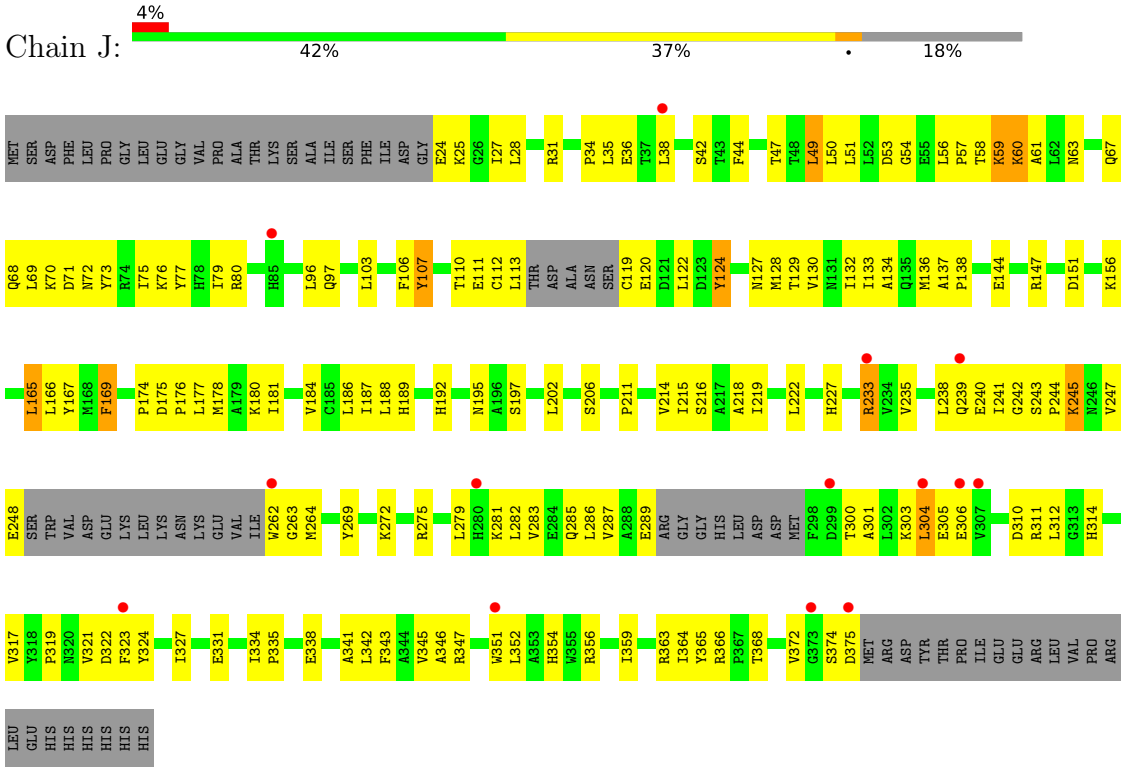
• Molecule 1: Citrate synthase

Chain I:

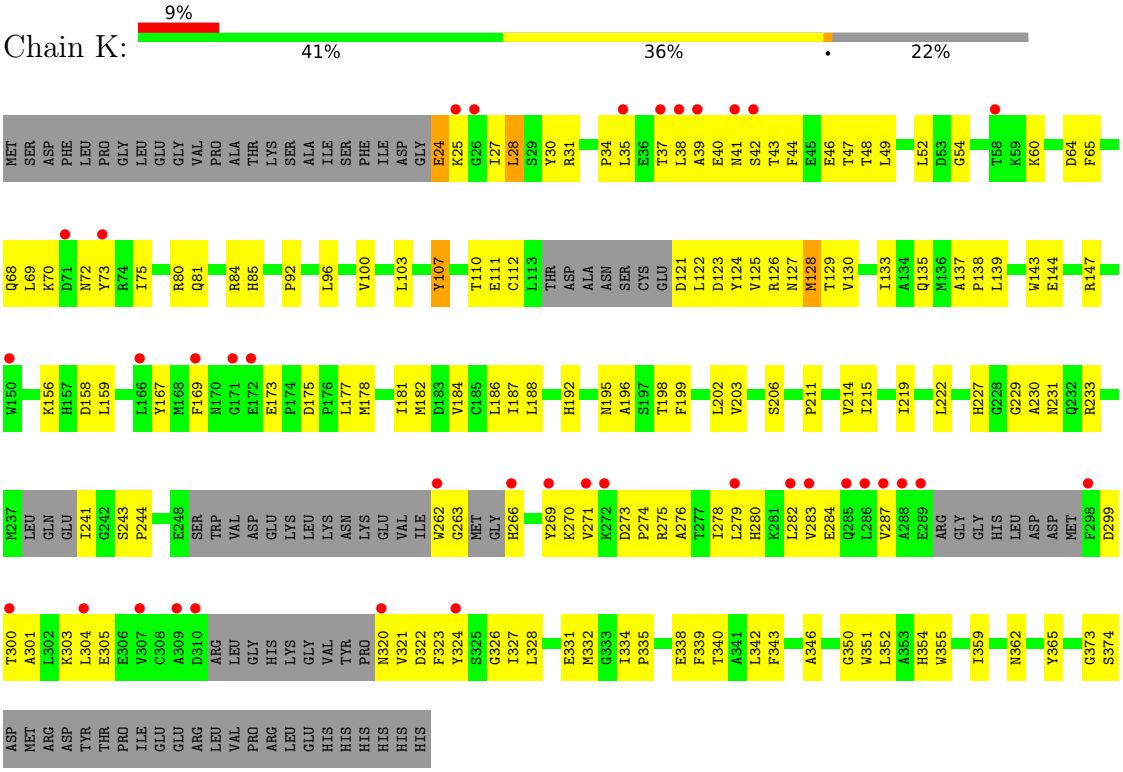


• Molecule 1: Citrate synthase

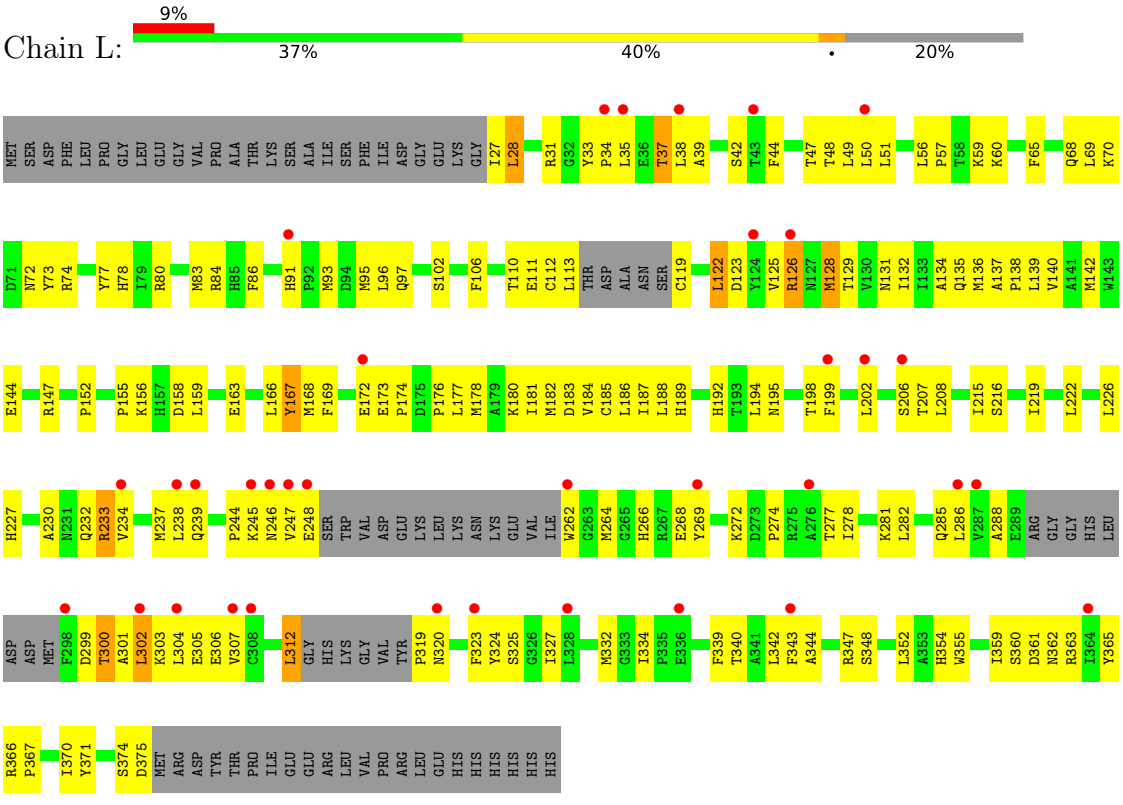
Chain J:



• Molecule 1: Citrate synthase



• Molecule 1: Citrate synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	155.69Å 96.61Å 203.10Å 90.00° 110.41° 90.00°	Depositor
Resolution (Å)	48.31 – 3.20 48.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.31-3.20) 99.0 (48.31-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.282 , 0.325 0.325 , 0.324	Depositor DCC
R_{free} test set	4638 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	114.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 126.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	30057	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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

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	0.61	0/2615	0.57	0/3547
1	B	0.60	0/2640	0.58	0/3580
1	C	0.59	0/2494	0.60	0/3385
1	D	0.60	0/2611	0.59	0/3542
1	E	0.60	0/2592	0.58	0/3515
1	F	0.59	0/2568	0.61	0/3482
1	G	0.61	0/2510	0.57	0/3404
1	H	0.61	0/2539	0.58	0/3444
1	I	0.60	0/2498	0.60	0/3384
1	J	0.60	0/2622	0.58	0/3557
1	K	0.60	0/2487	0.58	0/3372
1	L	0.61	0/2561	0.58	0/3474
All	All	0.60	0/30737	0.59	0/41686

There are no bond length outliers.

There are no bond angle outliers.

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	2555	0	2508	135	0
1	B	2580	0	2527	147	0
1	C	2441	0	2391	121	0
1	D	2552	0	2503	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2533	0	2482	145	0
1	F	2509	0	2452	156	0
1	G	2457	0	2415	149	0
1	H	2484	0	2443	152	0
1	I	2446	0	2402	156	0
1	J	2563	0	2507	141	0
1	K	2433	0	2377	148	0
1	L	2504	0	2452	170	0
All	All	30057	0	29459	1660	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 28.

All (1660) 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:F:264:MET:HA	1:F:319:PRO:HB3	1.34	1.05
1:A:28:LEU:HD12	1:A:35:LEU:HB2	1.42	1.02
1:A:334:ILE:HG21	1:A:342:LEU:HD11	1.42	0.99
1:K:266:HIS:HB3	1:K:269:TYR:HB2	1.45	0.98
1:I:233:ARG:HB2	1:I:323:PHE:HA	1.47	0.96
1:D:28:LEU:HA	1:D:35:LEU:HD13	1.47	0.96
1:J:28:LEU:HG	1:J:35:LEU:H	1.31	0.95
1:I:28:LEU:HB3	1:I:34:PRO:HA	1.50	0.94
1:D:239:GLN:HA	1:D:303:LYS:HD2	1.51	0.93
1:K:52:LEU:HD22	1:K:126:ARG:HH22	1.34	0.92
1:K:28:LEU:HB3	1:K:34:PRO:HA	1.51	0.91
1:A:28:LEU:HB3	1:A:34:PRO:HA	1.53	0.91
1:A:233:ARG:HG2	1:A:262:TRP:HB3	1.53	0.91
1:C:28:LEU:HA	1:C:35:LEU:HD13	1.52	0.90
1:G:369:GLN:HA	1:G:375:ASP:HB3	1.51	0.90
1:K:334:ILE:HG21	1:K:342:LEU:HD11	1.54	0.90
1:L:266:HIS:HB3	1:L:269:TYR:HB2	1.52	0.90
1:J:363:ARG:HG2	1:J:365:TYR:H	1.37	0.89
1:B:27:ILE:HG13	1:B:274:PRO:HG3	1.53	0.88
1:B:202:LEU:HD21	1:B:354:HIS:HB3	1.54	0.88
1:A:266:HIS:HB3	1:A:269:TYR:HB2	1.55	0.87
1:B:28:LEU:HB3	1:B:34:PRO:HA	1.53	0.87
1:H:166:LEU:HB2	1:H:174:PRO:HG3	1.57	0.87
1:B:233:ARG:HG2	1:B:263:GLY:HA3	1.54	0.86
1:F:189:HIS:CE1	1:F:321:VAL:HG21	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:129:THR:HG23	1:I:352:LEU:HD13	1.58	0.86
1:B:27:ILE:HG12	1:B:28:LEU:HD13	1.58	0.85
1:G:68:GLN:HG2	1:G:130:VAL:HG11	1.59	0.85
1:D:181:ILE:HD13	1:D:286:LEU:HD11	1.58	0.85
1:I:28:LEU:HA	1:I:35:LEU:HD13	1.59	0.85
1:F:233:ARG:HH21	1:F:327:ILE:HD11	1.41	0.84
1:F:96:LEU:HG	1:F:219:ILE:HD13	1.58	0.84
1:G:233:ARG:HE	1:G:323:PHE:HA	1.43	0.83
1:F:202:LEU:HD21	1:F:354:HIS:HB3	1.59	0.82
1:G:286:LEU:HD21	1:G:331:GLU:HG2	1.61	0.82
1:J:202:LEU:HD21	1:J:354:HIS:HB3	1.61	0.82
1:G:238:LEU:HD23	1:G:238:LEU:H	1.43	0.81
1:D:202:LEU:HD21	1:D:354:HIS:HB3	1.61	0.81
1:D:178:MET:HA	1:D:181:ILE:HD12	1.63	0.81
1:H:129:THR:HG23	1:H:352:LEU:HD13	1.61	0.80
1:A:241:ILE:HG22	1:A:244:PRO:HG2	1.64	0.80
1:J:272:LYS:HE3	1:J:319:PRO:HB2	1.64	0.79
1:F:27:ILE:HG13	1:F:274:PRO:HG3	1.63	0.79
1:F:80:ARG:HD3	1:F:84:ARG:HE	1.46	0.79
1:J:113:LEU:HD22	1:J:119:CYS:HB3	1.64	0.79
1:A:27:ILE:HG12	1:A:28:LEU:HD13	1.64	0.79
1:H:369:GLN:HE21	1:H:375:ASP:HB3	1.45	0.79
1:K:129:THR:HG23	1:K:352:LEU:HD13	1.65	0.79
1:B:304:LEU:HG	1:B:327:ILE:HD11	1.63	0.78
1:I:307:VAL:HA	1:I:311:ARG:HB2	1.64	0.78
1:B:312:LEU:H	1:B:312:LEU:HD22	1.49	0.78
1:A:102:SER:HB2	1:C:86:PHE:CE2	2.19	0.78
1:E:24:GLU:HB2	1:E:27:ILE:HG23	1.65	0.78
1:D:28:LEU:HG	1:D:35:LEU:H	1.49	0.78
1:A:222:LEU:HD11	1:A:343:PHE:HD1	1.46	0.77
1:F:27:ILE:HG12	1:F:28:LEU:HD13	1.66	0.77
1:F:267:ARG:HH21	1:H:363:ARG:HE	1.30	0.77
1:D:189:HIS:HB3	1:D:343:PHE:HD1	1.49	0.77
1:E:197:SER:H	1:E:227:HIS:HE1	1.33	0.76
1:F:233:ARG:HG3	1:F:323:PHE:HA	1.67	0.76
1:K:25:LYS:HE2	1:K:271:VAL:H	1.51	0.76
1:H:192:HIS:CE1	1:H:266:HIS:HE2	2.03	0.76
1:F:335:PRO:HG2	1:F:338:GLU:HG3	1.68	0.76
1:I:367:PRO:HG2	1:L:194:LEU:HB3	1.65	0.76
1:E:79:ILE:O	1:E:82:MET:HG3	1.85	0.75
1:G:129:THR:HG23	1:G:352:LEU:HD13	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:MET:HG2	1:E:319:PRO:HA	1.68	0.75
1:G:177:LEU:HD22	1:G:177:LEU:H	1.51	0.74
1:J:312:LEU:H	1:J:312:LEU:HD12	1.52	0.74
1:K:68:GLN:HG2	1:K:130:VAL:HG11	1.68	0.74
1:F:327:ILE:HD12	1:F:327:ILE:H	1.53	0.74
1:J:311:ARG:HA	1:J:314:HIS:HB2	1.67	0.74
1:J:137:ALA:HB3	1:J:138:PRO:HD3	1.69	0.74
1:A:129:THR:HB	1:A:352:LEU:HD13	1.70	0.74
1:E:286:LEU:HB3	1:E:331:GLU:HG2	1.70	0.74
1:G:47:THR:HG21	1:G:187:ILE:HG23	1.70	0.74
1:C:196:ALA:HB3	1:C:227:HIS:HD2	1.52	0.73
1:L:327:ILE:H	1:L:327:ILE:HD12	1.52	0.73
1:I:304:LEU:HD13	1:I:324:TYR:CE2	2.24	0.73
1:B:75:ILE:HD11	1:B:138:PRO:HB2	1.71	0.72
1:D:189:HIS:HB3	1:D:343:PHE:CD1	2.24	0.72
1:E:126:ARG:HH21	1:E:356:ARG:HH12	1.34	0.72
1:H:303:LYS:HD3	1:H:327:ILE:HG21	1.68	0.72
1:L:239:GLN:HA	1:L:303:LYS:HB3	1.71	0.72
1:B:193:THR:HG22	1:B:194:LEU:H	1.53	0.72
1:D:96:LEU:HG	1:D:219:ILE:HD13	1.71	0.72
1:E:334:ILE:HG21	1:E:342:LEU:HD11	1.69	0.72
1:A:202:LEU:HD21	1:A:354:HIS:HB3	1.70	0.72
1:L:334:ILE:HG21	1:L:342:LEU:HD11	1.72	0.72
1:D:102:SER:HB2	1:E:86:PHE:CE1	2.24	0.72
1:H:49:LEU:HD23	1:H:57:PRO:HG3	1.70	0.72
1:I:334:ILE:HG21	1:I:342:LEU:HD11	1.72	0.72
1:F:181:ILE:HG22	1:F:328:LEU:HD21	1.72	0.72
1:B:368:THR:HA	1:B:372:VAL:HA	1.71	0.71
1:D:34:PRO:HB2	1:D:36:GLU:OE1	1.90	0.71
1:A:311:ARG:HA	1:A:314:HIS:NE2	2.05	0.71
1:E:245:LYS:HE3	1:E:245:LYS:HA	1.70	0.71
1:B:314:HIS:HB3	1:B:317:VAL:HG23	1.71	0.71
1:F:241:ILE:HD11	1:F:306:GLU:HB2	1.72	0.71
1:G:350:GLY:O	1:G:354:HIS:HD2	1.74	0.71
1:B:68:GLN:HG2	1:B:130:VAL:HG11	1.72	0.71
1:B:300:THR:HA	1:B:327:ILE:HD13	1.72	0.71
1:B:368:THR:HA	1:B:372:VAL:CA	2.21	0.71
1:G:140:VAL:HG12	1:G:169:PHE:HZ	1.56	0.71
1:G:181:ILE:HG21	1:G:328:LEU:HD11	1.72	0.71
1:B:239:GLN:HG2	1:B:298:PHE:CE1	2.26	0.70
1:J:364:ILE:HG23	1:J:366:ARG:HG2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:LYS:HG2	1:G:273:ASP:H	1.55	0.70
1:H:233:ARG:HE	1:H:323:PHE:HA	1.56	0.70
1:I:126:ARG:HH22	1:I:356:ARG:HH11	1.39	0.70
1:J:58:THR:HG23	1:J:61:ALA:H	1.57	0.70
1:F:28:LEU:HB3	1:F:35:LEU:H	1.54	0.70
1:A:96:LEU:HG	1:A:219:ILE:HD13	1.72	0.70
1:L:232:GLN:HB2	1:L:262:TRP:CE2	2.27	0.70
1:H:48:THR:HG22	1:H:349:ALA:HB2	1.73	0.70
1:D:312:LEU:H	1:D:312:LEU:HD22	1.57	0.70
1:K:137:ALA:HB3	1:K:138:PRO:HD3	1.72	0.70
1:J:245:LYS:HA	1:J:245:LYS:HE3	1.73	0.70
1:L:97:GLN:HA	1:L:219:ILE:HD11	1.73	0.69
1:J:28:LEU:HB3	1:J:34:PRO:HA	1.74	0.69
1:L:96:LEU:HG	1:L:219:ILE:HD12	1.74	0.69
1:K:202:LEU:HD21	1:K:354:HIS:HB3	1.72	0.69
1:J:314:HIS:HB3	1:J:317:VAL:O	1.93	0.69
1:A:34:PRO:HG2	1:A:37:THR:HB	1.74	0.69
1:D:354:HIS:O	1:D:357:GLU:HG2	1.92	0.69
1:F:194:LEU:HB3	1:H:367:PRO:HD2	1.74	0.69
1:K:44:PHE:CD1	1:K:186:LEU:HB3	2.27	0.69
1:I:103:LEU:HG	1:I:107:TYR:HE1	1.58	0.69
1:D:192:HIS:HB2	1:D:347:ARG:NH2	2.08	0.69
1:I:233:ARG:HH11	1:I:234:VAL:HA	1.57	0.69
1:D:366:ARG:NE	1:E:195:ASN:HA	2.09	0.68
1:J:177:LEU:HD22	1:J:177:LEU:H	1.58	0.68
1:A:304:LEU:HG	1:A:327:ILE:HD11	1.74	0.68
1:F:334:ILE:HG12	1:F:342:LEU:HD21	1.75	0.68
1:J:233:ARG:HH21	1:J:322:ASP:HB2	1.58	0.68
1:E:129:THR:HG23	1:E:352:LEU:HD13	1.76	0.68
1:E:197:SER:H	1:E:227:HIS:CE1	2.12	0.68
1:J:129:THR:HG23	1:J:352:LEU:HD13	1.75	0.68
1:L:264:MET:HA	1:L:320:ASN:H	1.58	0.68
1:H:70:LYS:HE3	1:H:157:HIS:CE1	2.29	0.68
1:C:96:LEU:HG	1:C:219:ILE:HD13	1.73	0.68
1:F:96:LEU:HD13	1:F:139:LEU:HD11	1.76	0.68
1:H:197:SER:H	1:H:227:HIS:CE1	2.12	0.68
1:K:28:LEU:HA	1:K:35:LEU:HD13	1.74	0.68
1:L:181:ILE:HG13	1:L:286:LEU:HD11	1.74	0.68
1:L:264:MET:HA	1:L:319:PRO:HA	1.75	0.68
1:D:68:GLN:HG2	1:D:130:VAL:HG11	1.76	0.68
1:E:195:ASN:ND2	1:E:198:THR:H	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:ARG:HH12	1:L:325:SER:HB2	1.58	0.67
1:B:307:VAL:HG13	1:B:323:PHE:HZ	1.58	0.67
1:D:229:GLY:HA3	1:D:262:TRP:HE1	1.60	0.67
1:F:113:LEU:HD21	1:F:120:GLU:HB2	1.75	0.67
1:I:233:ARG:NH1	1:I:234:VAL:HA	2.10	0.67
1:J:286:LEU:HD22	1:J:331:GLU:HB3	1.76	0.67
1:K:229:GLY:HA3	1:K:262:TRP:HE1	1.60	0.67
1:B:311:ARG:HD2	1:B:318:TYR:HD1	1.58	0.67
1:A:238:LEU:HD11	1:A:241:ILE:HB	1.77	0.67
1:E:137:ALA:HB3	1:E:138:PRO:HD3	1.77	0.67
1:E:271:VAL:HG22	1:E:272:LYS:H	1.60	0.67
1:G:308:CYS:HA	1:G:319:PRO:HG3	1.77	0.67
1:I:202:LEU:HD22	1:I:358:GLN:HE21	1.58	0.67
1:L:334:ILE:HG12	1:L:342:LEU:HD11	1.77	0.67
1:B:70:LYS:HD3	1:B:157:HIS:O	1.95	0.67
1:C:233:ARG:HD2	1:C:323:PHE:HA	1.77	0.67
1:F:304:LEU:HD12	1:F:323:PHE:CZ	2.29	0.67
1:J:335:PRO:HG2	1:J:338:GLU:HG2	1.76	0.67
1:B:192:HIS:HD2	1:B:195:ASN:HD21	1.42	0.66
1:D:137:ALA:HB3	1:D:138:PRO:HD3	1.77	0.66
1:B:300:THR:HB	1:B:327:ILE:HG21	1.77	0.66
1:D:28:LEU:HB3	1:D:34:PRO:HA	1.75	0.66
1:I:230:ALA:HA	1:I:322:ASP:HB3	1.77	0.66
1:D:334:ILE:HG12	1:D:342:LEU:HD21	1.76	0.66
1:A:77:TYR:O	1:A:80:ARG:HG2	1.94	0.66
1:H:35:LEU:HD21	1:H:188:LEU:HG	1.77	0.66
1:I:25:LYS:NZ	1:I:274:PRO:HD3	2.09	0.66
1:I:70:LYS:HA	1:I:73:TYR:CE2	2.31	0.66
1:I:233:ARG:HD3	1:I:234:VAL:N	2.11	0.66
1:L:264:MET:HA	1:L:320:ASN:N	2.10	0.66
1:F:177:LEU:H	1:F:177:LEU:HD22	1.61	0.66
1:I:34:PRO:O	1:I:37:THR:HG22	1.96	0.66
1:B:368:THR:HA	1:B:372:VAL:HB	1.77	0.66
1:D:52:LEU:HD22	1:D:126:ARG:HH22	1.60	0.66
1:E:177:LEU:HD22	1:E:177:LEU:H	1.61	0.66
1:J:132:ILE:HG21	1:J:215:ILE:HG13	1.78	0.66
1:E:188:LEU:HD21	1:E:278:ILE:HB	1.77	0.65
1:H:70:LYS:HA	1:H:73:TYR:CE2	2.32	0.65
1:K:75:ILE:HD11	1:K:138:PRO:HB2	1.78	0.65
1:L:370:ILE:HG22	1:L:371:TYR:H	1.60	0.65
1:A:206:SER:HA	1:A:361:ASP:OD1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:280:HIS:O	1:I:283:VAL:HG22	1.96	0.65
1:C:196:ALA:HB3	1:C:227:HIS:CD2	2.32	0.65
1:G:79:ILE:HD11	1:G:106:PHE:HE2	1.62	0.65
1:J:28:LEU:HG	1:J:35:LEU:N	2.09	0.65
1:C:129:THR:HG23	1:C:352:LEU:HD13	1.79	0.65
1:I:216:SER:HA	1:I:219:ILE:HD11	1.78	0.65
1:L:129:THR:HG23	1:L:352:LEU:HD13	1.78	0.65
1:B:206:SER:HB2	1:B:364:ILE:HA	1.79	0.65
1:C:334:ILE:HG12	1:C:342:LEU:HD21	1.78	0.65
1:G:202:LEU:HD21	1:G:354:HIS:HB3	1.79	0.65
1:F:363:ARG:HG2	1:F:365:TYR:H	1.63	0.64
1:G:97:GLN:HA	1:G:219:ILE:HD11	1.78	0.64
1:G:196:ALA:HB3	1:G:227:HIS:HD2	1.62	0.64
1:I:31:ARG:HD3	1:I:54:GLY:HA2	1.78	0.64
1:J:156:LYS:HE3	1:J:167:TYR:CZ	2.32	0.64
1:L:31:ARG:HD2	1:L:35:LEU:HB2	1.77	0.64
1:L:70:LYS:HA	1:L:73:TYR:CE2	2.32	0.64
1:H:222:LEU:HD13	1:H:227:HIS:HD2	1.61	0.64
1:K:28:LEU:HD12	1:K:35:LEU:HD13	1.79	0.64
1:I:301:ALA:O	1:I:304:LEU:HG	1.96	0.64
1:B:129:THR:HG23	1:B:352:LEU:HD13	1.78	0.64
1:L:137:ALA:HB3	1:L:138:PRO:HD3	1.80	0.64
1:L:206:SER:HB2	1:L:363:ARG:O	1.96	0.64
1:B:247:VAL:HG22	1:B:248:GLU:HG2	1.79	0.64
1:D:182:MET:HB2	1:D:332:MET:HE1	1.79	0.64
1:J:301:ALA:O	1:J:305:GLU:HG2	1.98	0.64
1:G:176:PRO:O	1:G:180:LYS:HG2	1.97	0.64
1:D:70:LYS:HA	1:D:73:TYR:CE2	2.32	0.63
1:K:222:LEU:HD12	1:K:351:TRP:HZ2	1.63	0.63
1:J:243:SER:HB3	1:J:244:PRO:HD3	1.79	0.63
1:C:200:ALA:O	1:C:203:VAL:HG22	1.99	0.63
1:G:189:HIS:HB3	1:G:343:PHE:HD1	1.62	0.63
1:H:271:VAL:HG22	1:H:272:LYS:H	1.62	0.63
1:A:38:LEU:O	1:A:42:SER:HB3	1.98	0.63
1:A:102:SER:HB2	1:C:86:PHE:HE2	1.61	0.63
1:B:34:PRO:O	1:B:37:THR:HG22	1.99	0.63
1:J:111:GLU:OE2	1:J:120:GLU:HG2	1.98	0.63
1:C:38:LEU:HD21	1:C:50:LEU:HD23	1.81	0.63
1:D:58:THR:HG23	1:D:61:ALA:H	1.64	0.63
1:D:328:LEU:O	1:D:332:MET:HG3	1.99	0.63
1:H:96:LEU:HG	1:H:219:ILE:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:238:LEU:HA	1:H:304:LEU:HD11	1.81	0.63
1:J:49:LEU:HD13	1:J:57:PRO:HG3	1.80	0.63
1:L:244:PRO:HD2	1:L:245:LYS:NZ	2.14	0.63
1:G:189:HIS:HB3	1:G:343:PHE:CD1	2.34	0.63
1:K:75:ILE:HD13	1:K:139:LEU:HD23	1.80	0.63
1:L:93:MET:HE2	1:L:340:THR:HG22	1.80	0.63
1:L:177:LEU:O	1:L:181:ILE:HG12	1.99	0.63
1:C:304:LEU:O	1:C:307:VAL:HG22	1.99	0.62
1:H:192:HIS:HE2	1:H:269:TYR:HE2	1.46	0.62
1:C:177:LEU:O	1:C:181:ILE:HG12	1.99	0.62
1:G:206:SER:HB3	1:G:365:TYR:CD2	2.34	0.62
1:J:132:ILE:O	1:J:136:MET:HG2	1.99	0.62
1:J:197:SER:H	1:J:227:HIS:CE1	2.18	0.62
1:L:83:MET:HA	1:L:95:MET:HE1	1.80	0.62
1:A:156:LYS:HE3	1:A:167:TYR:CZ	2.34	0.62
1:G:166:LEU:HB3	1:G:174:PRO:HB3	1.81	0.62
1:L:266:HIS:CE1	1:L:268:GLU:HB2	2.34	0.62
1:H:25:LYS:HE3	1:H:270:LYS:H	1.65	0.62
1:L:222:LEU:HA	1:L:227:HIS:HD1	1.64	0.62
1:L:304:LEU:HB3	1:L:324:TYR:CE1	2.35	0.62
1:A:264:MET:HG3	1:A:319:PRO:HA	1.81	0.62
1:D:105:MET:HE1	1:E:86:PHE:HB3	1.80	0.62
1:J:127:ASN:O	1:J:130:VAL:HG12	1.99	0.62
1:A:86:PHE:CE1	1:C:102:SER:HB2	2.34	0.62
1:E:34:PRO:O	1:E:37:THR:HG22	1.99	0.62
1:I:137:ALA:HB3	1:I:138:PRO:HD3	1.81	0.62
1:B:132:ILE:HG21	1:B:215:ILE:HG13	1.82	0.62
1:D:27:ILE:HG13	1:D:274:PRO:HG3	1.81	0.62
1:E:238:LEU:HB3	1:E:241:ILE:HG23	1.80	0.62
1:F:47:THR:HG21	1:F:187:ILE:HG23	1.80	0.62
1:H:192:HIS:HE1	1:H:266:HIS:HE2	1.48	0.62
1:L:44:PHE:O	1:L:48:THR:HG23	2.00	0.62
1:A:27:ILE:HG23	1:A:28:LEU:HD22	1.82	0.62
1:A:267:ARG:HD2	1:C:366:ARG:HB3	1.81	0.62
1:B:79:ILE:O	1:B:82:MET:HG2	1.99	0.62
1:J:240:GLU:H	1:J:303:LYS:HD3	1.64	0.62
1:F:137:ALA:HB3	1:F:138:PRO:HD3	1.82	0.61
1:I:25:LYS:HD3	1:I:27:ILE:HD13	1.82	0.61
1:H:28:LEU:HD23	1:H:35:LEU:HD22	1.82	0.61
1:A:226:LEU:HD12	1:C:206:SER:O	2.00	0.61
1:D:106:PHE:O	1:D:108:PRO:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:ALA:HB3	1:G:138:PRO:HD3	1.81	0.61
1:F:27:ILE:HG12	1:F:28:LEU:HD22	1.81	0.61
1:G:24:GLU:HB2	1:G:270:LYS:HB3	1.82	0.61
1:H:47:THR:HG21	1:H:187:ILE:HG23	1.83	0.61
1:J:275:ARG:HB2	1:J:321:VAL:HG22	1.82	0.61
1:K:206:SER:HA	1:K:362:ASN:OD1	2.01	0.61
1:K:230:ALA:HA	1:K:233:ARG:HH22	1.65	0.61
1:K:328:LEU:O	1:K:332:MET:HG3	2.01	0.61
1:F:267:ARG:HH12	1:H:366:ARG:HB3	1.64	0.61
1:G:311:ARG:HD2	1:G:318:TYR:CE2	2.36	0.61
1:E:75:ILE:HD11	1:E:138:PRO:HB2	1.83	0.61
1:F:364:ILE:HG12	1:H:226:LEU:HD23	1.81	0.61
1:G:233:ARG:NE	1:G:323:PHE:HA	2.12	0.61
1:C:206:SER:HA	1:C:362:ASN:OD1	2.01	0.61
1:E:286:LEU:HD12	1:E:328:LEU:HD12	1.81	0.61
1:K:222:LEU:HD12	1:K:351:TRP:CZ2	2.36	0.61
1:C:47:THR:HG21	1:C:187:ILE:HG23	1.82	0.61
1:F:264:MET:HA	1:F:319:PRO:CB	2.21	0.61
1:G:193:THR:HG22	1:G:194:LEU:H	1.66	0.61
1:G:46:GLU:HB2	1:G:62:LEU:HD11	1.82	0.61
1:F:279:LEU:HD23	1:F:282:LEU:HD12	1.83	0.60
1:F:336:GLU:HA	1:F:339:PHE:CE2	2.36	0.60
1:I:243:SER:N	1:I:311:ARG:HE	1.99	0.60
1:B:25:LYS:NZ	1:B:27:ILE:HD12	2.16	0.60
1:A:105:MET:HE3	1:C:90:GLY:HA3	1.83	0.60
1:J:97:GLN:HA	1:J:219:ILE:HD11	1.83	0.60
1:K:233:ARG:HH21	1:K:326:GLY:H	1.49	0.60
1:L:131:ASN:O	1:L:135:GLN:HG2	2.02	0.60
1:L:239:GLN:CG	1:L:299:ASP:HA	2.32	0.60
1:B:125:VAL:HG23	1:B:126:ARG:H	1.66	0.60
1:B:140:VAL:HG12	1:B:169:PHE:HZ	1.65	0.60
1:F:189:HIS:HB3	1:F:343:PHE:CD1	2.37	0.60
1:F:233:ARG:NH1	1:F:234:VAL:HA	2.16	0.60
1:I:28:LEU:HG	1:I:35:LEU:H	1.66	0.60
1:J:241:ILE:O	1:J:244:PRO:HD2	2.01	0.60
1:B:369:GLN:HG3	1:B:370:ILE:HG12	1.83	0.60
1:C:70:LYS:HA	1:C:73:TYR:CE2	2.37	0.60
1:D:131:ASN:O	1:D:135:GLN:HG2	2.01	0.60
1:F:28:LEU:HD12	1:F:35:LEU:HB3	1.83	0.60
1:F:233:ARG:HD3	1:F:234:VAL:N	2.16	0.60
1:J:197:SER:H	1:J:227:HIS:HE1	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:TYR:HA	1:L:172:GLU:O	2.00	0.60
1:L:177:LEU:H	1:L:177:LEU:HD22	1.67	0.60
1:A:102:SER:HB2	1:C:86:PHE:CZ	2.37	0.60
1:H:156:LYS:HE3	1:H:167:TYR:CZ	2.36	0.60
1:J:189:HIS:HB3	1:J:343:PHE:CD1	2.37	0.60
1:J:189:HIS:HB3	1:J:343:PHE:HD1	1.67	0.60
1:L:34:PRO:O	1:L:37:THR:HG22	2.01	0.60
1:D:28:LEU:HG	1:D:35:LEU:N	2.16	0.60
1:D:271:VAL:HG22	1:D:272:LYS:H	1.66	0.60
1:G:76:LYS:HB2	1:G:79:ILE:HG12	1.83	0.60
1:G:369:GLN:HA	1:G:375:ASP:CB	2.30	0.60
1:H:328:LEU:O	1:H:332:MET:HG3	2.01	0.60
1:B:77:TYR:O	1:B:80:ARG:HG2	2.02	0.60
1:C:356:ARG:O	1:C:359:ILE:HG12	2.02	0.60
1:E:238:LEU:HG	1:E:240:GLU:H	1.67	0.60
1:H:369:GLN:HE22	1:H:372:VAL:HG22	1.67	0.60
1:A:243:SER:HB3	1:A:244:PRO:HD3	1.84	0.59
1:H:181:ILE:HG22	1:H:328:LEU:HD21	1.84	0.59
1:K:355:TRP:O	1:K:359:ILE:HG12	2.02	0.59
1:G:24:GLU:HG3	1:G:25:LYS:N	2.15	0.59
1:I:38:LEU:O	1:I:42:SER:HB3	2.02	0.59
1:L:300:THR:HG23	1:L:301:ALA:H	1.67	0.59
1:C:323:PHE:CD1	1:C:324:TYR:N	2.70	0.59
1:D:113:LEU:HD22	1:D:119:CYS:HB3	1.84	0.59
1:F:70:LYS:HA	1:F:73:TYR:CE2	2.37	0.59
1:F:363:ARG:HG3	1:H:267:ARG:HH22	1.66	0.59
1:B:132:ILE:O	1:B:136:MET:HG2	2.01	0.59
1:G:25:LYS:NZ	1:G:272:LYS:HB2	2.16	0.59
1:I:25:LYS:HE2	1:I:271:VAL:CG2	2.32	0.59
1:C:303:LYS:O	1:C:307:VAL:HG13	2.03	0.59
1:F:189:HIS:HE1	1:F:321:VAL:HG21	1.66	0.59
1:F:266:HIS:CE1	1:F:268:GLU:HB3	2.38	0.59
1:D:369:GLN:OE1	1:E:193:THR:HG23	2.03	0.59
1:H:319:PRO:HB3	1:H:323:PHE:CG	2.37	0.59
1:D:25:LYS:HE2	1:D:271:VAL:HG11	1.84	0.59
1:L:176:PRO:O	1:L:180:LYS:HG3	2.02	0.59
1:L:300:THR:HA	1:L:303:LYS:HZ3	1.66	0.59
1:A:222:LEU:HD11	1:A:343:PHE:CD1	2.34	0.59
1:F:28:LEU:HD13	1:F:28:LEU:H	1.68	0.59
1:G:24:GLU:HG3	1:G:25:LYS:H	1.67	0.59
1:B:195:ASN:ND2	1:B:347:ARG:HH21	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ILE:HG21	1:F:328:LEU:HD11	1.84	0.59
1:F:206:SER:O	1:H:226:LEU:HD22	2.03	0.59
1:K:75:ILE:HA	1:K:135:GLN:NE2	2.18	0.59
1:A:70:LYS:HA	1:A:73:TYR:CE2	2.37	0.58
1:G:33:TYR:HB3	1:G:38:LEU:HD21	1.85	0.58
1:J:275:ARG:HH12	1:J:347:ARG:HH22	1.51	0.58
1:D:363:ARG:HE	1:D:365:TYR:HA	1.67	0.58
1:H:239:GLN:HG3	1:H:304:LEU:HD22	1.85	0.58
1:L:69:LEU:HD12	1:L:134:ALA:HB2	1.84	0.58
1:G:70:LYS:HA	1:G:73:TYR:CE2	2.39	0.58
1:L:38:LEU:O	1:L:42:SER:HB3	2.03	0.58
1:L:122:LEU:HD13	1:L:123:ASP:N	2.19	0.58
1:L:359:ILE:HG13	1:L:360:SER:N	2.18	0.58
1:H:159:LEU:HD21	1:H:173:GLU:HG2	1.86	0.58
1:J:77:TYR:O	1:J:80:ARG:HG2	2.03	0.58
1:E:192:HIS:CE1	1:E:266:HIS:HE2	2.22	0.58
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.86	0.58
1:C:166:LEU:HB2	1:C:174:PRO:HG3	1.84	0.58
1:E:276:ALA:HB2	1:E:321:VAL:HA	1.86	0.58
1:G:34:PRO:O	1:G:37:THR:HG22	2.04	0.58
1:G:225:PRO:HG2	1:G:226:LEU:HD12	1.86	0.58
1:H:329:TYR:HB3	1:H:334:ILE:HB	1.86	0.58
1:I:328:LEU:O	1:I:332:MET:HG3	2.03	0.58
1:J:47:THR:HG21	1:J:187:ILE:HG23	1.86	0.58
1:K:276:ALA:HA	1:K:279:LEU:HD12	1.86	0.58
1:I:233:ARG:CB	1:I:323:PHE:HA	2.28	0.58
1:A:356:ARG:O	1:A:359:ILE:HG23	2.04	0.58
1:B:334:ILE:HG12	1:B:342:LEU:HD11	1.85	0.58
1:G:75:ILE:HD11	1:G:138:PRO:HB2	1.86	0.58
1:K:156:LYS:HB2	1:K:159:LEU:HB2	1.85	0.58
1:D:196:ALA:HB3	1:D:227:HIS:CD2	2.38	0.57
1:E:140:VAL:HG12	1:E:169:PHE:HZ	1.69	0.57
1:B:126:ARG:HH21	1:B:129:THR:HG21	1.68	0.57
1:B:311:ARG:HA	1:B:314:HIS:ND1	2.19	0.57
1:B:328:LEU:O	1:B:332:MET:HG3	2.04	0.57
1:C:34:PRO:HB2	1:C:37:THR:HG23	1.86	0.57
1:H:231:ASN:OD1	1:H:336:GLU:HB3	2.05	0.57
1:K:299:ASP:HA	1:K:303:LYS:HD2	1.86	0.57
1:L:230:ALA:HA	1:L:233:ARG:HG2	1.87	0.57
1:D:369:GLN:HB2	1:E:194:LEU:HD23	1.85	0.57
1:G:195:ASN:HB2	1:G:227:HIS:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:241:ILE:O	1:K:244:PRO:HD2	2.04	0.57
1:A:211:PRO:O	1:A:214:VAL:HG22	2.05	0.57
1:C:92:PRO:HA	1:C:143:TRP:CD1	2.39	0.57
1:K:27:ILE:HG12	1:K:28:LEU:HD22	1.85	0.57
1:L:38:LEU:HA	1:L:42:SER:HB3	1.87	0.57
1:D:196:ALA:HB3	1:D:227:HIS:HD2	1.70	0.57
1:E:230:ALA:HA	1:E:233:ARG:HD3	1.87	0.57
1:K:28:LEU:HG	1:K:35:LEU:H	1.70	0.57
1:K:70:LYS:HA	1:K:73:TYR:CE2	2.39	0.57
1:C:44:PHE:CD1	1:C:186:LEU:HB3	2.40	0.57
1:C:233:ARG:NH2	1:C:234:VAL:HB	2.19	0.57
1:D:33:TYR:HB3	1:D:38:LEU:HD11	1.87	0.57
1:F:370:ILE:HD12	1:F:370:ILE:H	1.70	0.57
1:G:156:LYS:HE2	1:G:167:TYR:CE1	2.40	0.57
1:J:47:THR:O	1:J:51:LEU:HG	2.05	0.57
1:L:136:MET:SD	1:L:348:SER:HB3	2.44	0.57
1:H:195:ASN:HB2	1:H:227:HIS:HE1	1.70	0.57
1:J:133:ILE:HG13	1:J:352:LEU:HD12	1.86	0.57
1:E:367:PRO:O	1:E:369:GLN:HG2	2.03	0.57
1:G:226:LEU:HD12	1:G:226:LEU:H	1.68	0.57
1:J:75:ILE:HD11	1:J:138:PRO:HB2	1.87	0.57
1:H:233:ARG:NE	1:H:323:PHE:HA	2.18	0.57
1:I:58:THR:HG23	1:I:61:ALA:H	1.69	0.57
1:K:192:HIS:HE1	1:K:266:HIS:CE1	2.22	0.57
1:A:28:LEU:CD1	1:A:35:LEU:HB2	2.28	0.56
1:A:136:MET:HG2	1:A:345:VAL:HA	1.87	0.56
1:B:79:ILE:HD11	1:B:106:PHE:CE2	2.40	0.56
1:B:368:THR:HA	1:B:372:VAL:CB	2.35	0.56
1:G:103:LEU:HD21	1:G:135:GLN:HG3	1.86	0.56
1:H:52:LEU:HD13	1:H:353:ALA:HA	1.87	0.56
1:B:159:LEU:HD21	1:B:173:GLU:HG2	1.85	0.56
1:D:92:PRO:HG2	1:D:338:GLU:HG2	1.86	0.56
1:G:328:LEU:O	1:G:332:MET:HG3	2.06	0.56
1:G:335:PRO:HG2	1:G:338:GLU:HG2	1.86	0.56
1:H:44:PHE:O	1:H:48:THR:HG23	2.05	0.56
1:K:211:PRO:O	1:K:214:VAL:HG22	2.05	0.56
1:B:167:TYR:HA	1:B:172:GLU:O	2.06	0.56
1:B:298:PHE:HA	1:B:302:LEU:HD12	1.87	0.56
1:F:28:LEU:HD13	1:F:28:LEU:N	2.20	0.56
1:F:232:GLN:HB3	1:F:262:TRP:NE1	2.21	0.56
1:B:28:LEU:HD12	1:B:35:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:ASN:HD21	1:E:198:THR:H	1.53	0.56
1:F:267:ARG:HD3	1:H:364:ILE:HD11	1.86	0.56
1:L:132:ILE:HD12	1:L:352:LEU:HD21	1.86	0.56
1:B:366:ARG:HH11	1:B:367:PRO:HD2	1.70	0.56
1:D:190:ALA:O	1:D:347:ARG:HA	2.05	0.56
1:C:231:ASN:O	1:C:234:VAL:HG12	2.05	0.56
1:F:272:LYS:HA	1:F:318:TYR:HB3	1.87	0.56
1:H:145:HIS:CD2	1:H:153:VAL:H	2.22	0.56
1:I:304:LEU:HD13	1:I:324:TYR:HE2	1.69	0.56
1:B:156:LYS:HE3	1:B:167:TYR:CZ	2.40	0.56
1:D:286:LEU:HB3	1:D:331:GLU:HG2	1.88	0.56
1:K:231:ASN:ND2	1:K:339:PHE:HB2	2.21	0.56
1:A:311:ARG:HA	1:A:314:HIS:CE1	2.41	0.56
1:C:202:LEU:HD21	1:C:354:HIS:HB3	1.87	0.56
1:H:177:LEU:O	1:H:181:ILE:HG13	2.06	0.56
1:J:113:LEU:HD11	1:J:120:GLU:HB2	1.87	0.56
1:D:311:ARG:HD3	1:D:311:ARG:H	1.70	0.56
1:E:194:LEU:O	1:E:198:THR:HB	2.06	0.56
1:G:234:VAL:HG11	1:G:336:GLU:HG2	1.87	0.56
1:J:314:HIS:CD2	1:J:317:VAL:HG23	2.41	0.56
1:K:156:LYS:HB3	1:K:158:ASP:OD1	2.06	0.56
1:I:194:LEU:HB3	1:L:367:PRO:HD2	1.88	0.56
1:L:264:MET:CA	1:L:319:PRO:HA	2.36	0.56
1:E:92:PRO:HG3	1:E:147:ARG:NH1	2.21	0.55
1:E:150:TRP:CH2	1:I:74:ARG:HG3	2.42	0.55
1:L:49:LEU:HD12	1:L:57:PRO:HG3	1.88	0.55
1:L:304:LEU:HD12	1:L:323:PHE:CE1	2.42	0.55
1:A:27:ILE:HG13	1:A:274:PRO:HG3	1.88	0.55
1:A:28:LEU:HD13	1:A:28:LEU:N	2.21	0.55
1:I:102:SER:HB2	1:L:86:PHE:CZ	2.41	0.55
1:J:44:PHE:CZ	1:J:346:ALA:HA	2.42	0.55
1:J:327:ILE:H	1:J:327:ILE:HD12	1.71	0.55
1:K:31:ARG:CD	1:K:54:GLY:HA2	2.37	0.55
1:D:28:LEU:HB3	1:D:34:PRO:CA	2.35	0.55
1:D:129:THR:HG23	1:D:352:LEU:HD13	1.88	0.55
1:I:25:LYS:HE2	1:I:271:VAL:HG23	1.88	0.55
1:J:303:LYS:O	1:J:306:GLU:HG2	2.05	0.55
1:L:266:HIS:CB	1:L:269:TYR:HB2	2.30	0.55
1:A:272:LYS:HG3	1:A:319:PRO:HB2	1.88	0.55
1:C:203:VAL:HA	1:C:365:TYR:CD2	2.41	0.55
1:E:126:ARG:HH21	1:E:356:ARG:NH1	2.01	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:LEU:HG	1:K:219:ILE:HD13	1.87	0.55
1:K:103:LEU:HD22	1:K:135:GLN:HG2	1.88	0.55
1:L:216:SER:O	1:L:219:ILE:HG12	2.06	0.55
1:D:86:PHE:CE1	1:E:102:SER:HB2	2.41	0.55
1:F:335:PRO:HG2	1:F:338:GLU:CG	2.35	0.55
1:G:206:SER:HB3	1:G:365:TYR:HD2	1.71	0.55
1:H:67:GLN:HA	1:H:70:LYS:HD3	1.88	0.55
1:I:231:ASN:OD1	1:I:336:GLU:HB3	2.07	0.55
1:K:31:ARG:NE	1:K:54:GLY:HA2	2.21	0.55
1:K:279:LEU:HA	1:K:282:LEU:HD12	1.88	0.55
1:L:91:HIS:CE1	1:L:93:MET:HB2	2.42	0.55
1:A:359:ILE:HD13	1:A:359:ILE:H	1.71	0.55
1:B:156:LYS:HE3	1:B:167:TYR:CE1	2.42	0.55
1:E:365:TYR:O	1:E:367:PRO:HD3	2.06	0.55
1:H:326:GLY:HA2	1:H:329:TYR:CD2	2.42	0.55
1:L:303:LYS:O	1:L:307:VAL:HG23	2.06	0.55
1:E:68:GLN:HG2	1:E:130:VAL:HG21	1.88	0.55
1:F:167:TYR:HA	1:F:172:GLU:O	2.07	0.55
1:I:371:TYR:HB2	1:L:268:GLU:OE2	2.07	0.55
1:K:47:THR:HG21	1:K:187:ILE:HG23	1.89	0.55
1:L:33:TYR:CE1	1:L:50:LEU:HD11	2.41	0.55
1:C:106:PHE:O	1:C:108:PRO:HD3	2.07	0.55
1:D:28:LEU:CG	1:D:35:LEU:H	2.19	0.55
1:D:364:ILE:HB	1:E:267:ARG:HH12	1.71	0.55
1:G:272:LYS:HG2	1:G:273:ASP:N	2.20	0.55
1:B:233:ARG:CG	1:B:263:GLY:HA3	2.32	0.55
1:C:77:TYR:O	1:C:80:ARG:HG2	2.06	0.55
1:F:102:SER:HB2	1:H:86:PHE:CE1	2.42	0.55
1:F:167:TYR:O	1:F:171:GLY:N	2.40	0.55
1:F:334:ILE:H	1:F:334:ILE:HD12	1.72	0.55
1:G:44:PHE:O	1:G:48:THR:HG23	2.07	0.55
1:G:69:LEU:HA	1:G:130:VAL:HG22	1.88	0.55
1:K:273:ASP:OD2	1:K:275:ARG:HB2	2.07	0.55
1:A:232:GLN:O	1:A:235:VAL:HG12	2.07	0.54
1:B:230:ALA:HA	1:B:322:ASP:HB3	1.89	0.54
1:C:206:SER:HB2	1:C:364:ILE:HA	1.89	0.54
1:F:272:LYS:HZ2	1:F:319:PRO:CD	2.20	0.54
1:G:131:ASN:O	1:G:135:GLN:HG2	2.07	0.54
1:H:100:VAL:HG21	1:H:219:ILE:HD11	1.89	0.54
1:I:82:MET:HG2	1:I:86:PHE:HE2	1.72	0.54
1:J:166:LEU:HD21	1:J:178:MET:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:222:LEU:HD11	1:K:343:PHE:CD2	2.43	0.54
1:G:113:LEU:CD2	1:G:120:GLU:HB3	2.37	0.54
1:J:27:ILE:HG22	1:J:269:TYR:HE1	1.71	0.54
1:J:31:ARG:NE	1:J:54:GLY:HA2	2.22	0.54
1:K:334:ILE:H	1:K:334:ILE:HD12	1.72	0.54
1:D:238:LEU:HD11	1:D:241:ILE:HB	1.89	0.54
1:E:235:VAL:HG23	1:E:304:LEU:HD22	1.90	0.54
1:G:113:LEU:HD21	1:G:120:GLU:HB3	1.89	0.54
1:K:75:ILE:HA	1:K:135:GLN:HE22	1.71	0.54
1:L:140:VAL:HG12	1:L:169:PHE:HZ	1.72	0.54
1:L:247:VAL:O	1:L:248:GLU:C	2.46	0.54
1:B:272:LYS:HD2	1:B:311:ARG:HH22	1.73	0.54
1:D:234:VAL:HG21	1:D:303:LYS:HE2	1.88	0.54
1:G:77:TYR:O	1:G:80:ARG:HG2	2.07	0.54
1:G:127:ASN:O	1:G:130:VAL:HG12	2.08	0.54
1:L:166:LEU:HB3	1:L:174:PRO:HG3	1.89	0.54
1:B:38:LEU:O	1:B:42:SER:HB3	2.08	0.54
1:G:33:TYR:CD1	1:G:50:LEU:HD11	2.42	0.54
1:G:350:GLY:O	1:G:354:HIS:CD2	2.58	0.54
1:J:216:SER:O	1:J:219:ILE:HG12	2.07	0.54
1:A:53:ASP:OD1	1:A:54:GLY:N	2.40	0.54
1:C:305:GLU:O	1:C:308:CYS:HB3	2.07	0.54
1:D:49:LEU:HD23	1:D:57:PRO:HB3	1.88	0.54
1:D:301:ALA:O	1:D:305:GLU:HG2	2.07	0.54
1:F:371:TYR:CE1	1:F:373:GLY:HA3	2.43	0.54
1:J:63:ASN:O	1:J:67:GLN:HG2	2.08	0.54
1:C:33:TYR:CE1	1:C:50:LEU:HD11	2.43	0.54
1:C:100:VAL:HG21	1:C:219:ILE:CD1	2.38	0.54
1:I:86:PHE:CZ	1:L:102:SER:HB2	2.42	0.54
1:L:195:ASN:ND2	1:L:347:ARG:HE	2.06	0.54
1:C:318:TYR:N	1:C:319:PRO:HD2	2.23	0.54
1:F:132:ILE:O	1:F:136:MET:HG2	2.08	0.54
1:H:103:LEU:HG	1:H:107:TYR:HE2	1.71	0.54
1:H:369:GLN:NE2	1:H:372:VAL:HG22	2.23	0.54
1:I:243:SER:H	1:I:311:ARG:HE	1.55	0.54
1:I:266:HIS:CE1	1:I:268:GLU:HB2	2.43	0.54
1:J:327:ILE:O	1:J:331:GLU:HG2	2.07	0.54
1:B:137:ALA:HB3	1:B:138:PRO:HD3	1.90	0.54
1:I:98:THR:HG21	1:L:102:SER:HB3	1.90	0.54
1:J:264:MET:SD	1:J:319:PRO:HA	2.48	0.54
1:B:27:ILE:CG1	1:B:28:LEU:HD13	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ILE:HG13	1:D:28:LEU:HD13	1.90	0.54
1:F:86:PHE:CZ	1:H:102:SER:HB2	2.42	0.54
1:F:280:HIS:HD1	1:F:324:TYR:HE2	1.53	0.54
1:I:28:LEU:HD23	1:I:34:PRO:HB3	1.89	0.54
1:C:27:ILE:HG23	1:C:274:PRO:HG3	1.89	0.53
1:C:100:VAL:HG21	1:C:219:ILE:HD11	1.90	0.53
1:K:196:ALA:HB3	1:K:227:HIS:HD2	1.72	0.53
1:L:334:ILE:HG21	1:L:342:LEU:CD1	2.37	0.53
1:A:369:GLN:HB2	1:C:193:THR:CG2	2.38	0.53
1:F:96:LEU:CD1	1:F:139:LEU:HD11	2.37	0.53
1:I:160:SER:H	1:I:163:GLU:HB2	1.73	0.53
1:K:373:GLY:O	1:K:374:SER:C	2.46	0.53
1:L:244:PRO:HD2	1:L:245:LYS:HZ2	1.72	0.53
1:B:273:ASP:CG	1:B:275:ARG:HE	2.12	0.53
1:F:181:ILE:HB	1:F:332:MET:HE2	1.91	0.53
1:I:28:LEU:HG	1:I:35:LEU:N	2.23	0.53
1:K:144:GLU:HG2	1:K:147:ARG:NH2	2.24	0.53
1:L:159:LEU:HD21	1:L:173:GLU:HG2	1.90	0.53
1:D:34:PRO:HG2	1:D:37:THR:HG22	1.91	0.53
1:E:100:VAL:HG21	1:E:219:ILE:HD11	1.89	0.53
1:F:77:TYR:HB3	1:J:151:ASP:OD1	2.07	0.53
1:F:102:SER:HA	1:F:105:MET:HE2	1.91	0.53
1:L:300:THR:HA	1:L:303:LYS:NZ	2.24	0.53
1:A:225:PRO:HD2	1:C:208:LEU:O	2.08	0.53
1:D:140:VAL:HG12	1:D:169:PHE:HZ	1.73	0.53
1:D:175:ASP:OD1	1:D:178:MET:HB2	2.09	0.53
1:F:264:MET:SD	1:F:319:PRO:HD3	2.47	0.53
1:G:182:MET:HB2	1:G:332:MET:HE3	1.91	0.53
1:K:335:PRO:HG2	1:K:338:GLU:HG2	1.91	0.53
1:L:365:TYR:O	1:L:367:PRO:HD3	2.08	0.53
1:A:162:ALA:HA	1:A:165:LEU:HD12	1.91	0.53
1:K:34:PRO:HG2	1:K:37:THR:HB	1.89	0.53
1:E:196:ALA:HB3	1:E:227:HIS:ND1	2.24	0.53
1:G:222:LEU:HD11	1:G:343:PHE:HD2	1.73	0.53
1:E:233:ARG:HH12	1:E:326:GLY:HA3	1.72	0.53
1:F:27:ILE:CG1	1:F:28:LEU:HD13	2.37	0.53
1:F:275:ARG:HB3	1:F:321:VAL:CG1	2.39	0.53
1:G:276:ALA:HB2	1:G:321:VAL:HA	1.91	0.53
1:F:102:SER:HB2	1:H:86:PHE:CZ	2.44	0.53
1:F:225:PRO:HG2	1:F:226:LEU:HD13	1.91	0.53
1:G:92:PRO:HA	1:G:143:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:ARG:HD2	1:G:318:TYR:HE2	1.74	0.53
1:I:206:SER:O	1:L:226:LEU:HD12	2.09	0.53
1:K:69:LEU:HA	1:K:130:VAL:HG22	1.91	0.53
1:K:195:ASN:HB3	1:K:227:HIS:NE2	2.23	0.53
1:K:327:ILE:O	1:K:331:GLU:HG2	2.09	0.53
1:L:28:LEU:HD11	1:L:192:HIS:CE1	2.44	0.53
1:B:182:MET:O	1:B:186:LEU:HG	2.09	0.53
1:I:44:PHE:HA	1:I:187:ILE:HG12	1.90	0.53
1:I:370:ILE:HG13	1:I:370:ILE:O	2.09	0.53
1:L:132:ILE:HG21	1:L:215:ILE:HG13	1.90	0.53
1:L:142:MET:HG3	1:L:152:PRO:HB3	1.90	0.53
1:F:113:LEU:HD22	1:F:119:CYS:HB3	1.91	0.52
1:F:226:LEU:HD22	1:H:208:LEU:HG	1.90	0.52
1:J:68:GLN:HG2	1:J:130:VAL:HG11	1.91	0.52
1:J:76:LYS:HB2	1:J:79:ILE:HG12	1.90	0.52
1:D:206:SER:O	1:E:226:LEU:HD12	2.09	0.52
1:E:127:ASN:O	1:E:130:VAL:HG12	2.08	0.52
1:E:156:LYS:HE3	1:E:167:TYR:CZ	2.44	0.52
1:F:31:ARG:HG3	1:F:50:LEU:O	2.09	0.52
1:F:177:LEU:O	1:F:181:ILE:HG13	2.08	0.52
1:K:127:ASN:O	1:K:130:VAL:HG12	2.09	0.52
1:K:241:ILE:HB	1:K:244:PRO:HG2	1.92	0.52
1:B:63:ASN:HD21	1:B:67:GLN:HE21	1.57	0.52
1:C:30:TYR:HD2	1:C:38:LEU:HD22	1.74	0.52
1:I:28:LEU:HB3	1:I:34:PRO:CA	2.32	0.52
1:K:28:LEU:HD13	1:K:28:LEU:N	2.24	0.52
1:C:198:THR:HA	1:C:351:TRP:CD1	2.44	0.52
1:C:279:LEU:O	1:C:283:VAL:HG23	2.09	0.52
1:J:211:PRO:O	1:J:214:VAL:HG22	2.10	0.52
1:J:222:LEU:HD13	1:J:343:PHE:CD2	2.44	0.52
1:J:335:PRO:HG2	1:J:338:GLU:CG	2.39	0.52
1:L:126:ARG:HA	1:L:129:THR:HB	1.89	0.52
1:B:27:ILE:O	1:B:28:LEU:HB2	2.09	0.52
1:D:366:ARG:HB3	1:E:267:ARG:HD2	1.92	0.52
1:H:137:ALA:HB3	1:H:138:PRO:HD3	1.91	0.52
1:I:125:VAL:HG13	1:I:355:TRP:CZ3	2.44	0.52
1:I:279:LEU:HD23	1:I:282:LEU:HD12	1.92	0.52
1:L:239:GLN:HG2	1:L:299:ASP:HA	1.90	0.52
1:I:304:LEU:HD12	1:I:305:GLU:N	2.24	0.52
1:K:25:LYS:HE2	1:K:271:VAL:HG12	1.92	0.52
1:B:76:LYS:NZ	1:B:106:PHE:HB3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:THR:O	1:H:202:LEU:HG	2.09	0.52
1:I:126:ARG:HA	1:I:129:THR:HB	1.91	0.52
1:J:243:SER:HB2	1:J:306:GLU:OE1	2.09	0.52
1:J:363:ARG:HG2	1:J:365:TYR:N	2.17	0.52
1:A:166:LEU:HB2	1:A:174:PRO:HG3	1.92	0.52
1:A:177:LEU:O	1:A:181:ILE:HG13	2.10	0.52
1:G:272:LYS:NZ	1:G:272:LYS:HB3	2.24	0.52
1:K:30:TYR:CD1	1:K:35:LEU:HD11	2.45	0.52
1:K:222:LEU:HD11	1:K:343:PHE:HD2	1.75	0.52
1:B:195:ASN:HB3	1:B:227:HIS:HE1	1.74	0.52
1:E:222:LEU:HD13	1:E:343:PHE:HD2	1.75	0.52
1:E:275:ARG:HH12	1:E:347:ARG:HH22	1.58	0.52
1:K:203:VAL:HA	1:K:365:TYR:CD2	2.45	0.52
1:K:211:PRO:HG3	1:K:355:TRP:CH2	2.45	0.52
1:L:83:MET:HG2	1:L:95:MET:HE2	1.92	0.52
1:A:63:ASN:O	1:A:67:GLN:HG2	2.10	0.52
1:D:183:ASP:O	1:D:187:ILE:HG13	2.10	0.52
1:G:66:SER:O	1:G:70:LYS:HG3	2.10	0.52
1:G:144:GLU:HG2	1:G:147:ARG:NH2	2.25	0.52
1:H:192:HIS:HE1	1:H:266:HIS:NE2	2.08	0.52
1:H:278:ILE:O	1:H:282:LEU:HG	2.10	0.52
1:A:72:ASN:HB3	1:A:131:ASN:HA	1.93	0.51
1:D:311:ARG:HA	1:D:314:HIS:HB2	1.91	0.51
1:E:49:LEU:HD11	1:E:65:PHE:HB3	1.91	0.51
1:H:355:TRP:NE1	1:H:359:ILE:HD11	2.25	0.51
1:I:368:THR:HA	1:I:371:TYR:HB3	1.92	0.51
1:J:24:GLU:OE1	1:J:25:LYS:HG3	2.10	0.51
1:G:48:THR:HG22	1:G:349:ALA:HB2	1.92	0.51
1:G:278:ILE:O	1:G:282:LEU:HG	2.10	0.51
1:K:233:ARG:HH21	1:K:326:GLY:N	2.08	0.51
1:L:198:THR:O	1:L:202:LEU:HG	2.10	0.51
1:B:195:ASN:HB3	1:B:227:HIS:CE1	2.45	0.51
1:B:215:ILE:HD11	1:B:352:LEU:HG	1.92	0.51
1:C:70:LYS:HE3	1:C:157:HIS:CD2	2.45	0.51
1:C:231:ASN:OD1	1:C:336:GLU:HB3	2.11	0.51
1:E:264:MET:HA	1:E:319:PRO:HA	1.91	0.51
1:F:129:THR:HG23	1:F:352:LEU:HD13	1.91	0.51
1:G:97:GLN:HA	1:G:219:ILE:CD1	2.39	0.51
1:H:266:HIS:CG	1:H:269:TYR:HB2	2.44	0.51
1:B:70:LYS:HA	1:B:73:TYR:CE2	2.44	0.51
1:B:206:SER:HB3	1:B:365:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:HB3	1:B:324:TYR:CE1	2.46	0.51
1:F:272:LYS:HZ1	1:F:319:PRO:CG	2.24	0.51
1:G:356:ARG:O	1:G:359:ILE:HG12	2.11	0.51
1:J:70:LYS:HA	1:J:73:TYR:CZ	2.45	0.51
1:J:334:ILE:HG12	1:J:342:LEU:HD21	1.91	0.51
1:L:59:LYS:HG3	1:L:60:LYS:HD2	1.92	0.51
1:L:233:ARG:NH1	1:L:325:SER:HB2	2.25	0.51
1:B:303:LYS:O	1:B:307:VAL:HG12	2.11	0.51
1:F:314:HIS:HB3	1:F:317:VAL:HB	1.93	0.51
1:I:70:LYS:HA	1:I:73:TYR:CZ	2.45	0.51
1:J:96:LEU:HG	1:J:219:ILE:HD12	1.92	0.51
1:L:312:LEU:HD22	1:L:312:LEU:C	2.31	0.51
1:A:32:GLY:HA2	1:C:374:SER:O	2.10	0.51
1:B:82:MET:HG3	1:B:83:MET:N	2.26	0.51
1:D:28:LEU:O	1:D:34:PRO:HA	2.11	0.51
1:D:124:TYR:HE2	1:D:211:PRO:HD2	1.76	0.51
1:I:194:LEU:HD12	1:L:367:PRO:HG2	1.92	0.51
1:K:43:THR:H	1:K:46:GLU:HB3	1.75	0.51
1:L:272:LYS:HD3	1:L:277:THR:HG22	1.93	0.51
1:D:43:THR:HG23	1:D:46:GLU:H	1.75	0.51
1:I:241:ILE:HA	1:I:311:ARG:NH2	2.26	0.51
1:A:215:ILE:O	1:A:219:ILE:HG13	2.11	0.51
1:D:28:LEU:HG	1:D:35:LEU:HB2	1.93	0.51
1:D:367:PRO:HG2	1:E:194:LEU:HD12	1.92	0.51
1:E:132:ILE:HG21	1:E:215:ILE:HG13	1.93	0.51
1:I:127:ASN:O	1:I:130:VAL:HG22	2.11	0.51
1:K:263:GLY:O	1:K:323:PHE:HB2	2.11	0.51
1:B:197:SER:H	1:B:227:HIS:CE1	2.28	0.51
1:B:199:PHE:HA	1:B:202:LEU:HD12	1.93	0.51
1:C:149:GLY:HA2	1:L:77:TYR:CE2	2.45	0.51
1:G:49:LEU:CD1	1:G:62:LEU:HA	2.41	0.51
1:G:238:LEU:H	1:G:238:LEU:CD2	2.19	0.51
1:G:334:ILE:HG21	1:G:342:LEU:HD11	1.93	0.51
1:L:47:THR:O	1:L:51:LEU:HG	2.10	0.51
1:F:272:LYS:HZ2	1:F:319:PRO:HD2	1.75	0.51
1:I:73:TYR:HD1	1:I:134:ALA:HB1	1.76	0.51
1:K:275:ARG:O	1:K:279:LEU:HG	2.11	0.51
1:G:167:TYR:HA	1:G:172:GLU:O	2.11	0.50
1:G:279:LEU:HD23	1:G:282:LEU:HD12	1.92	0.50
1:K:28:LEU:HG	1:K:35:LEU:N	2.26	0.50
1:K:215:ILE:O	1:K:219:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:303:LYS:HG3	1:L:304:LEU:HD22	1.94	0.50
1:A:222:LEU:HD12	1:A:351:TRP:CZ2	2.46	0.50
1:B:366:ARG:O	1:B:369:GLN:HG2	2.12	0.50
1:E:308:CYS:HB3	1:E:323:PHE:CE2	2.46	0.50
1:F:206:SER:HA	1:F:361:ASP:CG	2.31	0.50
1:F:323:PHE:HD2	1:F:324:TYR:CE1	2.29	0.50
1:F:366:ARG:HB3	1:H:267:ARG:HD2	1.92	0.50
1:G:369:GLN:CA	1:G:375:ASP:HB3	2.34	0.50
1:I:97:GLN:HA	1:I:219:ILE:CD1	2.41	0.50
1:I:302:LEU:O	1:I:305:GLU:HG3	2.11	0.50
1:J:238:LEU:HB3	1:J:303:LYS:HE3	1.92	0.50
1:A:269:TYR:CE1	1:A:274:PRO:HD2	2.46	0.50
1:E:24:GLU:CB	1:E:27:ILE:HG23	2.36	0.50
1:G:25:LYS:HZ2	1:G:272:LYS:HB2	1.75	0.50
1:H:237:MET:SD	1:H:237:MET:N	2.80	0.50
1:D:47:THR:HG21	1:D:187:ILE:HG23	1.93	0.50
1:I:156:LYS:HD3	1:I:159:LEU:HD11	1.94	0.50
1:K:52:LEU:HB3	1:K:126:ARG:HH12	1.76	0.50
1:K:203:VAL:HA	1:K:365:TYR:HD2	1.76	0.50
1:A:30:TYR:CE1	1:A:35:LEU:HD21	2.46	0.50
1:A:125:VAL:O	1:A:126:ARG:HB2	2.11	0.50
1:A:231:ASN:HA	1:A:234:VAL:HG23	1.91	0.50
1:A:238:LEU:HD21	1:A:242:GLY:HA2	1.93	0.50
1:A:271:VAL:HG22	1:A:272:LYS:H	1.77	0.50
1:B:31:ARG:NE	1:B:54:GLY:HA2	2.26	0.50
1:C:309:ALA:O	1:C:310:ASP:C	2.50	0.50
1:E:38:LEU:O	1:E:42:SER:HB3	2.11	0.50
1:E:138:PRO:HA	1:E:168:MET:HE1	1.93	0.50
1:F:181:ILE:HB	1:F:332:MET:CE	2.41	0.50
1:F:311:ARG:HE	1:F:318:TYR:HE1	1.60	0.50
1:H:206:SER:HB2	1:H:364:ILE:HA	1.93	0.50
1:K:110:THR:HG22	1:K:112:CYS:H	1.77	0.50
1:K:243:SER:HB2	1:K:244:PRO:HD3	1.93	0.50
1:L:156:LYS:HE2	1:L:167:TYR:CZ	2.46	0.50
1:A:156:LYS:HB2	1:A:159:LEU:HB2	1.92	0.50
1:H:327:ILE:O	1:H:331:GLU:HG2	2.11	0.50
1:I:279:LEU:O	1:I:283:VAL:HG13	2.12	0.50
1:E:167:TYR:HB2	1:E:174:PRO:HD3	1.93	0.50
1:F:28:LEU:HD12	1:F:35:LEU:CB	2.42	0.50
1:H:47:THR:O	1:H:50:LEU:HG	2.11	0.50
1:H:358:GLN:HE22	1:H:365:TYR:HE1	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:LEU:HG	1:I:35:LEU:HB2	1.94	0.50
1:I:311:ARG:O	1:I:312:LEU:C	2.49	0.50
1:K:199:PHE:HA	1:K:202:LEU:HD12	1.92	0.50
1:L:195:ASN:HD21	1:L:347:ARG:HE	1.59	0.50
1:L:264:MET:CB	1:L:319:PRO:HA	2.41	0.50
1:B:311:ARG:HD2	1:B:318:TYR:CD1	2.44	0.50
1:G:153:VAL:HG21	1:G:168:MET:O	2.12	0.50
1:H:241:ILE:O	1:H:242:GLY:C	2.50	0.50
1:I:104:GLY:O	1:I:108:PRO:HB3	2.11	0.50
1:J:372:VAL:HB	1:J:375:ASP:CA	2.41	0.50
1:K:222:LEU:HG	1:K:227:HIS:CE1	2.46	0.50
1:A:111:GLU:O	1:A:113:LEU:HG	2.12	0.50
1:C:199:PHE:O	1:C:203:VAL:HG13	2.12	0.50
1:D:91:HIS:HD2	1:D:93:MET:HB2	1.77	0.50
1:L:33:TYR:CZ	1:L:50:LEU:HD11	2.46	0.50
1:C:198:THR:O	1:C:202:LEU:HD23	2.13	0.49
1:E:70:LYS:C	1:E:72:ASN:H	2.15	0.49
1:H:70:LYS:HB3	1:H:157:HIS:CD2	2.47	0.49
1:I:86:PHE:CE1	1:L:102:SER:HB2	2.47	0.49
1:K:49:LEU:HD11	1:K:65:PHE:HB3	1.94	0.49
1:L:246:ASN:O	1:L:248:GLU:HG3	2.12	0.49
1:B:301:ALA:HA	1:B:305:GLU:CD	2.33	0.49
1:C:206:SER:HB3	1:C:365:TYR:CD2	2.47	0.49
1:D:28:LEU:CD1	1:D:35:LEU:HB2	2.41	0.49
1:D:335:PRO:HG2	1:D:338:GLU:HG3	1.93	0.49
1:E:182:MET:O	1:E:186:LEU:HG	2.13	0.49
1:G:233:ARG:HE	1:G:323:PHE:CA	2.19	0.49
1:B:271:VAL:HA	1:B:318:TYR:CD2	2.47	0.49
1:D:85:HIS:HD2	1:E:81:GLN:NE2	2.09	0.49
1:E:198:THR:O	1:E:202:LEU:HG	2.13	0.49
1:F:27:ILE:CG1	1:F:274:PRO:HG3	2.40	0.49
1:F:109:GLY:HA3	1:F:210:THR:HG22	1.94	0.49
1:H:233:ARG:HB3	1:H:233:ARG:CZ	2.42	0.49
1:J:31:ARG:CZ	1:J:54:GLY:HA2	2.42	0.49
1:J:112:CYS:O	1:J:113:LEU:C	2.50	0.49
1:K:156:LYS:HD2	1:K:159:LEU:CD1	2.42	0.49
1:A:34:PRO:HG2	1:A:37:THR:CB	2.39	0.49
1:C:156:LYS:HE3	1:C:167:TYR:CZ	2.47	0.49
1:C:273:ASP:OD1	1:C:274:PRO:HD2	2.12	0.49
1:D:47:THR:O	1:D:51:LEU:HG	2.12	0.49
1:D:314:HIS:HB3	1:D:317:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:PRO:HG3	1:E:199:PHE:CD1	2.47	0.49
1:I:68:GLN:HG2	1:I:130:VAL:HG21	1.94	0.49
1:L:285:GLN:O	1:L:288:ALA:HB3	2.12	0.49
1:B:135:GLN:C	1:B:138:PRO:HD2	2.32	0.49
1:B:368:THR:HG23	1:B:372:VAL:HB	1.93	0.49
1:C:75:ILE:HD11	1:C:138:PRO:HB2	1.93	0.49
1:F:235:VAL:O	1:F:236:GLY:C	2.50	0.49
1:H:195:ASN:HB2	1:H:227:HIS:CE1	2.47	0.49
1:L:156:LYS:HB3	1:L:158:ASP:OD1	2.12	0.49
1:C:302:LEU:O	1:C:306:GLU:HG2	2.13	0.49
1:J:175:ASP:OD1	1:J:175:ASP:N	2.46	0.49
1:A:79:ILE:O	1:A:82:MET:HG2	2.13	0.49
1:D:364:ILE:HG13	1:E:267:ARG:HH22	1.78	0.49
1:H:80:ARG:O	1:H:84:ARG:HG3	2.12	0.49
1:D:334:ILE:H	1:D:334:ILE:HD12	1.78	0.49
1:J:304:LEU:HD12	1:J:323:PHE:CE1	2.47	0.49
1:K:177:LEU:O	1:K:181:ILE:HG13	2.12	0.49
1:A:100:VAL:HG21	1:A:219:ILE:HD11	1.93	0.49
1:A:135:GLN:C	1:A:138:PRO:HD2	2.33	0.49
1:E:363:ARG:NH2	1:E:365:TYR:HA	2.28	0.49
1:G:222:LEU:HD23	1:G:344:ALA:HB2	1.94	0.49
1:G:271:VAL:HB	1:G:318:TYR:CE1	2.48	0.49
1:H:334:ILE:HD13	1:H:342:LEU:CD1	2.42	0.49
1:K:299:ASP:H	1:K:303:LYS:HE2	1.78	0.49
1:L:28:LEU:HD12	1:L:31:ARG:HH21	1.78	0.49
1:B:75:ILE:HG21	1:B:142:MET:HE1	1.95	0.49
1:D:354:HIS:O	1:D:358:GLN:HG2	2.13	0.49
1:J:176:PRO:O	1:J:180:LYS:HG2	2.13	0.49
1:J:241:ILE:HD12	1:J:242:GLY:N	2.27	0.49
1:A:120:GLU:H	1:A:120:GLU:CD	2.15	0.48
1:B:215:ILE:O	1:B:219:ILE:HG13	2.14	0.48
1:B:222:LEU:HD23	1:B:344:ALA:HB2	1.94	0.48
1:F:69:LEU:HD12	1:F:134:ALA:HB2	1.93	0.48
1:F:124:TYR:O	1:F:128:MET:HG2	2.13	0.48
1:F:267:ARG:NH1	1:H:366:ARG:HB3	2.27	0.48
1:I:123:ASP:HB2	1:I:127:ASN:CG	2.34	0.48
1:J:27:ILE:O	1:J:28:LEU:HB2	2.13	0.48
1:L:59:LYS:HG3	1:L:60:LYS:N	2.28	0.48
1:L:125:VAL:HG13	1:L:355:TRP:CZ3	2.48	0.48
1:A:238:LEU:HB3	1:A:303:LYS:HD2	1.94	0.48
1:C:27:ILE:HD12	1:C:274:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ASN:O	1:D:130:VAL:HG12	2.13	0.48
1:F:24:GLU:OE1	1:F:25:LYS:HG3	2.13	0.48
1:G:272:LYS:HE2	1:G:274:PRO:HD3	1.95	0.48
1:I:338:GLU:O	1:I:342:LEU:HG	2.13	0.48
1:H:63:ASN:O	1:H:67:GLN:HG2	2.13	0.48
1:I:75:ILE:HD11	1:I:138:PRO:HB2	1.95	0.48
1:L:188:LEU:HD21	1:L:278:ILE:HB	1.95	0.48
1:C:120:GLU:CD	1:C:120:GLU:H	2.16	0.48
1:D:233:ARG:CZ	1:D:233:ARG:HA	2.43	0.48
1:E:35:LEU:O	1:E:39:ALA:N	2.46	0.48
1:H:93:MET:SD	1:H:341:ALA:HA	2.54	0.48
1:H:222:LEU:CD1	1:H:227:HIS:HD2	2.25	0.48
1:I:198:THR:O	1:I:202:LEU:HG	2.13	0.48
1:J:192:HIS:HB3	1:J:195:ASN:HD22	1.78	0.48
1:L:183:ASP:O	1:L:187:ILE:HG13	2.12	0.48
1:A:343:PHE:CE1	1:A:347:ARG:HG3	2.48	0.48
1:C:31:ARG:NE	1:C:54:GLY:HA2	2.28	0.48
1:D:91:HIS:CD2	1:D:93:MET:H	2.32	0.48
1:F:194:LEU:O	1:H:367:PRO:HD2	2.14	0.48
1:F:233:ARG:HH21	1:F:327:ILE:CD1	2.21	0.48
1:F:356:ARG:O	1:F:359:ILE:HG23	2.13	0.48
1:J:347:ARG:HB3	1:J:351:TRP:CE2	2.49	0.48
1:K:335:PRO:HG2	1:K:338:GLU:CG	2.43	0.48
1:L:34:PRO:HB2	1:L:37:THR:HB	1.96	0.48
1:L:303:LYS:O	1:L:306:GLU:HG2	2.13	0.48
1:A:318:TYR:HB3	1:A:319:PRO:HD2	1.95	0.48
1:B:181:ILE:HD13	1:B:286:LEU:HG	1.96	0.48
1:E:144:GLU:O	1:E:147:ARG:HG2	2.13	0.48
1:F:139:LEU:HD12	1:F:140:VAL:N	2.28	0.48
1:H:77:TYR:O	1:H:80:ARG:HG2	2.13	0.48
1:I:245:LYS:H	1:I:245:LYS:HD3	1.78	0.48
1:J:363:ARG:NE	1:J:365:TYR:HA	2.28	0.48
1:K:25:LYS:HD3	1:K:269:TYR:HA	1.94	0.48
1:K:320:ASN:CG	1:K:321:VAL:H	2.17	0.48
1:L:49:LEU:HD11	1:L:65:PHE:HB3	1.94	0.48
1:L:239:GLN:CA	1:L:303:LYS:HB3	2.42	0.48
1:A:86:PHE:CZ	1:C:102:SER:HB2	2.49	0.48
1:A:192:HIS:HE1	1:A:266:HIS:CE1	2.32	0.48
1:C:31:ARG:CD	1:C:54:GLY:HA2	2.44	0.48
1:C:150:TRP:CE2	1:L:74:ARG:HD3	2.49	0.48
1:E:28:LEU:HD23	1:E:35:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:HIS:CD2	1:E:193:THR:H	2.31	0.48
1:E:206:SER:HB2	1:E:363:ARG:O	2.13	0.48
1:F:273:ASP:OD2	1:F:320:ASN:HA	2.14	0.48
1:G:216:SER:O	1:G:219:ILE:HG12	2.13	0.48
1:H:182:MET:HB2	1:H:332:MET:HE1	1.94	0.48
1:I:82:MET:HG2	1:I:86:PHE:CE2	2.48	0.48
1:I:245:LYS:HD3	1:I:245:LYS:N	2.29	0.48
1:K:323:PHE:O	1:K:324:TYR:HB2	2.14	0.48
1:A:241:ILE:O	1:A:244:PRO:HD2	2.14	0.48
1:B:156:LYS:HD2	1:B:159:LEU:HD22	1.95	0.48
1:C:304:LEU:HB3	1:C:324:TYR:CE1	2.48	0.48
1:E:318:TYR:HB3	1:E:319:PRO:HD2	1.95	0.48
1:G:49:LEU:HD11	1:G:65:PHE:HB3	1.96	0.48
1:G:215:ILE:HD11	1:G:352:LEU:HD23	1.95	0.48
1:I:202:LEU:HB3	1:I:365:TYR:CZ	2.49	0.48
1:A:91:HIS:HD2	1:A:93:MET:HB2	1.78	0.48
1:B:96:LEU:HG	1:B:219:ILE:HD13	1.95	0.48
1:E:243:SER:N	1:E:244:PRO:HD2	2.29	0.48
1:F:264:MET:O	1:F:318:TYR:C	2.52	0.48
1:H:239:GLN:H	1:H:239:GLN:CD	2.17	0.48
1:H:323:PHE:O	1:H:324:TYR:HB2	2.13	0.48
1:I:31:ARG:H	1:L:374:SER:HA	1.77	0.48
1:A:277:THR:O	1:A:281:LYS:HD3	2.14	0.48
1:B:366:ARG:NH1	1:B:367:PRO:HD2	2.28	0.48
1:E:166:LEU:HB3	1:E:174:PRO:HB3	1.96	0.48
1:E:356:ARG:O	1:E:359:ILE:HG12	2.14	0.48
1:F:194:LEU:HD12	1:H:367:PRO:HG2	1.95	0.48
1:F:272:LYS:HZ1	1:F:319:PRO:HG3	1.78	0.48
1:F:367:PRO:HG2	1:H:194:LEU:HB3	1.95	0.48
1:H:92:PRO:HA	1:H:143:TRP:CD1	2.49	0.48
1:K:156:LYS:HE3	1:K:167:TYR:CZ	2.48	0.48
1:L:129:THR:HG23	1:L:352:LEU:HB3	1.96	0.48
1:B:324:TYR:HD1	1:B:327:ILE:HD12	1.78	0.47
1:E:266:HIS:HB3	1:E:269:TYR:HB2	1.95	0.47
1:G:72:ASN:HD22	1:G:130:VAL:HG13	1.79	0.47
1:G:202:LEU:HD22	1:G:358:GLN:HB2	1.96	0.47
1:H:233:ARG:O	1:H:235:VAL:HG23	2.14	0.47
1:I:135:GLN:O	1:I:136:MET:C	2.53	0.47
1:A:144:GLU:O	1:A:147:ARG:HG2	2.15	0.47
1:C:281:LYS:C	1:C:281:LYS:HD3	2.34	0.47
1:D:178:MET:HG3	1:D:332:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:VAL:O	1:E:126:ARG:HB3	2.12	0.47
1:L:324:TYR:HA	1:L:327:ILE:HD13	1.95	0.47
1:A:91:HIS:CD2	1:A:93:MET:H	2.32	0.47
1:D:363:ARG:HG3	1:D:365:TYR:H	1.78	0.47
1:G:53:ASP:OD1	1:G:54:GLY:N	2.47	0.47
1:G:320:ASN:H	1:G:323:PHE:HE2	1.61	0.47
1:J:356:ARG:O	1:J:359:ILE:HG12	2.14	0.47
1:K:24:GLU:CG	1:K:25:LYS:H	2.27	0.47
1:A:359:ILE:HG12	1:A:360:SER:N	2.30	0.47
1:B:304:LEU:CG	1:B:327:ILE:HD11	2.39	0.47
1:C:124:TYR:HE2	1:C:211:PRO:HD2	1.80	0.47
1:E:135:GLN:C	1:E:138:PRO:HD2	2.34	0.47
1:F:207:THR:HA	1:H:226:LEU:HB2	1.96	0.47
1:G:33:TYR:CB	1:G:38:LEU:HD21	2.45	0.47
1:A:68:GLN:NE2	1:A:130:VAL:HG11	2.29	0.47
1:A:175:ASP:OD1	1:A:178:MET:HB2	2.14	0.47
1:C:202:LEU:HD21	1:C:354:HIS:CB	2.45	0.47
1:D:86:PHE:CZ	1:E:102:SER:HB2	2.49	0.47
1:D:222:LEU:HD11	1:D:343:PHE:CD2	2.49	0.47
1:E:279:LEU:HD12	1:E:321:VAL:O	2.15	0.47
1:F:27:ILE:HG12	1:F:28:LEU:CD1	2.40	0.47
1:G:79:ILE:HD11	1:G:106:PHE:CE2	2.46	0.47
1:G:137:ALA:HB1	1:G:165:LEU:HG	1.96	0.47
1:I:28:LEU:O	1:I:34:PRO:HA	2.15	0.47
1:K:175:ASP:OD2	1:K:177:LEU:HB3	2.13	0.47
1:L:202:LEU:HD21	1:L:354:HIS:HB3	1.95	0.47
1:L:274:PRO:O	1:L:278:ILE:HG13	2.15	0.47
1:D:177:LEU:O	1:D:181:ILE:HG13	2.15	0.47
1:E:122:LEU:HG	1:E:123:ASP:N	2.29	0.47
1:E:280:HIS:O	1:E:283:VAL:HG22	2.14	0.47
1:E:328:LEU:O	1:E:332:MET:HG3	2.14	0.47
1:F:28:LEU:O	1:F:34:PRO:HA	2.15	0.47
1:I:30:TYR:CE1	1:I:191:GLU:HB3	2.49	0.47
1:J:314:HIS:HD2	1:J:317:VAL:HG23	1.77	0.47
1:L:155:PRO:HG3	1:L:168:MET:SD	2.55	0.47
1:A:142:MET:HA	1:A:152:PRO:HB3	1.96	0.47
1:C:283:VAL:HG21	1:C:327:ILE:HD11	1.97	0.47
1:C:327:ILE:HG13	1:C:328:LEU:N	2.29	0.47
1:D:267:ARG:NH1	1:E:366:ARG:HB3	2.29	0.47
1:E:232:GLN:HG2	1:E:262:TRP:CZ2	2.49	0.47
1:I:31:ARG:CD	1:I:54:GLY:HA2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:100:VAL:HG21	1:K:219:ILE:HD11	1.97	0.47
1:K:196:ALA:HB3	1:K:227:HIS:CD2	2.49	0.47
1:B:222:LEU:HD12	1:B:227:HIS:HD2	1.80	0.47
1:D:49:LEU:HD23	1:D:57:PRO:CB	2.44	0.47
1:F:28:LEU:CB	1:F:35:LEU:H	2.24	0.47
1:H:53:ASP:HB2	1:H:356:ARG:NH1	2.30	0.47
1:H:128:MET:O	1:H:132:ILE:HG13	2.14	0.47
1:I:70:LYS:HE3	1:I:157:HIS:CE1	2.50	0.47
1:I:233:ARG:NE	1:I:326:GLY:HA3	2.30	0.47
1:J:206:SER:HB2	1:J:363:ARG:O	2.15	0.47
1:K:24:GLU:C	1:K:25:LYS:HG3	2.35	0.47
1:L:184:VAL:O	1:L:188:LEU:HD13	2.15	0.47
1:B:53:ASP:OD1	1:B:54:GLY:N	2.47	0.47
1:B:125:VAL:HG23	1:B:126:ARG:N	2.30	0.47
1:B:232:GLN:HG2	1:B:262:TRP:CZ2	2.50	0.47
1:C:159:LEU:HB2	1:C:164:ASN:OD1	2.15	0.47
1:D:206:SER:HB2	1:D:363:ARG:O	2.15	0.47
1:F:272:LYS:NZ	1:F:319:PRO:CD	2.78	0.47
1:G:48:THR:HG22	1:G:349:ALA:CB	2.45	0.47
1:H:182:MET:O	1:H:186:LEU:HG	2.15	0.47
1:I:226:LEU:HD12	1:L:206:SER:O	2.14	0.47
1:K:35:LEU:O	1:K:39:ALA:N	2.45	0.47
1:L:132:ILE:HB	1:L:352:LEU:HD11	1.97	0.47
1:B:177:LEU:O	1:B:181:ILE:HG13	2.15	0.47
1:B:204:ALA:O	1:B:207:THR:HG22	2.14	0.47
1:F:31:ARG:CD	1:F:54:GLY:HA2	2.45	0.47
1:F:266:HIS:HE1	1:F:268:GLU:HB3	1.79	0.47
1:G:358:GLN:OE1	1:G:363:ARG:HB3	2.15	0.47
1:J:272:LYS:HD3	1:J:319:PRO:HD2	1.96	0.47
1:K:169:PHE:HE2	1:K:338:GLU:HG3	1.80	0.47
1:A:27:ILE:HG12	1:A:28:LEU:CD1	2.41	0.46
1:A:47:THR:HG21	1:A:187:ILE:HG23	1.98	0.46
1:A:369:GLN:NE2	1:A:371:TYR:HB3	2.30	0.46
1:B:192:HIS:HB2	1:B:275:ARG:NH1	2.30	0.46
1:C:137:ALA:HB3	1:C:138:PRO:HD3	1.97	0.46
1:F:97:GLN:HG3	1:F:216:SER:O	2.14	0.46
1:H:167:TYR:HA	1:H:172:GLU:O	2.15	0.46
1:J:31:ARG:HG3	1:J:50:LEU:HG	1.97	0.46
1:L:27:ILE:CD1	1:L:269:TYR:HA	2.45	0.46
1:A:184:VAL:O	1:A:188:LEU:HG	2.14	0.46
1:F:47:THR:O	1:F:51:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:LYS:HB2	1:G:159:LEU:HB2	1.97	0.46
1:H:222:LEU:HD13	1:H:227:HIS:CD2	2.47	0.46
1:I:30:TYR:HA	1:L:374:SER:OG	2.15	0.46
1:J:238:LEU:CB	1:J:303:LYS:HE3	2.45	0.46
1:K:31:ARG:HD2	1:K:54:GLY:HA2	1.98	0.46
1:K:278:ILE:O	1:K:282:LEU:HG	2.15	0.46
1:L:239:GLN:CG	1:L:302:LEU:HD13	2.45	0.46
1:B:43:THR:HA	1:B:183:ASP:OD2	2.14	0.46
1:D:102:SER:HB2	1:E:86:PHE:CZ	2.50	0.46
1:D:238:LEU:CD1	1:D:241:ILE:HB	2.45	0.46
1:F:221:THR:HG22	1:H:207:THR:HG21	1.97	0.46
1:F:299:ASP:HA	1:F:303:LYS:HG2	1.98	0.46
1:G:29:SER:HA	1:G:31:ARG:HH22	1.80	0.46
1:J:364:ILE:CG2	1:J:366:ARG:HG2	2.44	0.46
1:K:72:ASN:HD22	1:K:130:VAL:HG13	1.80	0.46
1:L:80:ARG:O	1:L:84:ARG:HG3	2.15	0.46
1:L:182:MET:O	1:L:186:LEU:HG	2.16	0.46
1:D:31:ARG:NE	1:D:54:GLY:HA2	2.31	0.46
1:D:264:MET:O	1:D:320:ASN:HB2	2.15	0.46
1:F:38:LEU:O	1:F:39:ALA:C	2.54	0.46
1:F:334:ILE:HD12	1:F:334:ILE:N	2.30	0.46
1:G:308:CYS:HA	1:G:319:PRO:CG	2.45	0.46
1:H:204:ALA:HB3	1:H:214:VAL:HG13	1.96	0.46
1:H:230:ALA:HA	1:H:233:ARG:HH11	1.81	0.46
1:I:111:GLU:H	1:I:111:GLU:CD	2.19	0.46
1:I:216:SER:HA	1:I:219:ILE:CD1	2.45	0.46
1:J:56:LEU:HD23	1:J:57:PRO:O	2.16	0.46
1:B:25:LYS:HZ2	1:B:27:ILE:HB	1.80	0.46
1:B:308:CYS:O	1:B:311:ARG:HG2	2.16	0.46
1:D:222:LEU:HD11	1:D:343:PHE:CE2	2.51	0.46
1:E:96:LEU:HG	1:E:219:ILE:HD13	1.97	0.46
1:F:264:MET:SD	1:F:319:PRO:HB3	2.55	0.46
1:G:35:LEU:HD11	1:G:188:LEU:HD23	1.97	0.46
1:G:125:VAL:O	1:G:126:ARG:HB3	2.15	0.46
1:I:191:GLU:OE1	1:I:354:HIS:HE1	1.97	0.46
1:J:166:LEU:HB2	1:J:174:PRO:HG3	1.97	0.46
1:K:121:ASP:C	1:K:122:LEU:HD12	2.35	0.46
1:A:25:LYS:HB2	1:A:25:LYS:NZ	2.30	0.46
1:E:156:LYS:HE3	1:E:167:TYR:CE1	2.51	0.46
1:F:347:ARG:HB3	1:F:351:TRP:CE2	2.50	0.46
1:G:347:ARG:HB3	1:G:351:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:LEU:HD11	1:H:188:LEU:HD12	1.97	0.46
1:H:336:GLU:HA	1:H:339:PHE:CZ	2.51	0.46
1:I:25:LYS:HZ1	1:I:274:PRO:HD3	1.77	0.46
1:I:25:LYS:HZ2	1:I:274:PRO:HD3	1.79	0.46
1:I:367:PRO:HB3	1:I:370:ILE:HG23	1.96	0.46
1:A:36:GLU:O	1:A:39:ALA:HB3	2.16	0.46
1:B:334:ILE:H	1:B:334:ILE:HD12	1.80	0.46
1:H:233:ARG:HB3	1:H:233:ARG:NH1	2.30	0.46
1:J:177:LEU:O	1:J:181:ILE:HG13	2.16	0.46
1:A:128:MET:O	1:A:132:ILE:HG13	2.15	0.46
1:A:238:LEU:HB3	1:A:303:LYS:CD	2.46	0.46
1:B:367:PRO:O	1:B:371:TYR:N	2.49	0.46
1:C:38:LEU:O	1:C:42:SER:HB3	2.16	0.46
1:D:229:GLY:CA	1:D:262:TRP:HE1	2.27	0.46
1:G:27:ILE:HG21	1:G:30:TYR:CZ	2.50	0.46
1:G:302:LEU:O	1:G:305:GLU:HG3	2.15	0.46
1:I:67:GLN:HA	1:I:70:LYS:HD3	1.97	0.46
1:I:123:ASP:HB2	1:I:127:ASN:ND2	2.30	0.46
1:J:184:VAL:O	1:J:188:LEU:HG	2.16	0.46
1:K:338:GLU:O	1:K:342:LEU:HG	2.15	0.46
1:L:78:HIS:HB2	1:L:106:PHE:HZ	1.81	0.46
1:A:278:ILE:O	1:A:282:LEU:HG	2.16	0.46
1:A:335:PRO:HG2	1:A:338:GLU:CG	2.46	0.46
1:B:80:ARG:O	1:B:84:ARG:HG3	2.15	0.46
1:B:126:ARG:NE	1:B:126:ARG:HA	2.31	0.46
1:B:307:VAL:HG13	1:B:323:PHE:CZ	2.44	0.46
1:D:267:ARG:HD2	1:E:366:ARG:HB3	1.98	0.46
1:G:33:TYR:CE1	1:G:50:LEU:HD11	2.51	0.46
1:H:67:GLN:HE22	1:H:157:HIS:CE1	2.34	0.46
1:H:124:TYR:O	1:H:128:MET:HG2	2.16	0.46
1:I:356:ARG:O	1:I:359:ILE:HG23	2.16	0.46
1:K:280:HIS:HB2	1:K:324:TYR:CZ	2.51	0.46
1:E:215:ILE:O	1:E:219:ILE:HG13	2.15	0.46
1:F:86:PHE:CE1	1:H:102:SER:HB2	2.51	0.46
1:G:133:ILE:HG13	1:G:352:LEU:CD1	2.46	0.46
1:H:35:LEU:O	1:H:39:ALA:N	2.47	0.46
1:H:215:ILE:O	1:H:219:ILE:HG13	2.16	0.46
1:I:27:ILE:HB	1:I:274:PRO:HG3	1.97	0.46
1:K:24:GLU:HB2	1:K:25:LYS:NZ	2.31	0.46
1:L:113:LEU:HG	1:L:119:CYS:HB3	1.97	0.46
1:A:196:ALA:HB3	1:A:227:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:SER:O	1:C:226:LEU:HD12	2.16	0.45
1:A:211:PRO:O	1:A:215:ILE:HG12	2.15	0.45
1:A:232:GLN:HB3	1:A:262:TRP:CD2	2.51	0.45
1:D:366:ARG:HH22	1:E:192:HIS:CE1	2.34	0.45
1:F:75:ILE:HD11	1:F:138:PRO:CB	2.46	0.45
1:J:53:ASP:OD1	1:J:54:GLY:N	2.49	0.45
1:J:312:LEU:H	1:J:312:LEU:CD1	2.27	0.45
1:K:52:LEU:HD13	1:K:126:ARG:HH12	1.80	0.45
1:K:65:PHE:CZ	1:K:69:LEU:HD12	2.51	0.45
1:K:123:ASP:CG	1:K:124:TYR:H	2.18	0.45
1:K:178:MET:HA	1:K:181:ILE:HD12	1.97	0.45
1:A:234:VAL:HG21	1:A:339:PHE:CE2	2.52	0.45
1:B:185:CYS:O	1:B:189:HIS:HD2	1.99	0.45
1:G:370:ILE:HG23	1:G:375:ASP:HB2	1.96	0.45
1:I:181:ILE:HG21	1:I:328:LEU:HD11	1.97	0.45
1:B:192:HIS:CD2	1:B:195:ASN:HD21	2.29	0.45
1:B:238:LEU:HD23	1:B:238:LEU:H	1.81	0.45
1:C:25:LYS:HD2	1:C:25:LYS:N	2.32	0.45
1:C:28:LEU:CA	1:C:35:LEU:HD13	2.35	0.45
1:F:181:ILE:HG23	1:F:282:LEU:HD22	1.98	0.45
1:G:70:LYS:HB3	1:G:157:HIS:CD2	2.52	0.45
1:I:301:ALA:HA	1:I:304:LEU:CD2	2.46	0.45
1:J:36:GLU:H	1:J:36:GLU:CD	2.19	0.45
1:K:48:THR:O	1:K:52:LEU:HG	2.17	0.45
1:L:363:ARG:HG2	1:L:365:TYR:H	1.81	0.45
1:A:230:ALA:HA	1:A:322:ASP:HB3	1.98	0.45
1:H:75:ILE:HD11	1:H:138:PRO:HB2	1.98	0.45
1:H:132:ILE:O	1:H:136:MET:HG2	2.16	0.45
1:I:245:LYS:HG2	1:I:247:VAL:H	1.81	0.45
1:K:81:GLN:O	1:K:85:HIS:HD2	1.99	0.45
1:K:301:ALA:O	1:K:305:GLU:HG2	2.16	0.45
1:A:69:LEU:HD12	1:A:134:ALA:HB2	1.99	0.45
1:D:69:LEU:HD12	1:D:134:ALA:HB2	1.98	0.45
1:D:185:CYS:O	1:D:189:HIS:HD2	1.99	0.45
1:E:70:LYS:O	1:E:71:ASP:HB2	2.17	0.45
1:F:267:ARG:HH21	1:H:363:ARG:NE	2.05	0.45
1:G:269:TYR:CD2	1:G:274:PRO:HD2	2.51	0.45
1:H:110:THR:HG22	1:H:112:CYS:H	1.82	0.45
1:I:305:GLU:HA	1:I:308:CYS:SG	2.56	0.45
1:K:159:LEU:HD11	1:K:173:GLU:HG2	1.98	0.45
1:D:43:THR:HA	1:D:187:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HD21	1:D:120:GLU:HG3	1.97	0.45
1:F:321:VAL:HG23	1:F:322:ASP:N	2.31	0.45
1:G:29:SER:HA	1:G:31:ARG:NH2	2.31	0.45
1:I:183:ASP:O	1:I:187:ILE:HG13	2.17	0.45
1:I:233:ARG:HE	1:I:339:PHE:HE2	1.64	0.45
1:L:181:ILE:HD12	1:L:282:LEU:HD22	1.99	0.45
1:D:36:GLU:OE1	1:D:36:GLU:N	2.49	0.45
1:J:133:ILE:CG1	1:J:352:LEU:HD12	2.47	0.45
1:J:247:VAL:O	1:J:248:GLU:C	2.54	0.45
1:K:44:PHE:CZ	1:K:346:ALA:HA	2.51	0.45
1:K:75:ILE:HD11	1:K:138:PRO:CB	2.46	0.45
1:C:125:VAL:O	1:C:126:ARG:HB3	2.17	0.45
1:F:271:VAL:O	1:F:272:LYS:HB2	2.17	0.45
1:F:370:ILE:HD12	1:F:370:ILE:N	2.32	0.45
1:G:75:ILE:HD13	1:G:135:GLN:OE1	2.16	0.45
1:G:122:LEU:HD13	1:G:124:TYR:H	1.82	0.45
1:G:144:GLU:HG2	1:G:147:ARG:HH21	1.81	0.45
1:H:36:GLU:H	1:H:36:GLU:CD	2.20	0.45
1:J:44:PHE:CD1	1:J:186:LEU:HB3	2.52	0.45
1:J:60:LYS:HB3	1:J:60:LYS:HE3	1.76	0.45
1:J:233:ARG:NE	1:J:263:GLY:HA3	2.32	0.45
1:J:323:PHE:HD2	1:J:324:TYR:CZ	2.35	0.45
1:J:372:VAL:O	1:J:375:ASP:HB2	2.17	0.45
1:A:78:HIS:HA	1:A:81:GLN:NE2	2.32	0.45
1:B:266:HIS:HE1	1:B:268:GLU:HB2	1.82	0.45
1:E:206:SER:HB3	1:E:365:TYR:HD1	1.82	0.45
1:I:27:ILE:HD12	1:I:274:PRO:HG3	1.98	0.45
1:I:125:VAL:HG22	1:I:355:TRP:CH2	2.52	0.45
1:J:103:LEU:HG	1:J:107:TYR:HE1	1.82	0.45
1:J:133:ILE:HG13	1:J:352:LEU:CD1	2.47	0.45
1:A:156:LYS:HB3	1:A:158:ASP:OD1	2.17	0.45
1:B:63:ASN:O	1:B:67:GLN:HG2	2.17	0.45
1:F:185:CYS:O	1:F:189:HIS:HD2	1.99	0.45
1:H:142:MET:HA	1:H:152:PRO:HB3	1.98	0.45
1:I:27:ILE:HG13	1:I:28:LEU:HD13	1.98	0.45
1:I:241:ILE:HG22	1:I:244:PRO:HD3	1.98	0.45
1:J:69:LEU:HD12	1:J:134:ALA:HB2	1.99	0.45
1:J:218:ALA:HB1	1:J:351:TRP:CE2	2.52	0.45
1:J:233:ARG:O	1:J:235:VAL:HG12	2.17	0.45
1:J:279:LEU:HA	1:J:282:LEU:HD12	1.99	0.45
1:L:156:LYS:HE3	1:L:159:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:300:THR:O	1:L:304:LEU:HD23	2.17	0.45
1:A:192:HIS:CE1	1:C:366:ARG:HH22	2.35	0.44
1:C:28:LEU:O	1:C:34:PRO:HA	2.17	0.44
1:C:269:TYR:CE1	1:C:273:ASP:HB2	2.53	0.44
1:F:192:HIS:HE1	1:F:266:HIS:CE1	2.35	0.44
1:J:57:PRO:HB2	1:J:61:ALA:HB3	1.98	0.44
1:L:239:GLN:HG2	1:L:302:LEU:HD13	2.00	0.44
1:B:113:LEU:HA	1:B:119:CYS:HB3	1.99	0.44
1:C:38:LEU:O	1:C:39:ALA:C	2.55	0.44
1:D:27:ILE:CG1	1:D:28:LEU:HD13	2.47	0.44
1:E:71:ASP:CG	1:E:157:HIS:HE1	2.21	0.44
1:E:113:LEU:HD21	1:E:120:GLU:HB3	1.99	0.44
1:G:192:HIS:HB3	1:G:347:ARG:HH22	1.82	0.44
1:H:35:LEU:HA	1:H:38:LEU:HB2	1.99	0.44
1:I:49:LEU:HD13	1:I:57:PRO:HB3	1.98	0.44
1:J:310:ASP:HB2	1:J:314:HIS:CE1	2.52	0.44
1:L:50:LEU:HB2	1:L:56:LEU:HD23	1.99	0.44
1:A:269:TYR:C	1:A:271:VAL:N	2.71	0.44
1:B:133:ILE:HG13	1:B:352:LEU:HD12	2.00	0.44
1:B:158:ASP:HB2	1:F:315:LYS:HG2	1.99	0.44
1:C:238:LEU:HD12	1:C:238:LEU:N	2.33	0.44
1:E:36:GLU:N	1:E:36:GLU:OE1	2.51	0.44
1:E:192:HIS:HB2	1:E:347:ARG:NH2	2.32	0.44
1:E:287:VAL:HG11	1:E:305:GLU:OE1	2.17	0.44
1:F:195:ASN:HB2	1:F:227:HIS:NE2	2.33	0.44
1:I:159:LEU:HB2	1:I:164:ASN:OD1	2.17	0.44
1:I:160:SER:N	1:I:163:GLU:HB2	2.32	0.44
1:J:239:GLN:O	1:J:241:ILE:HG13	2.17	0.44
1:K:103:LEU:HG	1:K:107:TYR:HE1	1.82	0.44
1:B:31:ARG:HB2	1:B:50:LEU:HD21	1.98	0.44
1:E:192:HIS:HD2	1:E:193:THR:H	1.65	0.44
1:G:334:ILE:HG21	1:G:342:LEU:CD1	2.47	0.44
1:H:127:ASN:O	1:H:130:VAL:HG22	2.17	0.44
1:I:356:ARG:O	1:I:359:ILE:HG12	2.17	0.44
1:J:374:SER:O	1:J:375:ASP:C	2.56	0.44
1:C:273:ASP:OD2	1:C:275:ARG:HB2	2.17	0.44
1:E:264:MET:HG2	1:E:319:PRO:CA	2.44	0.44
1:G:63:ASN:O	1:G:67:GLN:HG2	2.17	0.44
1:G:192:HIS:HB3	1:G:347:ARG:NH2	2.32	0.44
1:G:274:PRO:O	1:G:278:ILE:HG13	2.17	0.44
1:H:329:TYR:HB2	1:H:339:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:SER:O	1:I:219:ILE:HG12	2.18	0.44
1:L:83:MET:HG2	1:L:95:MET:CE	2.47	0.44
1:L:239:GLN:HB3	1:L:302:LEU:HB3	1.99	0.44
1:B:192:HIS:HB3	1:B:347:ARG:NH2	2.32	0.44
1:C:30:TYR:CE1	1:C:191:GLU:HB3	2.53	0.44
1:E:338:GLU:O	1:E:342:LEU:HG	2.18	0.44
1:F:128:MET:O	1:F:132:ILE:HG13	2.18	0.44
1:F:233:ARG:HH11	1:F:234:VAL:HA	1.81	0.44
1:G:184:VAL:O	1:G:188:LEU:HG	2.18	0.44
1:J:327:ILE:HD12	1:J:327:ILE:N	2.31	0.44
1:A:78:HIS:HE1	1:I:149:GLY:HA2	1.83	0.44
1:B:75:ILE:HG21	1:B:142:MET:CE	2.48	0.44
1:B:156:LYS:HB3	1:B:158:ASP:OD1	2.18	0.44
1:B:192:HIS:CG	1:B:192:HIS:O	2.70	0.44
1:C:272:LYS:HG3	1:C:318:TYR:O	2.17	0.44
1:E:329:TYR:HB3	1:E:339:PHE:CE1	2.52	0.44
1:F:220:GLY:HA2	1:F:223:SER:HB3	1.99	0.44
1:H:202:LEU:HB3	1:H:358:GLN:OE1	2.17	0.44
1:J:124:TYR:CD2	1:J:128:MET:HG3	2.53	0.44
1:K:92:PRO:HA	1:K:143:TRP:CD1	2.53	0.44
1:K:300:THR:O	1:K:304:LEU:HD23	2.18	0.44
1:A:82:MET:HG3	1:A:83:MET:N	2.32	0.44
1:C:28:LEU:HB3	1:C:34:PRO:HA	2.00	0.44
1:E:238:LEU:N	1:E:241:ILE:HG12	2.32	0.44
1:G:34:PRO:HG2	1:G:37:THR:CG2	2.48	0.44
1:G:220:GLY:O	1:G:223:SER:HB3	2.17	0.44
1:H:76:LYS:HB2	1:H:79:ILE:HG12	1.99	0.44
1:J:72:ASN:HD22	1:J:130:VAL:HG13	1.82	0.44
1:K:301:ALA:HA	1:K:304:LEU:HB2	1.99	0.44
1:B:264:MET:HA	1:B:320:ASN:H	1.83	0.44
1:D:124:TYR:HE2	1:D:211:PRO:CD	2.31	0.44
1:F:271:VAL:O	1:F:318:TYR:CG	2.71	0.44
1:H:30:TYR:CD1	1:H:51:LEU:HD21	2.52	0.44
1:I:25:LYS:HE2	1:I:271:VAL:HG21	2.00	0.44
1:I:50:LEU:O	1:I:54:GLY:N	2.50	0.44
1:I:221:THR:O	1:L:207:THR:HG21	2.18	0.44
1:L:178:MET:SD	1:L:332:MET:HG2	2.58	0.44
1:C:304:LEU:HD12	1:C:327:ILE:HG21	1.98	0.43
1:F:28:LEU:HG	1:F:36:GLU:OE2	2.18	0.43
1:H:120:GLU:N	1:H:120:GLU:OE1	2.50	0.43
1:H:222:LEU:HD11	1:H:343:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:GLN:CD	1:J:130:VAL:HG11	2.38	0.43
1:K:34:PRO:O	1:K:38:LEU:HG	2.17	0.43
1:K:184:VAL:O	1:K:188:LEU:HD13	2.17	0.43
1:L:144:GLU:HG2	1:L:147:ARG:NH2	2.32	0.43
1:A:166:LEU:N	1:A:166:LEU:HD12	2.33	0.43
1:D:28:LEU:CB	1:D:35:LEU:H	2.30	0.43
1:D:243:SER:HA	1:D:245:LYS:NZ	2.33	0.43
1:E:72:ASN:ND2	1:E:130:VAL:HG13	2.33	0.43
1:F:86:PHE:HB3	1:F:87:PRO:HD2	2.00	0.43
1:F:144:GLU:HA	1:F:147:ARG:HE	1.82	0.43
1:F:148:ASN:HB2	1:F:150:TRP:CD1	2.53	0.43
1:F:304:LEU:HD22	1:F:304:LEU:N	2.33	0.43
1:H:206:SER:HB3	1:H:365:TYR:HD1	1.82	0.43
1:H:355:TRP:O	1:H:359:ILE:HG12	2.17	0.43
1:I:283:VAL:HA	1:I:286:LEU:HD12	1.99	0.43
1:K:274:PRO:O	1:K:278:ILE:HG13	2.18	0.43
1:L:35:LEU:O	1:L:39:ALA:N	2.40	0.43
1:L:319:PRO:HB3	1:L:323:PHE:CD2	2.53	0.43
1:A:44:PHE:CE1	1:A:346:ALA:HA	2.53	0.43
1:E:177:LEU:HD22	1:E:177:LEU:N	2.30	0.43
1:F:104:GLY:C	1:F:106:PHE:H	2.21	0.43
1:F:206:SER:HA	1:F:361:ASP:OD1	2.18	0.43
1:G:80:ARG:O	1:G:84:ARG:HG3	2.17	0.43
1:G:238:LEU:HD22	1:G:245:LYS:NZ	2.33	0.43
1:H:239:GLN:H	1:H:239:GLN:NE2	2.16	0.43
1:I:83:MET:SD	1:I:142:MET:HE3	2.58	0.43
1:I:233:ARG:NE	1:I:339:PHE:HE2	2.16	0.43
1:I:243:SER:HB2	1:I:244:PRO:HD3	2.00	0.43
1:J:300:THR:O	1:J:304:LEU:HD22	2.18	0.43
1:K:182:MET:O	1:K:186:LEU:HD13	2.18	0.43
1:A:207:THR:CG2	1:C:227:HIS:HB2	2.49	0.43
1:B:44:PHE:CZ	1:B:346:ALA:HA	2.53	0.43
1:B:44:PHE:CD1	1:B:186:LEU:HB3	2.53	0.43
1:B:224:GLY:O	1:B:228:GLY:N	2.51	0.43
1:B:231:ASN:O	1:B:234:VAL:HG12	2.17	0.43
1:E:34:PRO:O	1:E:38:LEU:HG	2.19	0.43
1:F:357:GLU:OE2	1:H:372:VAL:HG23	2.19	0.43
1:G:216:SER:HA	1:G:219:ILE:HD11	1.99	0.43
1:G:270:LYS:HG3	1:G:271:VAL:HG13	2.00	0.43
1:I:202:LEU:HD21	1:I:354:HIS:HB3	2.00	0.43
1:J:238:LEU:HB3	1:J:242:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:135:GLN:O	1:K:139:LEU:HG	2.18	0.43
1:A:269:TYR:C	1:A:271:VAL:H	2.21	0.43
1:B:184:VAL:O	1:B:188:LEU:HD13	2.18	0.43
1:B:347:ARG:HB3	1:B:351:TRP:CE2	2.53	0.43
1:C:182:MET:O	1:C:186:LEU:HD13	2.19	0.43
1:D:25:LYS:C	1:D:27:ILE:H	2.21	0.43
1:E:193:THR:O	1:E:195:ASN:N	2.45	0.43
1:F:182:MET:O	1:F:186:LEU:HG	2.19	0.43
1:H:124:TYR:HE2	1:H:211:PRO:HD2	1.83	0.43
1:H:358:GLN:HE21	1:H:358:GLN:HB3	1.51	0.43
1:J:122:LEU:HD12	1:J:127:ASN:HD22	1.83	0.43
1:J:233:ARG:HD2	1:J:323:PHE:HA	2.00	0.43
1:K:230:ALA:CA	1:K:233:ARG:HH22	2.31	0.43
1:C:332:MET:HB2	1:C:334:ILE:HD13	1.99	0.43
1:D:128:MET:O	1:D:132:ILE:HG13	2.19	0.43
1:E:336:GLU:HA	1:E:339:PHE:CE1	2.53	0.43
1:F:340:THR:O	1:F:343:PHE:HB3	2.19	0.43
1:I:112:CYS:SG	1:I:113:LEU:N	2.91	0.43
1:K:40:GLU:HG2	1:K:41:ASN:CG	2.39	0.43
1:L:135:GLN:C	1:L:138:PRO:HD2	2.39	0.43
1:L:177:LEU:HD22	1:L:177:LEU:N	2.32	0.43
1:A:232:GLN:HB3	1:A:262:TRP:CE2	2.54	0.43
1:B:69:LEU:HD12	1:B:134:ALA:HB2	2.01	0.43
1:B:222:LEU:CD1	1:B:227:HIS:HD2	2.32	0.43
1:C:222:LEU:CD2	1:C:343:PHE:HD2	2.32	0.43
1:D:68:GLN:CG	1:D:130:VAL:HG11	2.47	0.43
1:E:238:LEU:HB3	1:E:241:ILE:CG2	2.48	0.43
1:E:271:VAL:HG22	1:E:272:LYS:N	2.30	0.43
1:F:366:ARG:H	1:H:267:ARG:NH1	2.16	0.43
1:G:241:ILE:O	1:G:244:PRO:HD2	2.19	0.43
1:G:299:ASP:O	1:G:303:LYS:HB3	2.18	0.43
1:H:25:LYS:HE3	1:H:270:LYS:HG2	2.00	0.43
1:H:311:ARG:O	1:H:312:LEU:C	2.56	0.43
1:J:165:LEU:O	1:J:169:PHE:HB2	2.19	0.43
1:L:111:GLU:OE2	1:L:208:LEU:HB3	2.19	0.43
1:C:43:THR:HG23	1:C:46:GLU:H	1.84	0.43
1:C:175:ASP:OD1	1:C:178:MET:HG2	2.18	0.43
1:E:28:LEU:HD22	1:E:275:ARG:HD2	2.00	0.43
1:E:367:PRO:HB2	1:E:369:GLN:HE21	1.83	0.43
1:H:34:PRO:O	1:H:38:LEU:HG	2.17	0.43
1:H:279:LEU:HD23	1:H:282:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:340:THR:O	1:H:343:PHE:HB3	2.17	0.43
1:B:235:VAL:C	1:B:303:LYS:HZ2	2.21	0.43
1:C:203:VAL:HA	1:C:365:TYR:HD2	1.83	0.43
1:D:324:TYR:HD1	1:D:327:ILE:HD11	1.83	0.43
1:E:192:HIS:HB2	1:E:347:ARG:CZ	2.49	0.43
1:I:207:THR:HA	1:L:226:LEU:HB2	2.01	0.43
1:K:211:PRO:HG3	1:K:355:TRP:CZ2	2.54	0.43
1:L:327:ILE:H	1:L:327:ILE:CD1	2.28	0.43
1:B:334:ILE:HD12	1:B:334:ILE:N	2.33	0.43
1:E:31:ARG:CD	1:E:54:GLY:HA2	2.48	0.43
1:E:308:CYS:SG	1:E:327:ILE:HD11	2.59	0.43
1:F:92:PRO:HG2	1:F:337:ASP:O	2.17	0.43
1:H:55:GLU:O	1:H:56:LEU:C	2.57	0.43
1:K:49:LEU:HD11	1:K:65:PHE:CB	2.49	0.43
1:L:361:ASP:OD1	1:L:362:ASN:N	2.52	0.43
1:A:186:LEU:O	1:A:346:ALA:HB1	2.19	0.42
1:A:300:THR:O	1:A:304:LEU:HD23	2.19	0.42
1:B:183:ASP:O	1:B:187:ILE:HG13	2.18	0.42
1:D:273:ASP:CG	1:D:275:ARG:HE	2.22	0.42
1:G:30:TYR:HB3	1:G:33:TYR:O	2.19	0.42
1:H:142:MET:HG3	1:H:152:PRO:CG	2.49	0.42
1:J:144:GLU:OE1	1:J:147:ARG:NH2	2.52	0.42
1:A:235:VAL:HG13	1:A:235:VAL:O	2.19	0.42
1:C:65:PHE:CE2	1:C:69:LEU:HD11	2.54	0.42
1:F:201:ALA:HA	1:F:214:VAL:HG13	2.00	0.42
1:G:39:ALA:HB1	1:G:184:VAL:HG13	2.01	0.42
1:G:370:ILE:HG23	1:G:375:ASP:H	1.84	0.42
1:H:183:ASP:O	1:H:187:ILE:HG13	2.20	0.42
1:K:44:PHE:CG	1:K:186:LEU:HB3	2.53	0.42
1:K:231:ASN:HD21	1:K:340:THR:H	1.67	0.42
1:L:185:CYS:O	1:L:189:HIS:HD2	2.02	0.42
1:L:232:GLN:OE1	1:L:232:GLN:N	2.49	0.42
1:A:350:GLY:O	1:A:354:HIS:HD2	2.02	0.42
1:B:38:LEU:O	1:B:39:ALA:C	2.55	0.42
1:C:28:LEU:HG	1:C:35:LEU:HB2	2.01	0.42
1:C:82:MET:O	1:C:86:PHE:HD1	2.02	0.42
1:D:111:GLU:O	1:D:113:LEU:HG	2.19	0.42
1:F:323:PHE:HD2	1:F:324:TYR:HE1	1.63	0.42
1:G:132:ILE:O	1:G:136:MET:HG2	2.19	0.42
1:I:29:SER:HB2	1:L:375:ASP:OD1	2.19	0.42
1:J:233:ARG:NH1	1:J:262:TRP:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:25:LYS:HE3	1:K:270:LYS:H	1.84	0.42
1:L:128:MET:O	1:L:132:ILE:HG13	2.19	0.42
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.91	0.42
1:D:75:ILE:HD11	1:D:138:PRO:HB2	2.01	0.42
1:E:239:GLN:NE2	1:E:307:VAL:HA	2.35	0.42
1:G:233:ARG:HD3	1:G:233:ARG:C	2.40	0.42
1:H:271:VAL:HG22	1:H:272:LYS:N	2.32	0.42
1:H:371:TYR:CG	1:H:371:TYR:O	2.72	0.42
1:I:268:GLU:HG3	1:L:366:ARG:NH1	2.35	0.42
1:A:208:LEU:HD12	1:C:226:LEU:HD21	2.02	0.42
1:B:239:GLN:HG2	1:B:298:PHE:HE1	1.79	0.42
1:E:25:LYS:HA	1:E:25:LYS:CE	2.49	0.42
1:F:176:PRO:O	1:F:180:LYS:HG3	2.20	0.42
1:F:273:ASP:CG	1:F:275:ARG:HE	2.23	0.42
1:G:52:LEU:HD23	1:G:353:ALA:HA	2.00	0.42
1:H:135:GLN:C	1:H:138:PRO:HD2	2.40	0.42
1:I:230:ALA:O	1:I:233:ARG:HD2	2.19	0.42
1:J:341:ALA:O	1:J:345:VAL:HG23	2.20	0.42
1:J:372:VAL:HG12	1:J:374:SER:H	1.84	0.42
1:K:42:SER:HA	1:K:46:GLU:OE2	2.19	0.42
1:K:111:GLU:H	1:K:111:GLU:CD	2.23	0.42
1:K:222:LEU:O	1:K:222:LEU:HD23	2.19	0.42
1:L:352:LEU:O	1:L:355:TRP:HB3	2.20	0.42
1:A:121:ASP:C	1:A:122:LEU:HD12	2.40	0.42
1:B:247:VAL:O	1:B:248:GLU:C	2.58	0.42
1:B:300:THR:O	1:B:305:GLU:HG3	2.19	0.42
1:C:30:TYR:CD1	1:C:35:LEU:HD11	2.55	0.42
1:C:70:LYS:HE3	1:C:157:HIS:NE2	2.35	0.42
1:D:356:ARG:O	1:D:359:ILE:HG23	2.19	0.42
1:E:238:LEU:H	1:E:241:ILE:CD1	2.33	0.42
1:E:271:VAL:HA	1:E:318:TYR:CD2	2.54	0.42
1:G:335:PRO:HG2	1:G:338:GLU:CG	2.50	0.42
1:H:30:TYR:CE2	1:H:35:LEU:HD13	2.54	0.42
1:I:36:GLU:OE1	1:I:36:GLU:N	2.53	0.42
1:I:77:TYR:HE2	1:I:81:GLN:HE21	1.65	0.42
1:L:281:LYS:NZ	1:L:282:LEU:HG	2.35	0.42
1:A:239:GLN:HG3	1:A:241:ILE:HD11	2.02	0.42
1:B:278:ILE:O	1:B:282:LEU:HG	2.19	0.42
1:D:271:VAL:HG22	1:D:272:LYS:N	2.33	0.42
1:E:66:SER:O	1:E:70:LYS:HG3	2.19	0.42
1:E:156:LYS:HB3	1:E:158:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:TYR:O	1:E:171:GLY:N	2.52	0.42
1:F:27:ILE:O	1:F:28:LEU:C	2.56	0.42
1:F:31:ARG:HD3	1:H:374:SER:HB2	2.02	0.42
1:H:275:ARG:HB3	1:H:321:VAL:HG23	2.02	0.42
1:J:166:LEU:HB3	1:J:174:PRO:HB3	2.02	0.42
1:J:312:LEU:HD12	1:J:312:LEU:N	2.29	0.42
1:K:334:ILE:HD12	1:K:334:ILE:N	2.34	0.42
1:B:192:HIS:HB2	1:B:275:ARG:HH12	1.85	0.42
1:C:31:ARG:HG3	1:C:50:LEU:O	2.19	0.42
1:C:231:ASN:CG	1:C:336:GLU:HB3	2.40	0.42
1:C:347:ARG:HD3	1:C:347:ARG:HA	1.86	0.42
1:D:207:THR:HA	1:E:226:LEU:HB2	2.01	0.42
1:E:28:LEU:CD2	1:E:275:ARG:HD2	2.49	0.42
1:E:70:LYS:HD3	1:E:157:HIS:CD2	2.55	0.42
1:J:177:LEU:HD22	1:J:177:LEU:N	2.30	0.42
1:K:156:LYS:HE3	1:K:167:TYR:CE2	2.54	0.42
1:K:198:THR:O	1:K:202:LEU:HG	2.19	0.42
1:K:214:VAL:CG2	1:K:215:ILE:N	2.83	0.42
1:L:239:GLN:HG3	1:L:299:ASP:HA	1.99	0.42
1:B:275:ARG:O	1:B:279:LEU:HG	2.19	0.42
1:C:42:SER:HA	1:C:46:GLU:OE1	2.20	0.42
1:D:301:ALA:H	1:D:304:LEU:HD23	1.85	0.42
1:F:35:LEU:HD11	1:F:188:LEU:HD12	2.02	0.42
1:F:135:GLN:C	1:F:138:PRO:HD2	2.40	0.42
1:H:76:LYS:HE2	1:H:107:TYR:OH	2.20	0.42
1:I:135:GLN:O	1:I:139:LEU:HG	2.20	0.42
1:I:368:THR:O	1:I:371:TYR:HD1	2.03	0.42
1:K:60:LYS:HZ3	1:K:64:ASP:CG	2.22	0.42
1:L:68:GLN:HG2	1:L:72:ASN:ND2	2.35	0.42
1:L:181:ILE:CG1	1:L:286:LEU:HD11	2.46	0.42
1:L:303:LYS:HA	1:L:306:GLU:HG2	2.02	0.42
1:A:271:VAL:HG22	1:A:272:LYS:N	2.33	0.42
1:B:25:LYS:HZ1	1:B:27:ILE:HD12	1.83	0.42
1:C:144:GLU:OE1	1:C:147:ARG:NH2	2.53	0.42
1:C:183:ASP:O	1:C:186:LEU:HB2	2.19	0.42
1:F:27:ILE:HG12	1:F:28:LEU:N	2.35	0.42
1:G:128:MET:O	1:G:132:ILE:HG13	2.19	0.42
1:J:72:ASN:ND2	1:J:130:VAL:HG13	2.35	0.42
1:L:159:LEU:HA	1:L:163:GLU:OE1	2.20	0.42
1:L:181:ILE:HG13	1:L:286:LEU:HD21	2.02	0.42
1:A:337:ASP:OD1	1:A:337:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ARG:CZ	1:C:322:ASP:O	2.68	0.41
1:D:135:GLN:C	1:D:138:PRO:HD2	2.40	0.41
1:I:38:LEU:O	1:I:39:ALA:C	2.58	0.41
1:J:76:LYS:HE3	1:J:106:PHE:HB3	2.02	0.41
1:J:347:ARG:HB3	1:J:351:TRP:CZ2	2.55	0.41
1:L:122:LEU:HD22	1:L:123:ASP:H	1.85	0.41
1:B:47:THR:O	1:B:51:LEU:HG	2.20	0.41
1:C:48:THR:O	1:C:52:LEU:HG	2.20	0.41
1:D:226:LEU:HD22	1:E:208:LEU:HG	2.02	0.41
1:E:279:LEU:HD23	1:E:282:LEU:HD12	2.02	0.41
1:E:315:LYS:O	1:E:315:LYS:HD3	2.20	0.41
1:F:189:HIS:HB3	1:F:343:PHE:CE1	2.54	0.41
1:G:196:ALA:HB3	1:G:227:HIS:CD2	2.50	0.41
1:G:239:GLN:HE21	1:G:239:GLN:HB2	1.66	0.41
1:J:112:CYS:SG	1:J:113:LEU:N	2.93	0.41
1:L:110:THR:HG22	1:L:113:LEU:H	1.85	0.41
1:L:122:LEU:HD13	1:L:123:ASP:H	1.84	0.41
1:L:327:ILE:HD12	1:L:327:ILE:N	2.28	0.41
1:A:47:THR:O	1:A:51:LEU:HG	2.19	0.41
1:A:166:LEU:CB	1:A:174:PRO:HG3	2.50	0.41
1:E:336:GLU:HA	1:E:339:PHE:CD1	2.56	0.41
1:F:367:PRO:HD2	1:H:194:LEU:O	2.21	0.41
1:H:49:LEU:HD13	1:H:65:PHE:CD1	2.56	0.41
1:I:66:SER:O	1:I:70:LYS:HG3	2.20	0.41
1:I:336:GLU:HA	1:I:339:PHE:CD1	2.55	0.41
1:I:336:GLU:HA	1:I:339:PHE:CE1	2.55	0.41
1:J:363:ARG:CG	1:J:365:TYR:H	2.22	0.41
1:K:241:ILE:C	1:K:244:PRO:HD2	2.41	0.41
1:L:93:MET:HE1	1:L:344:ALA:HB2	2.01	0.41
1:L:199:PHE:HD1	1:L:202:LEU:HD12	1.85	0.41
1:A:110:THR:HG22	1:A:112:CYS:H	1.85	0.41
1:C:70:LYS:HA	1:C:73:TYR:CD2	2.55	0.41
1:C:269:TYR:CZ	1:C:273:ASP:HB2	2.56	0.41
1:D:299:ASP:O	1:D:303:LYS:HD3	2.21	0.41
1:E:138:PRO:HA	1:E:168:MET:CE	2.50	0.41
1:E:206:SER:HB3	1:E:365:TYR:CD1	2.56	0.41
1:E:206:SER:CB	1:E:365:TYR:HD1	2.34	0.41
1:E:247:VAL:O	1:E:248:GLU:HG2	2.21	0.41
1:F:366:ARG:HH22	1:H:192:HIS:CE1	2.39	0.41
1:F:367:PRO:HG3	1:H:199:PHE:CG	2.55	0.41
1:G:190:ALA:O	1:G:347:ARG:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:LYS:HB3	1:G:272:LYS:HZ3	1.85	0.41
1:I:211:PRO:O	1:I:215:ILE:HG12	2.21	0.41
1:I:222:LEU:HD11	1:I:351:TRP:CZ2	2.55	0.41
1:I:300:THR:N	1:I:303:LYS:HD3	2.36	0.41
1:K:24:GLU:HB2	1:K:25:LYS:HZ3	1.86	0.41
1:L:68:GLN:HG2	1:L:72:ASN:HD21	1.85	0.41
1:L:334:ILE:CG2	1:L:342:LEU:HD11	2.46	0.41
1:D:111:GLU:H	1:D:111:GLU:CD	2.21	0.41
1:G:34:PRO:O	1:G:38:LEU:HG	2.21	0.41
1:G:226:LEU:HD12	1:G:226:LEU:N	2.33	0.41
1:I:306:GLU:HG2	1:I:311:ARG:HD3	2.01	0.41
1:K:323:PHE:HD1	1:K:324:TYR:CD2	2.38	0.41
1:B:27:ILE:HG12	1:B:28:LEU:CD1	2.40	0.41
1:B:239:GLN:HG2	1:B:298:PHE:CZ	2.55	0.41
1:D:363:ARG:HG3	1:D:365:TYR:CD1	2.56	0.41
1:G:67:GLN:HA	1:G:70:LYS:HD2	2.02	0.41
1:G:148:ASN:HB2	1:G:150:TRP:CD1	2.55	0.41
1:G:280:HIS:O	1:G:284:GLU:HG3	2.20	0.41
1:H:103:LEU:HA	1:H:106:PHE:HD2	1.85	0.41
1:H:167:TYR:O	1:H:171:GLY:N	2.53	0.41
1:I:225:PRO:HG3	1:L:112:CYS:SG	2.61	0.41
1:I:362:ASN:N	1:I:362:ASN:HD22	2.18	0.41
1:K:27:ILE:HG12	1:K:28:LEU:HD13	2.02	0.41
1:K:28:LEU:CB	1:K:34:PRO:HA	2.35	0.41
1:K:273:ASP:CG	1:K:275:ARG:HE	2.24	0.41
1:K:280:HIS:O	1:K:284:GLU:HG3	2.20	0.41
1:L:59:LYS:NZ	1:L:60:LYS:HD2	2.36	0.41
1:B:70:LYS:C	1:B:72:ASN:H	2.24	0.41
1:B:312:LEU:H	1:B:312:LEU:CD2	2.25	0.41
1:C:234:VAL:HG11	1:C:339:PHE:HE2	1.85	0.41
1:D:100:VAL:HG21	1:D:219:ILE:HD11	2.02	0.41
1:E:177:LEU:O	1:E:181:ILE:HG13	2.21	0.41
1:H:326:GLY:HA2	1:H:329:TYR:HD2	1.85	0.41
1:I:135:GLN:C	1:I:138:PRO:HD2	2.41	0.41
1:J:31:ARG:NH2	1:J:51:LEU:O	2.53	0.41
1:J:38:LEU:O	1:J:42:SER:HB3	2.20	0.41
1:K:40:GLU:HG2	1:K:41:ASN:ND2	2.35	0.41
1:L:77:TYR:O	1:L:80:ARG:HG2	2.21	0.41
1:L:91:HIS:ND1	1:L:93:MET:HB2	2.36	0.41
1:L:125:VAL:O	1:L:126:ARG:HB2	2.21	0.41
1:A:324:TYR:HD1	1:A:327:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HD21	1:C:65:PHE:CG	2.56	0.41
1:C:338:GLU:O	1:C:342:LEU:HD13	2.21	0.41
1:D:126:ARG:HH21	1:D:129:THR:HG21	1.84	0.41
1:D:286:LEU:HD22	1:D:328:LEU:HD12	2.03	0.41
1:E:167:TYR:HA	1:E:172:GLU:O	2.20	0.41
1:E:178:MET:SD	1:E:332:MET:HG2	2.61	0.41
1:F:264:MET:SD	1:F:319:PRO:CG	3.09	0.41
1:H:196:ALA:HB3	1:H:227:HIS:ND1	2.35	0.41
1:H:363:ARG:O	1:H:364:ILE:C	2.59	0.41
1:J:59:LYS:HB3	1:J:59:LYS:HE3	1.89	0.41
1:J:211:PRO:O	1:J:215:ILE:HG12	2.20	0.41
1:J:285:GLN:O	1:J:289:GLU:HG2	2.21	0.41
1:K:233:ARG:NH2	1:K:322:ASP:O	2.53	0.41
1:A:111:GLU:CD	1:A:111:GLU:H	2.24	0.41
1:A:156:LYS:HE3	1:A:167:TYR:CE1	2.56	0.41
1:A:273:ASP:CG	1:A:275:ARG:HE	2.24	0.41
1:A:367:PRO:HG2	1:C:194:LEU:HB3	2.03	0.41
1:B:24:GLU:OE1	1:B:25:LYS:HB2	2.20	0.41
1:B:340:THR:O	1:B:343:PHE:HB3	2.21	0.41
1:C:304:LEU:HA	1:C:307:VAL:HG22	2.02	0.41
1:D:85:HIS:CD2	1:E:81:GLN:HE21	2.38	0.41
1:D:304:LEU:HD22	1:D:304:LEU:N	2.35	0.41
1:E:156:LYS:HB2	1:E:159:LEU:HB2	2.03	0.41
1:E:273:ASP:CG	1:E:275:ARG:HE	2.24	0.41
1:E:359:ILE:HG13	1:E:360:SER:N	2.36	0.41
1:F:28:LEU:N	1:F:28:LEU:CD1	2.84	0.41
1:G:88:HIS:O	1:G:147:ARG:HG3	2.20	0.41
1:G:306:GLU:O	1:G:307:VAL:HB	2.21	0.41
1:H:329:TYR:HA	1:H:334:ILE:HD12	2.02	0.41
1:I:42:SER:HA	1:I:46:GLU:OE1	2.20	0.41
1:I:76:LYS:HE3	1:I:106:PHE:HB3	2.03	0.41
1:I:102:SER:HB2	1:L:86:PHE:CE1	2.55	0.41
1:I:137:ALA:O	1:I:138:PRO:C	2.60	0.41
1:I:166:LEU:HD23	1:I:178:MET:HE2	2.03	0.41
1:I:283:VAL:O	1:I:287:VAL:HG23	2.21	0.41
1:J:59:LYS:HD2	1:J:59:LYS:C	2.41	0.41
1:J:68:GLN:HA	1:J:71:ASP:OD2	2.21	0.41
1:J:283:VAL:O	1:J:287:VAL:HG23	2.21	0.41
1:J:338:GLU:O	1:J:342:LEU:HD13	2.21	0.41
1:K:80:ARG:O	1:K:84:ARG:HG3	2.21	0.41
1:L:199:PHE:HA	1:L:202:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:202:LEU:CD2	1:L:354:HIS:HB3	2.51	0.41
1:L:237:MET:O	1:L:238:LEU:HB2	2.21	0.41
1:A:44:PHE:CD1	1:A:186:LEU:HB3	2.56	0.41
1:A:231:ASN:HA	1:A:234:VAL:CG2	2.50	0.41
1:A:241:ILE:CG2	1:A:244:PRO:HG2	2.45	0.41
1:A:267:ARG:NH1	1:C:366:ARG:HB3	2.36	0.41
1:A:275:ARG:O	1:A:279:LEU:HG	2.21	0.41
1:B:198:THR:HA	1:B:351:TRP:CD1	2.56	0.41
1:B:321:VAL:HG13	1:B:322:ASP:OD1	2.21	0.41
1:B:337:ASP:N	1:B:337:ASP:OD1	2.53	0.41
1:G:182:MET:HB2	1:G:332:MET:CE	2.51	0.41
1:I:69:LEU:HD12	1:I:130:VAL:O	2.20	0.41
1:I:278:ILE:O	1:I:282:LEU:HG	2.21	0.41
1:J:110:THR:HG22	1:J:112:CYS:H	1.86	0.41
1:J:233:ARG:HA	1:J:233:ARG:HH11	1.86	0.41
1:K:222:LEU:HG	1:K:227:HIS:ND1	2.36	0.41
1:K:305:GLU:OE2	1:K:324:TYR:HE1	2.04	0.41
1:C:358:GLN:O	1:C:362:ASN:HB2	2.21	0.40
1:E:46:GLU:HG3	1:E:57:PRO:HD2	2.02	0.40
1:E:69:LEU:HD12	1:E:134:ALA:HB2	2.03	0.40
1:E:189:HIS:HB3	1:E:343:PHE:CD1	2.56	0.40
1:F:359:ILE:HG13	1:F:360:SER:H	1.85	0.40
1:G:177:LEU:O	1:G:181:ILE:HG13	2.20	0.40
1:H:192:HIS:CE1	1:H:266:HIS:NE2	2.79	0.40
1:I:27:ILE:HD12	1:I:274:PRO:HB3	2.02	0.40
1:I:159:LEU:HA	1:I:163:GLU:OE1	2.22	0.40
1:J:372:VAL:HB	1:J:375:ASP:HA	2.03	0.40
1:K:24:GLU:HG3	1:K:25:LYS:H	1.86	0.40
1:B:126:ARG:NH2	1:B:129:THR:HG21	2.36	0.40
1:C:324:TYR:O	1:C:327:ILE:HG12	2.21	0.40
1:D:80:ARG:HG3	1:D:81:GLN:N	2.36	0.40
1:D:188:LEU:HD21	1:D:278:ILE:HB	2.04	0.40
1:E:159:LEU:HA	1:E:163:GLU:OE1	2.22	0.40
1:H:26:GLY:H	1:H:269:TYR:HE1	1.68	0.40
1:H:231:ASN:O	1:H:234:VAL:HG12	2.21	0.40
1:I:121:ASP:OD1	1:I:122:LEU:N	2.55	0.40
1:I:194:LEU:O	1:L:367:PRO:HD2	2.22	0.40
1:I:222:LEU:HD13	1:I:343:PHE:CD2	2.57	0.40
1:K:266:HIS:CB	1:K:269:TYR:HB2	2.34	0.40
1:K:273:ASP:OD2	1:K:321:VAL:HB	2.21	0.40
1:L:140:VAL:HG12	1:L:169:PHE:CZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:312:LEU:H	1:L:312:LEU:CD1	2.34	0.40
1:A:27:ILE:HD11	1:A:274:PRO:HB3	2.03	0.40
1:A:126:ARG:HH22	1:A:356:ARG:HD2	1.86	0.40
1:A:198:THR:O	1:A:202:LEU:HG	2.21	0.40
1:B:363:ARG:HH21	1:B:369:GLN:NE2	2.19	0.40
1:C:177:LEU:HD23	1:C:177:LEU:C	2.41	0.40
1:E:356:ARG:O	1:E:359:ILE:HG23	2.21	0.40
1:F:70:LYS:HD3	1:F:157:HIS:O	2.21	0.40
1:F:136:MET:O	1:F:140:VAL:HG23	2.21	0.40
1:G:156:LYS:HD2	1:G:159:LEU:HD22	2.04	0.40
1:G:243:SER:HB2	1:G:244:PRO:HD3	2.03	0.40
1:H:111:GLU:H	1:H:111:GLU:CD	2.25	0.40
1:I:195:ASN:O	1:I:196:ALA:C	2.59	0.40
1:I:207:THR:O	1:I:208:LEU:HB2	2.21	0.40
1:K:283:VAL:O	1:K:287:VAL:HG23	2.21	0.40
1:B:301:ALA:O	1:B:302:LEU:HD23	2.22	0.40
1:C:304:LEU:HD12	1:C:327:ILE:HD13	2.03	0.40
1:G:27:ILE:HG13	1:G:193:THR:OG1	2.21	0.40
1:H:162:ALA:HA	1:H:165:LEU:HD12	2.03	0.40
1:I:366:ARG:NH1	1:L:195:ASN:HA	2.36	0.40
1:K:350:GLY:O	1:K:354:HIS:HD2	2.04	0.40
1:A:80:ARG:O	1:A:84:ARG:HG3	2.21	0.40
1:A:176:PRO:HB2	1:A:180:LYS:NZ	2.37	0.40
1:B:178:MET:SD	1:B:332:MET:HE3	2.62	0.40
1:C:273:ASP:OD2	1:C:321:VAL:HB	2.21	0.40
1:D:177:LEU:HG	1:D:181:ILE:HD11	2.03	0.40
1:D:194:LEU:N	1:D:194:LEU:HD22	2.37	0.40
1:D:340:THR:O	1:D:343:PHE:HB3	2.22	0.40
1:E:80:ARG:HG3	1:E:81:GLN:N	2.37	0.40
1:F:95:MET:HE2	1:F:95:MET:HB2	1.98	0.40
1:G:49:LEU:HD11	1:G:62:LEU:HA	2.04	0.40
1:G:169:PHE:HE2	1:G:338:GLU:HG3	1.87	0.40
1:H:122:LEU:HD12	1:H:122:LEU:C	2.42	0.40
1:K:125:VAL:HA	1:K:128:MET:SD	2.61	0.40
1:K:129:THR:O	1:K:133:ILE:HG13	2.22	0.40
1:L:234:VAL:HG21	1:L:339:PHE:CE2	2.57	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	316/397 (80%)	297 (94%)	19 (6%)	0	100	100
1	B	319/397 (80%)	292 (92%)	27 (8%)	0	100	100
1	C	301/397 (76%)	283 (94%)	18 (6%)	0	100	100
1	D	316/397 (80%)	300 (95%)	16 (5%)	0	100	100
1	E	313/397 (79%)	297 (95%)	15 (5%)	1 (0%)	41	74
1	F	308/397 (78%)	284 (92%)	24 (8%)	0	100	100
1	G	301/397 (76%)	282 (94%)	19 (6%)	0	100	100
1	H	305/397 (77%)	283 (93%)	21 (7%)	1 (0%)	41	74
1	I	297/397 (75%)	280 (94%)	16 (5%)	1 (0%)	41	74
1	J	318/397 (80%)	299 (94%)	19 (6%)	0	100	100
1	K	295/397 (74%)	280 (95%)	15 (5%)	0	100	100
1	L	307/397 (77%)	286 (93%)	21 (7%)	0	100	100
All	All	3696/4764 (78%)	3463 (94%)	230 (6%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	242	GLY
1	I	108	PRO
1	E	367	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	275/340 (81%)	270 (98%)	5 (2%)	59	82
1	B	278/340 (82%)	270 (97%)	8 (3%)	42	74
1	C	265/340 (78%)	259 (98%)	6 (2%)	50	78
1	D	275/340 (81%)	269 (98%)	6 (2%)	52	79
1	E	273/340 (80%)	267 (98%)	6 (2%)	52	79
1	F	270/340 (79%)	265 (98%)	5 (2%)	57	81
1	G	266/340 (78%)	256 (96%)	10 (4%)	33	67
1	H	269/340 (79%)	260 (97%)	9 (3%)	38	71
1	I	264/340 (78%)	257 (97%)	7 (3%)	44	75
1	J	275/340 (81%)	263 (96%)	12 (4%)	28	64
1	K	262/340 (77%)	258 (98%)	4 (2%)	65	85
1	L	271/340 (80%)	258 (95%)	13 (5%)	25	61
All	All	3243/4080 (80%)	3152 (97%)	91 (3%)	43	74

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	136	MET
1	A	337	ASP
1	A	359	ILE
1	A	371	TYR
1	B	28	LEU
1	B	50	LEU
1	B	191	GLU
1	B	233	ARG
1	B	239	GLN
1	B	275	ARG
1	B	337	ASP
1	B	358	GLN
1	C	136	MET
1	C	186	LEU
1	C	233	ARG
1	C	240	GLU
1	C	303	LYS
1	C	323	PHE
1	D	28	LEU
1	D	233	ARG
1	D	275	ARG

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Mol	Chain	Res	Type
1	D	281	LYS
1	D	302	LEU
1	D	311	ARG
1	E	25	LYS
1	E	36	GLU
1	E	107	TYR
1	E	245	LYS
1	E	246	ASN
1	E	275	ARG
1	F	28	LEU
1	F	233	ARG
1	F	241	ILE
1	F	245	LYS
1	F	312	LEU
1	G	62	LEU
1	G	107	TYR
1	G	122	LEU
1	G	153	VAL
1	G	167	TYR
1	G	233	ARG
1	G	239	GLN
1	G	358	GLN
1	G	370	ILE
1	G	372	VAL
1	H	25	LYS
1	H	51	LEU
1	H	74	ARG
1	H	78	HIS
1	H	107	TYR
1	H	191	GLU
1	H	233	ARG
1	H	239	GLN
1	H	358	GLN
1	I	36	GLU
1	I	107	TYR
1	I	219	ILE
1	I	233	ARG
1	I	245	LYS
1	I	271	VAL
1	I	362	ASN
1	J	49	LEU
1	J	59	LYS

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Mol	Chain	Res	Type
1	J	60	LYS
1	J	107	TYR
1	J	124	TYR
1	J	165	LEU
1	J	169	PHE
1	J	233	ARG
1	J	245	LYS
1	J	281	LYS
1	J	304	LEU
1	J	368	THR
1	K	24	GLU
1	K	28	LEU
1	K	107	TYR
1	K	128	MET
1	L	28	LEU
1	L	37	THR
1	L	122	LEU
1	L	126	ARG
1	L	128	MET
1	L	139	LEU
1	L	167	TYR
1	L	233	ARG
1	L	300	THR
1	L	302	LEU
1	L	305	GLU
1	L	312	LEU
1	L	343	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	67	GLN
1	A	81	GLN
1	A	91	HIS
1	A	145	HIS
1	A	232	GLN
1	A	358	GLN
1	B	41	ASN
1	B	63	ASN
1	B	68	GLN
1	B	127	ASN

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Mol	Chain	Res	Type
1	B	195	ASN
1	B	227	HIS
1	B	232	GLN
1	B	239	GLN
1	B	358	GLN
1	B	369	GLN
1	C	41	ASN
1	C	72	ASN
1	C	81	GLN
1	C	154	ASN
1	C	170	ASN
1	D	91	HIS
1	D	157	HIS
1	D	246	ASN
1	E	41	ASN
1	E	81	GLN
1	E	192	HIS
1	E	195	ASN
1	E	227	HIS
1	E	239	GLN
1	E	246	ASN
1	E	369	GLN
1	F	148	ASN
1	F	157	HIS
1	F	189	HIS
1	F	358	GLN
1	G	72	ASN
1	G	148	ASN
1	G	154	ASN
1	G	157	HIS
1	G	170	ASN
1	G	189	HIS
1	G	232	GLN
1	G	239	GLN
1	G	354	HIS
1	G	358	GLN
1	H	67	GLN
1	H	145	HIS
1	H	148	ASN
1	H	192	HIS
1	H	227	HIS
1	H	239	GLN

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Mol	Chain	Res	Type
1	H	369	GLN
1	I	41	ASN
1	I	67	GLN
1	I	72	ASN
1	I	97	GLN
1	I	131	ASN
1	I	148	ASN
1	I	227	HIS
1	I	354	HIS
1	I	362	ASN
1	J	41	ASN
1	J	135	GLN
1	J	148	ASN
1	J	192	HIS
1	J	227	HIS
1	J	280	HIS
1	K	41	ASN
1	K	67	GLN
1	K	72	ASN
1	K	85	HIS
1	K	154	ASN
1	K	231	ASN
1	L	72	ASN
1	L	81	GLN
1	L	131	ASN
1	L	145	HIS
1	L	148	ASN
1	L	157	HIS
1	L	170	ASN
1	L	280	HIS
1	L	358	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

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, 95^{th} 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	324/397 (81%)	0.41	15 (4%) 32 20	86, 118, 157, 237	0
1	B	327/397 (82%)	0.54	33 (10%) 7 4	84, 114, 187, 280	0
1	C	311/397 (78%)	0.49	29 (9%) 8 5	89, 135, 208, 286	0
1	D	324/397 (81%)	0.46	20 (6%) 20 11	85, 117, 172, 218	0
1	E	321/397 (80%)	0.40	18 (5%) 24 13	85, 116, 171, 259	0
1	F	318/397 (80%)	0.36	19 (5%) 21 12	30, 122, 183, 255	0
1	G	313/397 (78%)	0.71	35 (11%) 5 3	96, 127, 207, 286	0
1	H	315/397 (79%)	0.61	33 (10%) 6 3	89, 140, 207, 271	0
1	I	311/397 (78%)	0.49	24 (7%) 13 7	94, 135, 209, 262	0
1	J	326/397 (82%)	0.42	14 (4%) 35 22	96, 131, 187, 285	0
1	K	309/397 (77%)	0.68	37 (11%) 4 2	92, 132, 205, 241	0
1	L	317/397 (79%)	0.73	35 (11%) 5 3	30, 147, 209, 288	0
All	All	3816/4764 (80%)	0.52	312 (8%) 11 6	30, 128, 199, 288	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	39	ALA	7.5
1	B	374	SER	7.2
1	G	269	TYR	6.8
1	K	288	ALA	6.6
1	L	320	ASN	6.5
1	G	302	LEU	6.4
1	C	231	ASN	6.3
1	B	310	ASP	6.3
1	F	304	LEU	5.7
1	K	38	LEU	5.6
1	G	289	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	41	ASN	5.4
1	L	304	LEU	5.2
1	H	310	ASP	5.2
1	J	304	LEU	5.1
1	K	271	VAL	4.9
1	I	266	HIS	4.8
1	L	202	LEU	4.7
1	G	299	ASP	4.7
1	H	188	LEU	4.7
1	F	318	TYR	4.6
1	D	320	ASN	4.5
1	G	246	ASN	4.5
1	L	248	GLU	4.5
1	I	302	LEU	4.5
1	E	310	ASP	4.5
1	K	310	ASP	4.4
1	G	233	ARG	4.4
1	H	287	VAL	4.4
1	L	323	PHE	4.3
1	I	270	LYS	4.3
1	E	286	LEU	4.2
1	G	42	SER	4.2
1	K	307	VAL	4.2
1	H	35	LEU	4.2
1	F	323	PHE	4.1
1	A	369	GLN	4.1
1	G	327	ILE	4.1
1	H	286	LEU	4.1
1	K	287	VAL	4.1
1	F	269	TYR	4.0
1	D	286	LEU	4.0
1	G	62	LEU	4.0
1	C	286	LEU	4.0
1	G	245	LYS	3.9
1	C	304	LEU	3.9
1	K	286	LEU	3.9
1	K	41	ASN	3.9
1	J	38	LEU	3.9
1	B	302	LEU	3.9
1	F	319	PRO	3.9
1	G	306	GLU	3.8
1	C	310	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	233	ARG	3.8
1	J	323	PHE	3.8
1	H	186	LEU	3.7
1	B	300	THR	3.7
1	F	266	HIS	3.7
1	G	27	ILE	3.7
1	H	187	ILE	3.7
1	I	305	GLU	3.7
1	B	313	GLY	3.6
1	K	262	TRP	3.6
1	G	29	SER	3.6
1	K	272	LYS	3.6
1	G	303	LYS	3.5
1	H	285	GLN	3.5
1	G	73	TYR	3.5
1	D	288	ALA	3.4
1	B	239	GLN	3.4
1	B	311	ARG	3.4
1	J	351	TRP	3.4
1	I	282	LEU	3.3
1	H	27	ILE	3.3
1	F	41	ASN	3.3
1	H	279	LEU	3.3
1	D	279	LEU	3.3
1	L	245	LYS	3.3
1	I	310	ASP	3.3
1	B	375	ASP	3.3
1	D	314	HIS	3.2
1	B	177	LEU	3.2
1	K	269	TYR	3.2
1	H	26	GLY	3.2
1	H	284	GLU	3.2
1	J	375	ASP	3.2
1	C	234	VAL	3.2
1	K	304	LEU	3.2
1	K	320	ASN	3.2
1	E	317	VAL	3.2
1	F	279	LEU	3.1
1	G	188	LEU	3.1
1	C	44	PHE	3.1
1	J	307	VAL	3.1
1	C	269	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	25	LYS	3.1
1	L	38	LEU	3.1
1	I	323	PHE	3.1
1	K	150	TRP	3.1
1	I	284	GLU	3.1
1	H	288	ALA	3.1
1	I	77	TYR	3.1
1	K	282	LEU	3.1
1	L	124	TYR	3.1
1	B	156	LYS	3.1
1	I	262	TRP	3.1
1	K	298	PHE	3.0
1	B	240	GLU	3.0
1	B	306	GLU	3.0
1	H	375	ASP	3.0
1	L	238	LEU	3.0
1	A	57	PRO	3.0
1	G	206	SER	3.0
1	L	239	GLN	3.0
1	C	197	SER	3.0
1	I	285	GLN	3.0
1	H	289	GLU	3.0
1	B	369	GLN	3.0
1	D	289	GLU	3.0
1	H	190	ALA	3.0
1	K	171	GLY	3.0
1	K	285	GLN	3.0
1	J	373	GLY	3.0
1	B	314	HIS	3.0
1	G	28	LEU	2.9
1	C	282	LEU	2.9
1	L	364	ILE	2.9
1	L	50	LEU	2.9
1	A	173	GLU	2.9
1	G	238	LEU	2.9
1	E	285	GLN	2.9
1	I	42	SER	2.9
1	L	307	VAL	2.9
1	K	300	THR	2.9
1	L	343	PHE	2.9
1	B	69	LEU	2.9
1	H	30	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	283	VAL	2.8
1	E	57	PRO	2.8
1	C	334	ILE	2.8
1	L	199	PHE	2.8
1	B	304	LEU	2.8
1	K	309	ALA	2.8
1	E	179	ALA	2.8
1	L	286	LEU	2.8
1	K	73	TYR	2.8
1	D	85	HIS	2.8
1	L	34	PRO	2.8
1	A	62	LEU	2.7
1	E	28	LEU	2.7
1	B	39	ALA	2.7
1	G	193	THR	2.7
1	D	39	ALA	2.7
1	C	280	HIS	2.7
1	F	320	ASN	2.7
1	H	339	PHE	2.7
1	K	172	GLU	2.7
1	G	272	LYS	2.7
1	C	284	GLU	2.7
1	K	37	THR	2.7
1	C	53	ASP	2.7
1	E	308	CYS	2.7
1	G	304	LEU	2.7
1	I	183	ASP	2.7
1	E	85	HIS	2.7
1	J	85	HIS	2.7
1	J	299	ASP	2.6
1	B	368	THR	2.6
1	H	283	VAL	2.6
1	B	371	TYR	2.6
1	A	365	TYR	2.6
1	F	282	LEU	2.6
1	K	324	TYR	2.6
1	H	41	ASN	2.6
1	A	304	LEU	2.6
1	B	187	ILE	2.6
1	C	27	ILE	2.6
1	J	239	GLN	2.6
1	A	361	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	81	GLN	2.6
1	E	186	LEU	2.6
1	K	279	LEU	2.6
1	L	328	LEU	2.6
1	L	126	ARG	2.5
1	F	276	ALA	2.5
1	K	26	GLY	2.5
1	L	247	VAL	2.5
1	C	189	HIS	2.5
1	D	239	GLN	2.5
1	G	305	GLU	2.5
1	H	157	HIS	2.5
1	L	43	THR	2.5
1	L	262	TRP	2.5
1	F	314	HIS	2.5
1	L	276	ALA	2.5
1	B	316	GLY	2.5
1	I	279	LEU	2.5
1	L	234	VAL	2.5
1	C	232	GLN	2.5
1	I	271	VAL	2.5
1	B	312	LEU	2.4
1	E	44	PHE	2.4
1	K	166	LEU	2.4
1	L	35	LEU	2.4
1	B	367	PRO	2.4
1	E	174	PRO	2.4
1	C	285	GLN	2.4
1	G	85	HIS	2.4
1	I	311	ARG	2.4
1	B	178	MET	2.4
1	L	308	CYS	2.4
1	G	237	MET	2.4
1	D	318	TYR	2.4
1	I	177	LEU	2.4
1	H	85	HIS	2.4
1	B	308	CYS	2.4
1	D	238	LEU	2.4
1	K	42	SER	2.4
1	K	71	ASP	2.4
1	L	269	TYR	2.4
1	A	85	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	LEU	2.4
1	H	238	LEU	2.4
1	C	287	VAL	2.4
1	D	124	TYR	2.4
1	C	227	HIS	2.4
1	C	343	PHE	2.3
1	A	240	GLU	2.3
1	F	187	ILE	2.3
1	H	189	HIS	2.3
1	A	107	TYR	2.3
1	C	270	LYS	2.3
1	L	91	HIS	2.3
1	E	183	ASP	2.3
1	K	289	GLU	2.3
1	D	38	LEU	2.3
1	L	172	GLU	2.3
1	J	280	HIS	2.3
1	E	239	GLN	2.3
1	D	240	GLU	2.3
1	H	110	THR	2.3
1	H	109	GLY	2.3
1	B	286	LEU	2.3
1	H	324	TYR	2.3
1	G	185	CYS	2.3
1	F	262	TRP	2.3
1	B	182	MET	2.2
1	G	198	THR	2.2
1	D	303	LYS	2.2
1	K	266	HIS	2.2
1	C	237	MET	2.2
1	D	62	LEU	2.2
1	A	124	TYR	2.2
1	G	186	LEU	2.2
1	H	38	LEU	2.2
1	G	362	ASN	2.2
1	K	58	THR	2.2
1	L	206	SER	2.2
1	L	298	PHE	2.2
1	E	110	THR	2.2
1	B	315	LYS	2.2
1	J	262	TRP	2.2
1	K	25	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	239	GLN	2.2
1	I	304	LEU	2.2
1	C	370	ILE	2.2
1	K	35	LEU	2.2
1	F	60	LYS	2.2
1	C	339	PHE	2.2
1	L	246	ASN	2.2
1	C	196	ALA	2.2
1	I	324	TYR	2.2
1	H	326	GLY	2.2
1	K	169	PHE	2.1
1	F	265	GLY	2.1
1	I	35	LEU	2.1
1	H	44	PHE	2.1
1	H	94	ASP	2.1
1	F	28	LEU	2.1
1	C	329	TYR	2.1
1	D	30	TYR	2.1
1	E	314	HIS	2.1
1	B	41	ASN	2.1
1	J	306	GLU	2.1
1	L	336	GLU	2.1
1	B	362	ASN	2.1
1	G	133	ILE	2.1
1	E	188	LEU	2.1
1	A	54	GLY	2.1
1	G	58	THR	2.1
1	I	188	LEU	2.1
1	L	302	LEU	2.1
1	C	222	LEU	2.1
1	E	262	TRP	2.1
1	H	49	LEU	2.1
1	I	300	THR	2.1
1	F	310	ASP	2.0
1	I	201	ALA	2.0
1	F	370	ILE	2.0
1	G	357	GLU	2.0
1	B	238	LEU	2.0
1	H	46	GLU	2.0
1	G	301	ALA	2.0
1	A	367	PRO	2.0
1	B	124	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	287	VAL	2.0
1	D	304	LEU	2.0
1	G	38	LEU	2.0
1	G	204	ALA	2.0
1	B	159	LEU	2.0
1	I	38	LEU	2.0
1	L	287	VAL	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.