



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:42 am GMT

PDB ID : 4AH6
Title : Human mitochondrial aspartyl-tRNA synthetase
Authors : Neuenfeldt, A.; Sissler, M.; Lorber, B.; Florentz, C.; Sauter, C.
Deposited on : 2012-02-03
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

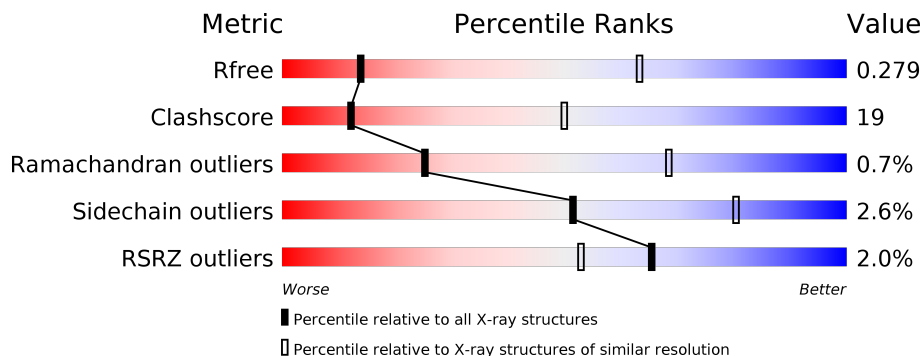
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	617	<div> <div>2%</div> <div>59% 35% • 5%</div> </div>
1	B	617	<div> <div>2%</div> <div>58% 36% • 5%</div> </div>
1	C	617	<div> <div>%</div> <div>58% 36% • 5%</div> </div>
1	D	617	<div> <div>2%</div> <div>57% 37% • 5%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18840 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 ASPARTATE-TRNA LIGASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4710	3007	813	867	23			
1	B	589	Total	C	N	O	S	0	0	0
			4710	3007	813	867	23			
1	C	589	Total	C	N	O	S	0	0	0
			4710	3007	813	867	23			
1	D	589	Total	C	N	O	S	0	0	0
			4710	3007	813	867	23			

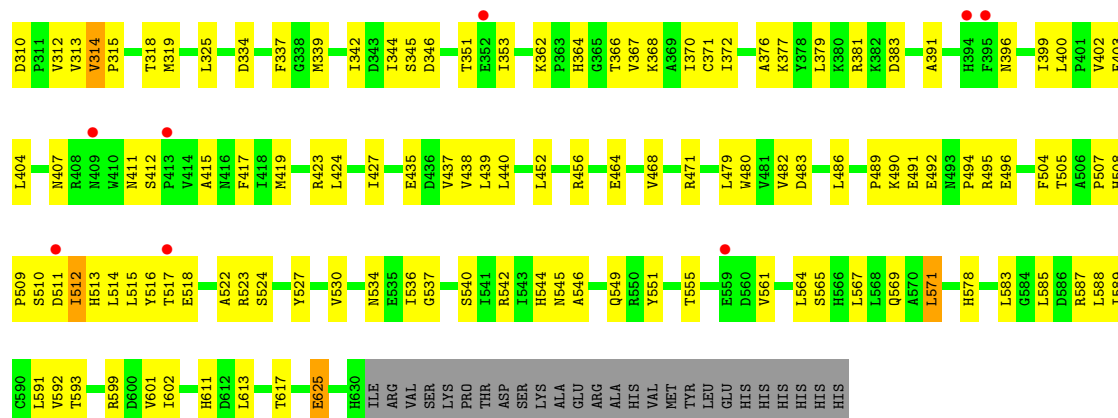
There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	EXPRESSION TAG	UNP Q6PI48
A	646	VAL	-	EXPRESSION TAG	UNP Q6PI48
A	647	MET	-	EXPRESSION TAG	UNP Q6PI48
A	648	TYR	-	EXPRESSION TAG	UNP Q6PI48
A	649	LEU	-	EXPRESSION TAG	UNP Q6PI48
A	650	GLU	-	EXPRESSION TAG	UNP Q6PI48
A	651	HIS	-	EXPRESSION TAG	UNP Q6PI48
A	652	HIS	-	EXPRESSION TAG	UNP Q6PI48
A	653	HIS	-	EXPRESSION TAG	UNP Q6PI48
A	654	HIS	-	EXPRESSION TAG	UNP Q6PI48
A	655	HIS	-	EXPRESSION TAG	UNP Q6PI48
A	656	HIS	-	EXPRESSION TAG	UNP Q6PI48
B	40	MET	-	EXPRESSION TAG	UNP Q6PI48
B	646	VAL	-	EXPRESSION TAG	UNP Q6PI48
B	647	MET	-	EXPRESSION TAG	UNP Q6PI48
B	648	TYR	-	EXPRESSION TAG	UNP Q6PI48
B	649	LEU	-	EXPRESSION TAG	UNP Q6PI48
B	650	GLU	-	EXPRESSION TAG	UNP Q6PI48
B	651	HIS	-	EXPRESSION TAG	UNP Q6PI48
B	652	HIS	-	EXPRESSION TAG	UNP Q6PI48
B	653	HIS	-	EXPRESSION TAG	UNP Q6PI48

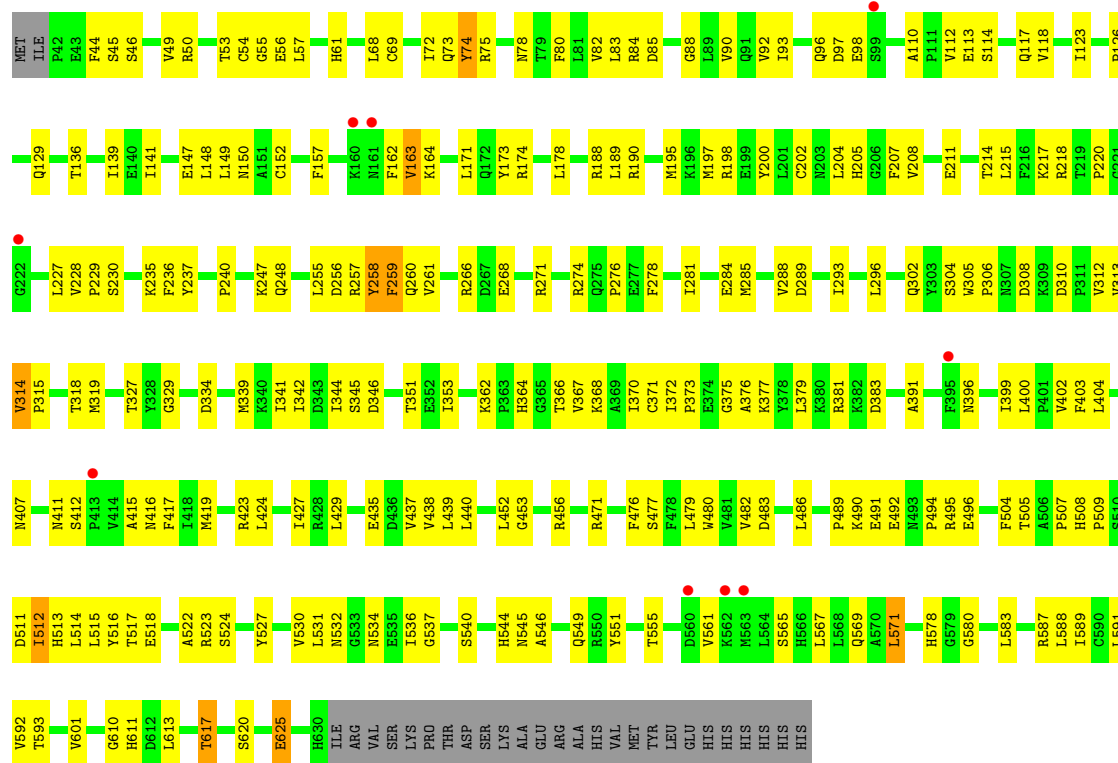
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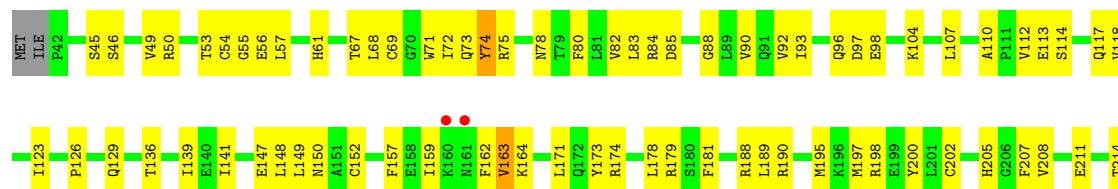
Chain	Residue	Modelled	Actual	Comment	Reference
B	654	HIS	-	EXPRESSION TAG	UNP Q6PI48
B	655	HIS	-	EXPRESSION TAG	UNP Q6PI48
B	656	HIS	-	EXPRESSION TAG	UNP Q6PI48
C	40	MET	-	EXPRESSION TAG	UNP Q6PI48
C	646	VAL	-	EXPRESSION TAG	UNP Q6PI48
C	647	MET	-	EXPRESSION TAG	UNP Q6PI48
C	648	TYR	-	EXPRESSION TAG	UNP Q6PI48
C	649	LEU	-	EXPRESSION TAG	UNP Q6PI48
C	650	GLU	-	EXPRESSION TAG	UNP Q6PI48
C	651	HIS	-	EXPRESSION TAG	UNP Q6PI48
C	652	HIS	-	EXPRESSION TAG	UNP Q6PI48
C	653	HIS	-	EXPRESSION TAG	UNP Q6PI48
C	654	HIS	-	EXPRESSION TAG	UNP Q6PI48
C	655	HIS	-	EXPRESSION TAG	UNP Q6PI48
C	656	HIS	-	EXPRESSION TAG	UNP Q6PI48
D	40	MET	-	EXPRESSION TAG	UNP Q6PI48
D	646	VAL	-	EXPRESSION TAG	UNP Q6PI48
D	647	MET	-	EXPRESSION TAG	UNP Q6PI48
D	648	TYR	-	EXPRESSION TAG	UNP Q6PI48
D	649	LEU	-	EXPRESSION TAG	UNP Q6PI48
D	650	GLU	-	EXPRESSION TAG	UNP Q6PI48
D	651	HIS	-	EXPRESSION TAG	UNP Q6PI48
D	652	HIS	-	EXPRESSION TAG	UNP Q6PI48
D	653	HIS	-	EXPRESSION TAG	UNP Q6PI48
D	654	HIS	-	EXPRESSION TAG	UNP Q6PI48
D	655	HIS	-	EXPRESSION TAG	UNP Q6PI48
D	656	HIS	-	EXPRESSION TAG	UNP Q6PI48



• Molecule 1: ASPARTATE-TRNA LIGASE, MITOCHONDRIAL



• Molecule 1: ASPARTATE-TRNA LIGASE, MITOCHONDRIAL



H508	H509	L400	P306	L215
	S510	F401	N307	F216
	D511	V402	D308	K217
	I512	F403	K309	R218
	H513	L404	D310	T219
	L514		P311	P220
	L515	M407	V312	
	L516	R408	V313	L227
	Y517	N409	V314	V228
	E518	W410	P315	P229
K521	N411	T318	R230	
A522	S412	M319	R231	
R523	F413		E232	
S524	V414		P233	
	A415	D334	G234	
Y527	N416	T335	K235	
	F417	R336	F236	
	I418	Y237	Y237	
V530	M339	S238	S238	
L531	M419	L239	L239	
		P240	P240	
N534		I342		
E535	R423	D343	K247	
I536	L424	S344	Q248	
G537	I427	S345		
		D346		
S540	E435	T351	L255	
I541	D436	E352	D256	
R542	V437	I353	R257	
GLU	V438	K362	Y258	
ARG	L439	P363	F259	
ALA	L440	H364	Q260	
HIS	N545	G365	V261	
VAL	A546	T366		
MET	E547	V367	Y265	
TYR	L548	K368	R266	
LEU	Q549			
GLU	R550	A369	S270	
HIS	Y551	I370	R271	
HIS		C371	P272	
HIS	T555	I372		
HIS	K558	P373	Q275	
HIS	E559	E374	P276	
		G375	E277	
		A376	F278	
		K377		
	S565	Y378	I281	
	H567	L379		
	L568	K380	E284	
	Q569	R381	M285	
	A570	K382		
L571	R493	D383	V288	
	P494			
H578	R495	A391	I293	
	E496	A392	L296	
	L583	D393		
	G584	H394	Q302	
	L585	F395	Y303	
		N396	S304	
	L588		W305	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.40Å 82.60Å 146.30Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	29.92 – 3.70 29.92 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.92-3.70) 98.8 (29.92-3.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.75Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.219 , 0.280 0.223 , 0.279	Depositor DCC
R_{free} test set	1780 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	88.0	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18840	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/4819	0.52	0/6529
1	B	0.29	0/4819	0.53	0/6529
1	C	0.29	0/4819	0.53	0/6529
1	D	0.29	0/4819	0.53	0/6529
All	All	0.29	0/19276	0.53	0/26116

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4710	0	4729	187	0
1	B	4710	0	4729	205	0
1	C	4710	0	4729	192	1
1	D	4710	0	4729	202	1
All	All	18840	0	18916	716	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (716) 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:A:195:MET:CE	1:B:198:ARG:HG3	1.46	1.43
1:C:198:ARG:HG3	1:D:195:MET:CE	1.52	1.37
1:A:195:MET:HE1	1:B:198:ARG:CG	1.54	1.36
1:C:198:ARG:CG	1:D:195:MET:HE1	1.74	1.17
1:D:162:PHE:CE1	1:D:181:PHE:HB3	1.91	1.05
1:C:198:ARG:HG3	1:D:195:MET:HE1	1.08	1.03
1:C:195:MET:CE	1:D:198:ARG:HG3	1.90	1.01
1:C:198:ARG:CG	1:D:195:MET:CE	2.31	1.01
1:C:198:ARG:HG3	1:D:195:MET:HE2	1.42	1.01
1:D:162:PHE:CZ	1:D:181:PHE:HB3	1.96	1.00
1:D:162:PHE:CE1	1:D:181:PHE:CB	2.46	0.98
1:C:293:ILE:HD11	1:C:527:TYR:CZ	2.02	0.94
1:C:195:MET:HE1	1:D:198:ARG:HG3	1.52	0.90
1:B:162:PHE:CE1	1:B:181:PHE:HB3	2.07	0.89
1:A:490:LYS:HB3	1:A:491:GLU:HA	1.53	0.88
1:D:490:LYS:HB3	1:D:491:GLU:HA	1.54	0.88
1:C:490:LYS:HB3	1:C:491:GLU:HA	1.54	0.88
1:D:403:PHE:CE2	1:D:437:VAL:HG11	2.09	0.88
1:B:490:LYS:HB3	1:B:491:GLU:HA	1.54	0.88
1:C:504:PHE:CD1	1:C:549:GLN:NE2	2.43	0.86
1:A:195:MET:HE2	1:B:198:ARG:HG3	1.55	0.85
1:C:195:MET:HE1	1:D:198:ARG:CG	2.06	0.85
1:C:403:PHE:CE2	1:C:437:VAL:HG11	2.13	0.84
1:A:195:MET:CE	1:B:198:ARG:CG	2.27	0.84
1:B:403:PHE:CE2	1:B:437:VAL:HG11	2.11	0.83
1:A:195:MET:HE1	1:B:198:ARG:HG3	0.85	0.82
1:A:608:PHE:CE2	1:D:414:VAL:HA	2.14	0.82
1:A:198:ARG:HG3	1:B:195:MET:CE	2.08	0.82
1:A:113:GLU:O	1:A:152:CYS:SG	2.39	0.81
1:A:504:PHE:CD1	1:A:549:GLN:NE2	2.50	0.80
1:D:207:PHE:HZ	1:D:296:LEU:HD11	1.47	0.79
1:C:504:PHE:CD1	1:C:549:GLN:CD	2.56	0.79
1:C:372:ILE:HG23	1:C:437:VAL:HG23	1.65	0.79
1:C:293:ILE:HD11	1:C:527:TYR:OH	1.83	0.79
1:C:207:PHE:HZ	1:C:296:LEU:HD11	1.49	0.78
1:B:314:VAL:HB	1:B:315:PRO:HD2	1.66	0.78
1:C:314:VAL:HB	1:C:315:PRO:HD2	1.66	0.78
1:C:195:MET:HE2	1:D:198:ARG:HG3	1.64	0.78
1:B:372:ILE:HG23	1:B:437:VAL:HG23	1.65	0.77
1:D:314:VAL:HB	1:D:315:PRO:HD2	1.66	0.77
1:A:314:VAL:HB	1:A:315:PRO:HD2	1.66	0.77
1:B:207:PHE:HZ	1:B:296:LEU:HD11	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLN:HE21	1:B:602:ILE:CD1	1.97	0.77
1:B:162:PHE:CE1	1:B:181:PHE:CB	2.69	0.75
1:D:372:ILE:HG23	1:D:437:VAL:HG23	1.67	0.75
1:D:403:PHE:CD2	1:D:437:VAL:HG12	2.22	0.74
1:B:403:PHE:CD2	1:B:437:VAL:HG12	2.23	0.73
1:C:195:MET:CE	1:D:198:ARG:CG	2.65	0.73
1:A:504:PHE:CD1	1:A:549:GLN:CD	2.62	0.73
1:D:162:PHE:CE1	1:D:181:PHE:HB2	2.22	0.73
1:B:275:GLN:NE2	1:B:602:ILE:CD1	2.52	0.72
1:C:403:PHE:CD2	1:C:437:VAL:HG12	2.25	0.72
1:A:372:ILE:HG23	1:A:437:VAL:HG13	1.71	0.71
1:C:202:CYS:HB3	1:D:195:MET:HE3	1.71	0.71
1:A:198:ARG:HG3	1:B:195:MET:HE2	1.72	0.70
1:B:275:GLN:NE2	1:B:602:ILE:HD12	2.06	0.70
1:B:412:SER:HB3	1:B:415:ALA:HB3	1.73	0.70
1:D:412:SER:HB3	1:D:415:ALA:HB3	1.74	0.70
1:B:113:GLU:O	1:B:152:CYS:SG	2.49	0.70
1:A:198:ARG:HG3	1:B:195:MET:HE1	1.74	0.69
1:C:412:SER:HB3	1:C:415:ALA:HB3	1.75	0.69
1:C:486:LEU:HD23	1:C:515:LEU:HD21	1.74	0.69
1:C:258:TYR:HD2	1:C:284:GLU:HB2	1.57	0.69
1:D:258:TYR:HD2	1:D:284:GLU:HB2	1.58	0.69
1:A:412:SER:HB3	1:A:415:ALA:HB3	1.75	0.69
1:D:162:PHE:HE1	1:D:181:PHE:HB2	1.57	0.69
1:B:486:LEU:HD23	1:B:515:LEU:HD21	1.75	0.69
1:C:527:TYR:OH	1:C:580:GLY:O	2.07	0.69
1:D:486:LEU:HD23	1:D:515:LEU:HD21	1.75	0.68
1:D:207:PHE:CZ	1:D:296:LEU:HD11	2.29	0.68
1:A:516:TYR:HE1	1:A:551:TYR:HD2	1.41	0.68
1:A:258:TYR:HD2	1:A:284:GLU:HB2	1.59	0.68
1:C:516:TYR:HE1	1:C:551:TYR:HD2	1.42	0.68
1:A:486:LEU:HD23	1:A:515:LEU:HD21	1.75	0.67
1:B:504:PHE:CD1	1:B:549:GLN:NE2	2.62	0.67
1:B:516:TYR:HE1	1:B:551:TYR:HD2	1.41	0.67
1:C:293:ILE:CD1	1:C:527:TYR:OH	2.41	0.67
1:C:198:ARG:CG	1:D:195:MET:HE2	2.14	0.67
1:B:258:TYR:HD2	1:B:284:GLU:HB2	1.58	0.67
1:C:207:PHE:CZ	1:C:296:LEU:HD11	2.29	0.67
1:B:207:PHE:CZ	1:B:296:LEU:HD11	2.30	0.66
1:D:113:GLU:O	1:D:152:CYS:SG	2.50	0.66
1:D:403:PHE:CE2	1:D:437:VAL:CG1	2.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:LYS:HG2	1:C:364:HIS:H	1.60	0.66
1:B:403:PHE:CE2	1:B:437:VAL:CG1	2.79	0.66
1:A:362:LYS:HG2	1:A:364:HIS:H	1.60	0.65
1:C:517:THR:HG22	1:C:518:GLU:HG3	1.78	0.65
1:A:198:ARG:CG	1:B:195:MET:HE1	2.25	0.65
1:D:362:LYS:HG2	1:D:364:HIS:H	1.61	0.65
1:D:516:TYR:HE1	1:D:551:TYR:HD2	1.42	0.65
1:A:57:LEU:HB3	1:A:139:ILE:HD11	1.78	0.65
1:B:362:LYS:HG2	1:B:364:HIS:H	1.61	0.65
1:C:403:PHE:CE2	1:C:437:VAL:CG1	2.80	0.65
1:D:84:ARG:NH2	1:D:113:GLU:OE2	2.30	0.65
1:A:195:MET:HE3	1:B:202:CYS:HB3	1.78	0.65
1:C:351:THR:HG22	1:C:353:ILE:HG22	1.79	0.64
1:C:84:ARG:NH2	1:C:113:GLU:OE2	2.29	0.64
1:C:504:PHE:CD1	1:C:549:GLN:OE1	2.50	0.64
1:A:351:THR:HG22	1:A:353:ILE:HG22	1.78	0.64
1:B:84:ARG:NH2	1:B:113:GLU:OE2	2.30	0.64
1:A:255:LEU:HA	1:B:188:ARG:HH22	1.62	0.64
1:A:517:THR:HG22	1:A:518:GLU:HG3	1.80	0.64
1:B:75:ARG:NH2	1:B:110:ALA:O	2.30	0.64
1:D:517:THR:HG22	1:D:518:GLU:HG3	1.80	0.64
1:B:587:ARG:O	1:B:591:LEU:HD13	1.98	0.64
1:D:351:THR:HG22	1:D:353:ILE:HG22	1.80	0.64
1:A:84:ARG:NH2	1:A:113:GLU:OE2	2.30	0.64
1:A:268:GLU:HG3	1:A:271:ARG:H	1.63	0.64
1:B:57:LEU:HB3	1:B:139:ILE:HD11	1.80	0.63
1:C:376:ALA:HB3	1:C:435:GLU:HB3	1.81	0.63
1:C:46:SER:H	1:D:257:ARG:NH2	1.96	0.63
1:C:54:CYS:SG	1:C:68:LEU:HD13	2.38	0.63
1:A:195:MET:HE1	1:B:198:ARG:CB	2.28	0.63
1:A:228:VAL:HG13	1:A:237:TYR:HB2	1.80	0.63
1:D:75:ARG:NH2	1:D:110:ALA:O	2.32	0.63
1:C:257:ARG:NH2	1:D:46:SER:H	1.96	0.63
1:C:228:VAL:HG13	1:C:237:TYR:HB2	1.81	0.63
1:C:507:PRO:HA	1:C:524:SER:HA	1.81	0.62
1:D:376:ALA:HB3	1:D:435:GLU:HB3	1.80	0.62
1:D:57:LEU:HB3	1:D:139:ILE:HD11	1.79	0.62
1:C:75:ARG:NH2	1:C:110:ALA:O	2.33	0.62
1:C:57:LEU:HB3	1:C:139:ILE:HD11	1.79	0.62
1:C:504:PHE:HD1	1:C:549:GLN:OE1	1.83	0.62
1:A:376:ALA:HB3	1:A:435:GLU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:PHE:CD2	1:D:437:VAL:CG1	2.82	0.62
1:A:516:TYR:HE1	1:A:551:TYR:CD2	2.17	0.62
1:A:75:ARG:NH2	1:A:110:ALA:O	2.33	0.62
1:A:372:ILE:HG23	1:A:437:VAL:CG1	2.30	0.62
1:B:403:PHE:CD2	1:B:437:VAL:CG1	2.83	0.61
1:B:507:PRO:HA	1:B:524:SER:HA	1.81	0.61
1:D:507:PRO:HA	1:D:524:SER:HA	1.82	0.61
1:B:162:PHE:CZ	1:B:181:PHE:HB3	2.35	0.61
1:C:268:GLU:HG3	1:C:271:ARG:H	1.63	0.61
1:B:517:THR:HG22	1:B:518:GLU:HG3	1.81	0.61
1:A:507:PRO:HA	1:A:524:SER:HA	1.81	0.61
1:B:351:THR:HG22	1:B:353:ILE:HG22	1.81	0.61
1:C:351:THR:HG23	1:C:417:PHE:HE2	1.66	0.61
1:D:516:TYR:HE1	1:D:551:TYR:CD2	2.18	0.61
1:B:376:ALA:HB3	1:B:435:GLU:HB3	1.82	0.61
1:B:534:ASN:HB2	1:B:591:LEU:HD21	1.82	0.61
1:D:162:PHE:CZ	1:D:181:PHE:CB	2.76	0.61
1:C:534:ASN:HB2	1:C:591:LEU:HD21	1.83	0.61
1:C:217:LYS:HB3	1:D:617:THR:HB	1.83	0.60
1:B:372:ILE:HG23	1:B:437:VAL:CG2	2.32	0.60
1:B:516:TYR:HE1	1:B:551:TYR:CD2	2.18	0.60
1:A:248:GLN:OE1	1:A:578:HIS:NE2	2.31	0.60
1:B:504:PHE:CD1	1:B:549:GLN:CD	2.74	0.60
1:C:516:TYR:HE1	1:C:551:TYR:CD2	2.19	0.60
1:B:302:GLN:HA	1:B:312:VAL:HG11	1.84	0.60
1:D:248:GLN:OE1	1:D:578:HIS:NE2	2.30	0.60
1:D:351:THR:HG23	1:D:417:PHE:HE2	1.66	0.60
1:B:54:CYS:HB2	1:B:85:ASP:HB2	1.83	0.60
1:C:255:LEU:HA	1:D:188:ARG:HH22	1.66	0.60
1:A:46:SER:H	1:B:257:ARG:NH2	1.99	0.60
1:C:372:ILE:HG23	1:C:437:VAL:CG2	2.31	0.60
1:C:302:GLN:HA	1:C:312:VAL:HG11	1.84	0.60
1:C:399:ILE:HD11	1:C:439:LEU:HB3	1.84	0.59
1:C:504:PHE:HD1	1:C:549:GLN:CD	2.05	0.59
1:B:400:LEU:HD23	1:B:440:LEU:HD12	1.84	0.59
1:C:73:GLN:HB3	1:C:82:VAL:HG13	1.84	0.59
1:D:228:VAL:HG13	1:D:237:TYR:HB2	1.83	0.59
1:B:228:VAL:HG13	1:B:237:TYR:HB2	1.84	0.59
1:B:351:THR:HG23	1:B:417:PHE:HE2	1.67	0.59
1:C:471:ARG:HG3	1:C:471:ARG:O	2.03	0.59
1:A:504:PHE:CD1	1:A:549:GLN:OE1	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLN:HB3	1:A:82:VAL:HG13	1.84	0.59
1:C:400:LEU:HD23	1:C:440:LEU:HD12	1.83	0.59
1:D:54:CYS:HB2	1:D:85:ASP:HB2	1.84	0.59
1:C:587:ARG:O	1:C:591:LEU:HD13	2.02	0.59
1:C:92:VAL:HG13	1:C:141:ILE:HG23	1.84	0.59
1:D:302:GLN:HA	1:D:312:VAL:HG11	1.85	0.59
1:D:49:VAL:O	1:D:49:VAL:HG13	2.03	0.59
1:D:73:GLN:HB3	1:D:82:VAL:HG13	1.85	0.59
1:A:400:LEU:HD23	1:A:440:LEU:HD12	1.84	0.59
1:D:400:LEU:HD23	1:D:440:LEU:HD12	1.84	0.59
1:D:92:VAL:HG13	1:D:141:ILE:HG23	1.84	0.59
1:A:302:GLN:HA	1:A:312:VAL:HG11	1.85	0.58
1:D:344:ILE:HD11	1:D:440:LEU:HD23	1.84	0.58
1:C:403:PHE:CD2	1:C:437:VAL:CG1	2.85	0.58
1:A:227:LEU:HD13	1:A:236:PHE:HE1	1.69	0.58
1:A:399:ILE:HD11	1:A:439:LEU:HB3	1.84	0.58
1:A:92:VAL:HG13	1:A:141:ILE:HG23	1.85	0.58
1:B:270:SER:HA	1:B:272:PRO:HD3	1.85	0.58
1:B:344:ILE:HD11	1:B:440:LEU:HD23	1.84	0.58
1:A:257:ARG:NH2	1:B:46:SER:H	2.00	0.58
1:C:49:VAL:O	1:C:49:VAL:HG13	2.04	0.58
1:A:351:THR:HG23	1:A:417:PHE:HE2	1.67	0.58
1:B:73:GLN:HB3	1:B:82:VAL:HG13	1.84	0.58
1:B:399:ILE:HD11	1:B:439:LEU:HB3	1.84	0.58
1:C:611:HIS:HA	1:C:617:THR:O	2.04	0.58
1:A:504:PHE:HD1	1:A:549:GLN:OE1	1.86	0.57
1:D:399:ILE:HD11	1:D:439:LEU:HB3	1.85	0.57
1:B:227:LEU:HD13	1:B:236:PHE:HE1	1.69	0.57
1:B:92:VAL:HG13	1:B:141:ILE:HG23	1.85	0.57
1:C:344:ILE:HD11	1:C:440:LEU:HD23	1.86	0.57
1:D:208:VAL:HG21	1:D:255:LEU:HD22	1.85	0.57
1:A:611:HIS:HA	1:A:617:THR:O	2.04	0.57
1:A:190:ARG:NH1	1:B:211:GLU:OE2	2.38	0.57
1:A:198:ARG:CG	1:B:195:MET:CE	2.80	0.57
1:B:49:VAL:HG13	1:B:49:VAL:O	2.05	0.57
1:B:611:HIS:HA	1:B:617:THR:O	2.05	0.57
1:C:339:MET:O	1:C:456:ARG:NE	2.37	0.57
1:B:54:CYS:SG	1:B:68:LEU:HD13	2.45	0.57
1:D:270:SER:HA	1:D:272:PRO:HD3	1.86	0.57
1:A:46:SER:O	1:B:257:ARG:NH2	2.35	0.57
1:A:211:GLU:OE2	1:B:190:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ILE:HG23	1:D:437:VAL:CG2	2.34	0.57
1:D:54:CYS:SG	1:D:68:LEU:HD13	2.44	0.57
1:B:208:VAL:HG21	1:B:255:LEU:HD22	1.87	0.57
1:A:49:VAL:HG13	1:A:49:VAL:O	2.04	0.56
1:C:248:GLN:OE1	1:C:578:HIS:NE2	2.30	0.56
1:A:217:LYS:HB3	1:B:617:THR:HB	1.87	0.56
1:C:190:ARG:NH1	1:D:211:GLU:OE2	2.38	0.56
1:B:275:GLN:HE21	1:B:602:ILE:HD13	1.68	0.56
1:A:608:PHE:HE2	1:D:414:VAL:HA	1.66	0.56
1:A:344:ILE:HD11	1:A:440:LEU:HD23	1.86	0.56
1:C:625:GLU:OE2	1:D:218:ARG:NH1	2.39	0.56
1:C:211:GLU:OE2	1:D:190:ARG:NH1	2.39	0.56
1:D:214:THR:O	1:D:240:PRO:HD3	2.05	0.56
1:D:197:MET:HG3	1:D:304:SER:OG	2.05	0.56
1:A:189:LEU:HD13	1:A:593:THR:HG22	1.88	0.56
1:B:189:LEU:HD13	1:B:593:THR:HG22	1.88	0.56
1:B:370:ILE:HG23	1:B:452:LEU:HD13	1.88	0.56
1:D:248:GLN:HB2	1:D:567:LEU:HD11	1.88	0.56
1:C:227:LEU:HD13	1:C:236:PHE:HE1	1.69	0.56
1:C:370:ILE:HG23	1:C:452:LEU:HD13	1.88	0.56
1:D:611:HIS:HA	1:D:617:THR:O	2.06	0.56
1:B:248:GLN:OE1	1:B:578:HIS:NE2	2.31	0.55
1:D:227:LEU:HD13	1:D:236:PHE:HE1	1.69	0.55
1:A:625:GLU:OE2	1:B:218:ARG:NH1	2.39	0.55
1:A:188:ARG:HH22	1:B:255:LEU:HA	1.71	0.55
1:C:248:GLN:HB2	1:C:567:LEU:HD11	1.88	0.55
1:C:198:ARG:CB	1:D:195:MET:HE1	2.35	0.55
1:C:188:ARG:HH22	1:D:255:LEU:HA	1.71	0.55
1:A:248:GLN:HB2	1:A:567:LEU:HD11	1.87	0.55
1:C:504:PHE:HD1	1:C:549:GLN:NE2	2.00	0.55
1:A:214:THR:O	1:A:240:PRO:HD3	2.06	0.55
1:A:208:VAL:HG21	1:A:255:LEU:HD22	1.88	0.55
1:C:126:PRO:HG2	1:C:129:GLN:HG3	1.89	0.55
1:C:214:THR:O	1:C:240:PRO:HD3	2.07	0.55
1:B:69:CYS:HB3	1:B:117:GLN:HG3	1.89	0.55
1:D:189:LEU:HD13	1:D:593:THR:HG22	1.88	0.55
1:A:339:MET:O	1:A:456:ARG:NE	2.40	0.54
1:C:54:CYS:HB2	1:C:85:ASP:HB2	1.90	0.54
1:C:97:ASP:OD1	1:C:98:GLU:N	2.38	0.54
1:A:247:LYS:HE2	1:A:284:GLU:HG2	1.89	0.54
1:D:391:ALA:O	1:D:396:ASN:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLN:HB2	1:B:567:LEU:HD11	1.88	0.54
1:C:189:LEU:HD13	1:C:593:THR:HG22	1.89	0.54
1:A:126:PRO:HG2	1:A:129:GLN:HG3	1.90	0.54
1:D:379:LEU:HB3	1:D:383:ASP:OD1	2.08	0.54
1:A:400:LEU:HD11	1:A:415:ALA:HB2	1.90	0.54
1:B:197:MET:HG3	1:B:304:SER:OG	2.07	0.54
1:C:208:VAL:HG21	1:C:255:LEU:HD22	1.89	0.54
1:C:402:VAL:HB	1:C:438:VAL:HG23	1.90	0.54
1:D:97:ASP:OD1	1:D:98:GLU:N	2.37	0.54
1:A:195:MET:HE1	1:B:198:ARG:HG2	1.78	0.53
1:A:534:ASN:HB2	1:A:591:LEU:HD21	1.90	0.53
1:C:197:MET:HG3	1:C:304:SER:OG	2.08	0.53
1:D:339:MET:O	1:D:456:ARG:NE	2.40	0.53
1:D:546:ALA:HB2	1:D:571:LEU:HB3	1.90	0.53
1:C:195:MET:HE3	1:D:202:CYS:HB3	1.90	0.53
1:C:257:ARG:NH2	1:D:46:SER:O	2.38	0.53
1:B:339:MET:O	1:B:456:ARG:NE	2.40	0.53
1:C:402:VAL:HG22	1:C:415:ALA:HB1	1.90	0.53
1:A:370:ILE:HG23	1:A:452:LEU:HD13	1.90	0.53
1:A:391:ALA:O	1:A:396:ASN:HA	2.09	0.53
1:A:546:ALA:HB2	1:A:571:LEU:HB3	1.90	0.53
1:C:391:ALA:O	1:C:396:ASN:HA	2.09	0.53
1:D:402:VAL:HG22	1:D:415:ALA:HB1	1.90	0.53
1:D:534:ASN:HB2	1:D:591:LEU:HD21	1.91	0.53
1:B:419:MET:O	1:B:423:ARG:HB2	2.08	0.53
1:D:419:MET:O	1:D:423:ARG:HB2	2.09	0.53
1:B:379:LEU:HB3	1:B:383:ASP:OD1	2.08	0.53
1:C:329:GLY:HA3	1:C:453:GLY:HA3	1.91	0.53
1:D:402:VAL:HB	1:D:438:VAL:HG23	1.90	0.53
1:B:247:LYS:HE2	1:B:284:GLU:HG2	1.89	0.53
1:B:400:LEU:HD11	1:B:415:ALA:HB2	1.91	0.53
1:D:514:LEU:HB2	1:D:522:ALA:HB2	1.91	0.53
1:D:126:PRO:HG2	1:D:129:GLN:HG3	1.90	0.53
1:D:247:LYS:HE2	1:D:284:GLU:HG2	1.90	0.53
1:A:419:MET:O	1:A:423:ARG:HB2	2.09	0.53
1:B:214:THR:O	1:B:240:PRO:HD3	2.08	0.53
1:D:486:LEU:HD22	1:D:507:PRO:HB3	1.91	0.53
1:A:514:LEU:HB2	1:A:522:ALA:HB2	1.91	0.53
1:B:504:PHE:HD1	1:B:549:GLN:OE1	1.92	0.53
1:C:400:LEU:HD11	1:C:415:ALA:HB2	1.90	0.53
1:A:486:LEU:HD22	1:A:507:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:HB3	1:A:383:ASP:OD1	2.09	0.52
1:A:402:VAL:HG22	1:A:415:ALA:HB1	1.89	0.52
1:D:200:TYR:CE1	1:D:205:HIS:CE1	2.96	0.52
1:A:198:ARG:HD3	1:A:259:PHE:CZ	2.44	0.52
1:A:197:MET:HG3	1:A:304:SER:OG	2.09	0.52
1:A:504:PHE:HD1	1:A:549:GLN:NE2	2.06	0.52
1:B:402:VAL:HB	1:B:438:VAL:HG23	1.91	0.52
1:B:509:PRO:O	1:B:512:ILE:N	2.42	0.52
1:C:69:CYS:HB3	1:C:117:GLN:HG3	1.91	0.52
1:A:69:CYS:HB3	1:A:117:GLN:HG3	1.92	0.52
1:D:370:ILE:HG23	1:D:452:LEU:HD13	1.90	0.52
1:B:126:PRO:HG2	1:B:129:GLN:HG3	1.90	0.52
1:B:391:ALA:O	1:B:396:ASN:HA	2.10	0.52
1:C:546:ALA:HB2	1:C:571:LEU:HB3	1.92	0.52
1:B:198:ARG:HD3	1:B:259:PHE:CZ	2.45	0.52
1:C:379:LEU:HB3	1:C:383:ASP:OD1	2.08	0.52
1:D:69:CYS:HB3	1:D:117:GLN:HG3	1.91	0.52
1:A:402:VAL:HB	1:A:438:VAL:HG23	1.91	0.52
1:A:509:PRO:O	1:A:512:ILE:N	2.42	0.52
1:D:400:LEU:HD11	1:D:415:ALA:HB2	1.92	0.52
1:C:419:MET:O	1:C:423:ARG:HB2	2.09	0.52
1:C:509:PRO:O	1:C:512:ILE:N	2.42	0.52
1:D:174:ARG:O	1:D:178:LEU:HG	2.10	0.52
1:A:198:ARG:HD3	1:A:259:PHE:HZ	1.74	0.52
1:B:546:ALA:HB2	1:B:571:LEU:HB3	1.90	0.52
1:C:198:ARG:HD3	1:C:259:PHE:HZ	1.75	0.52
1:B:198:ARG:HD3	1:B:259:PHE:HZ	1.75	0.52
1:B:93:ILE:HD11	1:B:123:ILE:HD11	1.92	0.51
1:C:247:LYS:HE2	1:C:284:GLU:HG2	1.92	0.51
1:C:46:SER:O	1:D:257:ARG:NH2	2.39	0.51
1:D:423:ARG:O	1:D:427:ILE:HG12	2.10	0.51
1:A:195:MET:CE	1:B:198:ARG:HG2	2.34	0.51
1:C:113:GLU:O	1:C:152:CYS:SG	2.65	0.51
1:D:198:ARG:HD3	1:D:259:PHE:CZ	2.46	0.51
1:C:198:ARG:HD3	1:C:259:PHE:CZ	2.45	0.51
1:C:508:HIS:HB3	1:C:523:ARG:HG3	1.92	0.51
1:D:509:PRO:O	1:D:512:ILE:N	2.42	0.51
1:D:71:TRP:HE1	1:D:179:ARG:HH21	1.59	0.51
1:B:508:HIS:HB3	1:B:523:ARG:HG3	1.92	0.51
1:B:514:LEU:HB2	1:B:522:ALA:HB2	1.92	0.51
1:B:97:ASP:OD1	1:B:98:GLU:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:CE1	1:A:205:HIS:CE1	2.98	0.51
1:B:402:VAL:HG22	1:B:415:ALA:HB1	1.92	0.51
1:C:218:ARG:NH1	1:D:625:GLU:OE2	2.44	0.51
1:D:377:LYS:HG2	1:D:407:ASN:HD21	1.76	0.51
1:A:174:ARG:O	1:A:178:LEU:HG	2.11	0.51
1:C:200:TYR:CE1	1:C:205:HIS:CE1	2.98	0.51
1:D:198:ARG:HD3	1:D:259:PHE:HZ	1.75	0.51
1:A:54:CYS:HB2	1:A:85:ASP:HB2	1.93	0.51
1:B:504:PHE:CD1	1:B:549:GLN:OE1	2.64	0.51
1:D:508:HIS:HB3	1:D:523:ARG:HG3	1.93	0.51
1:C:55:GLY:HA3	1:C:88:GLY:HA3	1.92	0.51
1:A:504:PHE:HD1	1:A:549:GLN:CD	2.10	0.50
1:C:93:ILE:HD11	1:C:123:ILE:HD11	1.93	0.50
1:C:227:LEU:O	1:D:229:PRO:HD2	2.11	0.50
1:C:589:ILE:HG23	1:C:601:VAL:HG21	1.93	0.50
1:D:265:TYR:HD1	1:D:277:GLU:HB3	1.76	0.50
1:A:329:GLY:HA3	1:A:453:GLY:HA3	1.91	0.50
1:C:514:LEU:HB2	1:C:522:ALA:HB2	1.93	0.50
1:A:97:ASP:OD1	1:A:98:GLU:N	2.37	0.50
1:A:113:GLU:C	1:A:152:CYS:HG	2.08	0.50
1:B:471:ARG:O	1:B:471:ARG:HG3	2.11	0.50
1:B:486:LEU:HD22	1:B:507:PRO:HB3	1.93	0.50
1:C:377:LYS:HG2	1:C:407:ASN:HD21	1.77	0.50
1:B:551:TYR:O	1:B:555:THR:HG23	2.12	0.50
1:C:423:ARG:O	1:C:427:ILE:HG12	2.11	0.50
1:A:314:VAL:HB	1:A:315:PRO:CD	2.40	0.50
1:A:508:HIS:HB3	1:A:523:ARG:HG3	1.93	0.50
1:B:366:THR:HG21	1:B:368:LYS:HE2	1.94	0.50
1:D:505:THR:HG23	1:D:540:SER:HB2	1.93	0.50
1:C:344:ILE:HG22	1:C:429:LEU:HD13	1.94	0.50
1:C:90:VAL:HG23	1:C:136:THR:HB	1.94	0.50
1:A:377:LYS:HG2	1:A:407:ASN:HD21	1.77	0.49
1:C:174:ARG:O	1:C:178:LEU:HG	2.11	0.49
1:B:265:TYR:HD1	1:B:277:GLU:HB3	1.77	0.49
1:B:377:LYS:HG2	1:B:407:ASN:HD21	1.76	0.49
1:A:45:SER:OG	1:A:50:ARG:NH2	2.45	0.49
1:B:171:LEU:HB2	1:B:613:LEU:HD12	1.95	0.49
1:B:314:VAL:HB	1:B:315:PRO:CD	2.40	0.49
1:B:589:ILE:HG23	1:B:601:VAL:HG21	1.94	0.49
1:A:218:ARG:NH1	1:B:625:GLU:OE2	2.45	0.49
1:A:274:ARG:CZ	1:A:587:ARG:HH21	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ARG:O	1:A:427:ILE:HG12	2.13	0.49
1:A:505:THR:HG23	1:A:540:SER:HB2	1.94	0.49
1:B:423:ARG:O	1:B:427:ILE:HG12	2.11	0.49
1:C:486:LEU:HD22	1:C:507:PRO:HB3	1.93	0.49
1:D:74:TYR:O	1:D:82:VAL:HG12	2.12	0.49
1:A:490:LYS:CB	1:A:491:GLU:HA	2.35	0.49
1:B:215:LEU:HD13	1:B:237:TYR:CE2	2.48	0.49
1:C:117:GLN:HB2	1:C:149:LEU:HD11	1.94	0.49
1:D:93:ILE:HD11	1:D:123:ILE:HD11	1.94	0.49
1:B:505:THR:HG23	1:B:540:SER:HB2	1.94	0.49
1:B:74:TYR:O	1:B:82:VAL:HG12	2.13	0.49
1:C:504:PHE:CE1	1:C:549:GLN:CD	2.85	0.49
1:A:55:GLY:HA3	1:A:88:GLY:HA3	1.95	0.49
1:A:93:ILE:HD11	1:A:123:ILE:HD11	1.95	0.49
1:D:312:VAL:HG22	1:D:313:VAL:H	1.77	0.49
1:A:293:ILE:HD11	1:A:527:TYR:CE1	2.47	0.49
1:B:117:GLN:HB2	1:B:149:LEU:HD11	1.94	0.49
1:D:366:THR:HG21	1:D:368:LYS:HE2	1.94	0.49
1:B:90:VAL:HG23	1:B:136:THR:HB	1.95	0.48
1:B:162:PHE:CE1	1:B:181:PHE:HB2	2.47	0.48
1:C:366:THR:HG21	1:C:368:LYS:HE2	1.94	0.48
1:C:74:TYR:O	1:C:82:VAL:HG12	2.12	0.48
1:D:117:GLN:HB2	1:D:149:LEU:HD11	1.95	0.48
1:A:366:THR:HG21	1:A:368:LYS:HE2	1.94	0.48
1:B:200:TYR:CE1	1:B:205:HIS:CE1	3.00	0.48
1:C:505:THR:HG23	1:C:540:SER:HB2	1.95	0.48
1:D:171:LEU:HB2	1:D:613:LEU:HD12	1.95	0.48
1:C:229:PRO:HA	1:C:236:PHE:HB3	1.96	0.48
1:D:229:PRO:HA	1:D:236:PHE:HB3	1.95	0.48
1:D:45:SER:OG	1:D:50:ARG:NH2	2.47	0.48
1:C:256:ASP:CG	1:D:50:ARG:HH22	2.17	0.48
1:A:90:VAL:HG23	1:A:136:THR:HB	1.95	0.48
1:B:55:GLY:HA3	1:B:88:GLY:HA3	1.96	0.48
1:D:314:VAL:HB	1:D:315:PRO:CD	2.40	0.48
1:D:293:ILE:HD11	1:D:527:TYR:CZ	2.49	0.48
1:D:275:GLN:NE2	1:D:602:ILE:HD12	2.29	0.48
1:A:312:VAL:HG22	1:A:313:VAL:H	1.79	0.48
1:C:163:VAL:HG12	1:C:164:LYS:HG2	1.96	0.48
1:A:74:TYR:O	1:A:82:VAL:HG12	2.14	0.48
1:B:174:ARG:O	1:B:178:LEU:HG	2.14	0.48
1:C:266:ARG:HD2	1:C:278:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:TYR:O	1:D:555:THR:HG23	2.14	0.48
1:D:571:LEU:HA	1:D:571:LEU:HD13	1.70	0.48
1:D:57:LEU:HA	1:D:61:HIS:ND1	2.29	0.48
1:D:589:ILE:HG23	1:D:601:VAL:HG21	1.95	0.48
1:A:117:GLN:HB2	1:A:149:LEU:HD11	1.95	0.48
1:A:229:PRO:HD2	1:B:227:LEU:O	2.14	0.48
1:A:617:THR:HB	1:B:217:LYS:HB3	1.94	0.48
1:B:312:VAL:HG22	1:B:313:VAL:H	1.79	0.48
1:D:163:VAL:HG12	1:D:164:LYS:HG2	1.96	0.48
1:D:504:PHE:CD1	1:D:549:GLN:NE2	2.82	0.48
1:A:171:LEU:HD23	1:A:174:ARG:HD3	1.96	0.47
1:D:90:VAL:HG23	1:D:136:THR:HB	1.95	0.47
1:A:511:ASP:OD2	1:A:513:HIS:HB3	2.14	0.47
1:B:171:LEU:HD23	1:B:174:ARG:HD3	1.96	0.47
1:C:171:LEU:HB2	1:C:613:LEU:HD12	1.95	0.47
1:C:306:PRO:C	1:C:308:ASP:H	2.18	0.47
1:C:617:THR:HB	1:D:217:LYS:HB3	1.95	0.47
1:D:319:MET:HB2	1:D:479:LEU:HD11	1.96	0.47
1:D:293:ILE:HD11	1:D:527:TYR:CE1	2.48	0.47
1:A:589:ILE:HG23	1:A:601:VAL:HG21	1.95	0.47
1:A:171:LEU:HB2	1:A:613:LEU:HD12	1.96	0.47
1:B:229:PRO:HA	1:B:236:PHE:HB3	1.96	0.47
1:B:489:PRO:HB2	1:B:494:PRO:HG3	1.97	0.47
1:C:274:ARG:CZ	1:C:587:ARG:HH21	2.27	0.47
1:A:114:SER:HB3	1:A:150:ASN:O	2.14	0.47
1:C:114:SER:HB3	1:C:150:ASN:O	2.15	0.47
1:C:511:ASP:OD2	1:C:513:HIS:HB3	2.15	0.47
1:A:163:VAL:HG12	1:A:164:LYS:HG2	1.96	0.47
1:A:489:PRO:HB2	1:A:494:PRO:HG3	1.97	0.47
1:B:293:ILE:HD11	1:B:527:TYR:CE1	2.49	0.47
1:B:319:MET:HB2	1:B:479:LEU:HD11	1.96	0.47
1:C:312:VAL:HG22	1:C:313:VAL:H	1.80	0.47
1:C:551:TYR:O	1:C:555:THR:HG23	2.14	0.47
1:C:50:ARG:HH22	1:D:256:ASP:CG	2.17	0.47
1:B:114:SER:HB3	1:B:150:ASN:O	2.14	0.47
1:B:270:SER:HA	1:B:271:ARG:HA	1.64	0.47
1:C:314:VAL:HB	1:C:315:PRO:CD	2.39	0.47
1:A:306:PRO:C	1:A:308:ASP:H	2.17	0.47
1:D:113:GLU:OE1	1:D:159:ILE:HG13	2.14	0.47
1:A:293:ILE:HD11	1:A:527:TYR:CZ	2.49	0.47
1:B:215:LEU:CD1	1:B:237:TYR:CE2	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:GLU:OE1	1:B:496:GLU:HG3	2.14	0.47
1:C:229:PRO:HD2	1:D:227:LEU:O	2.14	0.47
1:A:229:PRO:HA	1:A:236:PHE:HB3	1.96	0.47
1:B:306:PRO:C	1:B:308:ASP:H	2.18	0.47
1:B:57:LEU:HA	1:B:61:HIS:ND1	2.30	0.46
1:D:270:SER:HA	1:D:271:ARG:HA	1.64	0.46
1:A:85:ASP:OD1	1:A:86:PHE:CD1	2.68	0.46
1:D:55:GLY:HA3	1:D:88:GLY:HA3	1.96	0.46
1:C:319:MET:HB2	1:C:479:LEU:HD11	1.98	0.46
1:C:489:PRO:HB2	1:C:494:PRO:HG3	1.97	0.46
1:C:492:GLU:OE1	1:C:496:GLU:HG3	2.15	0.46
1:C:477:SER:N	1:C:532:ASN:OD1	2.34	0.46
1:D:305:TRP:HZ2	1:D:476:PHE:CD1	2.33	0.46
1:D:494:PRO:HA	1:D:495:ARG:HA	1.42	0.46
1:A:227:LEU:O	1:B:229:PRO:HD2	2.14	0.46
1:A:319:MET:HB2	1:A:479:LEU:HD11	1.97	0.46
1:A:424:LEU:HD12	1:A:424:LEU:H	1.81	0.46
1:B:157:PHE:CE1	1:B:173:TYR:HB2	2.51	0.46
1:B:163:VAL:HG12	1:B:164:LYS:HG2	1.97	0.46
1:B:45:SER:OG	1:B:50:ARG:NH2	2.48	0.46
1:B:510:SER:O	1:B:510:SER:OG	2.30	0.46
1:A:536:ILE:HG13	1:A:588:LEU:HB2	1.97	0.46
1:D:318:THR:HA	1:D:480:TRP:HB2	1.97	0.46
1:D:489:PRO:HB2	1:D:494:PRO:HG3	1.96	0.46
1:A:537:GLY:HA3	1:A:583:LEU:HD12	1.98	0.46
1:B:318:THR:HA	1:B:480:TRP:HB2	1.98	0.46
1:D:492:GLU:OE1	1:D:496:GLU:HG3	2.15	0.46
1:A:494:PRO:HA	1:A:495:ARG:HA	1.43	0.46
1:D:171:LEU:HD23	1:D:174:ARG:HD3	1.96	0.46
1:D:71:TRP:HE1	1:D:179:ARG:NH2	2.13	0.46
1:A:164:LYS:HB2	1:D:396:ASN:ND2	2.31	0.46
1:A:261:VAL:HG12	1:A:281:ILE:HG12	1.98	0.46
1:A:266:ARG:HD2	1:A:278:PHE:CE1	2.50	0.46
1:B:537:GLY:HA3	1:B:583:LEU:HD12	1.98	0.46
1:D:306:PRO:C	1:D:308:ASP:H	2.18	0.46
1:B:337:PHE:CZ	1:B:339:MET:HE3	2.51	0.45
1:C:424:LEU:H	1:C:424:LEU:HD12	1.81	0.45
1:A:218:ARG:NE	1:A:220:PRO:HG3	2.32	0.45
1:B:293:ILE:HD11	1:B:527:TYR:CZ	2.52	0.45
1:B:544:HIS:O	1:B:545:ASN:ND2	2.50	0.45
1:C:53:THR:O	1:C:56:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:SER:HB3	1:D:150:ASN:O	2.16	0.45
1:A:551:TYR:O	1:A:555:THR:HG23	2.16	0.45
1:A:57:LEU:HA	1:A:61:HIS:ND1	2.31	0.45
1:B:511:ASP:OD2	1:B:513:HIS:HB3	2.16	0.45
1:C:171:LEU:HD23	1:C:174:ARG:HD3	1.98	0.45
1:C:157:PHE:CE1	1:C:173:TYR:HB2	2.52	0.45
1:B:424:LEU:H	1:B:424:LEU:HD12	1.81	0.45
1:B:536:ILE:HG13	1:B:588:LEU:HB2	1.99	0.45
1:C:494:PRO:HA	1:C:495:ARG:HA	1.43	0.45
1:D:424:LEU:HD12	1:D:424:LEU:H	1.82	0.45
1:C:285:MET:HB2	1:C:288:VAL:HG11	1.99	0.45
1:A:475:LEU:HD12	1:A:476:PHE:H	1.82	0.45
1:C:218:ARG:NE	1:C:220:PRO:HG3	2.32	0.45
1:C:339:MET:H	1:C:456:ARG:HH21	1.65	0.45
1:C:45:SER:OG	1:C:50:ARG:NH2	2.49	0.45
1:C:536:ILE:HG13	1:C:588:LEU:HB2	1.98	0.45
1:C:565:SER:O	1:C:569:GLN:HB2	2.17	0.45
1:D:285:MET:HB2	1:D:288:VAL:HG11	1.99	0.45
1:A:492:GLU:OE1	1:A:496:GLU:HG3	2.16	0.45
1:D:275:GLN:NE2	1:D:602:ILE:CD1	2.80	0.45
1:A:256:ASP:CG	1:B:50:ARG:HH22	2.20	0.45
1:B:266:ARG:HD2	1:B:278:PHE:HE2	1.82	0.45
1:B:339:MET:H	1:B:456:ARG:HH21	1.65	0.45
1:C:147:GLU:HG2	1:C:148:LEU:N	2.32	0.45
1:C:258:TYR:CD2	1:C:284:GLU:HB2	2.46	0.45
1:C:379:LEU:HD12	1:C:379:LEU:H	1.82	0.45
1:A:202:CYS:HB3	1:B:195:MET:HE3	1.98	0.44
1:B:228:VAL:O	1:B:236:PHE:HB2	2.17	0.44
1:C:57:LEU:HA	1:C:61:HIS:ND1	2.32	0.44
1:C:198:ARG:HG2	1:D:195:MET:CE	2.36	0.44
1:C:589:ILE:HA	1:C:592:VAL:HG12	1.99	0.44
1:D:334:ASP:OD1	1:D:336:ARG:NE	2.37	0.44
1:A:54:CYS:SG	1:A:68:LEU:HD13	2.58	0.44
1:B:162:PHE:HE1	1:B:181:PHE:HB2	1.81	0.44
1:B:379:LEU:H	1:B:379:LEU:HD12	1.81	0.44
1:C:198:ARG:C	1:D:195:MET:HE1	2.37	0.44
1:D:266:ARG:HD2	1:D:278:PHE:HE2	1.82	0.44
1:B:53:THR:O	1:B:56:GLU:HG2	2.17	0.44
1:D:510:SER:OG	1:D:510:SER:O	2.31	0.44
1:C:537:GLY:HA3	1:C:583:LEU:HD12	1.98	0.44
1:A:404:LEU:HA	1:A:419:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:SER:O	1:A:569:GLN:HB2	2.18	0.44
1:B:218:ARG:NE	1:B:220:PRO:HG3	2.33	0.44
1:B:72:ILE:O	1:B:113:GLU:HA	2.18	0.44
1:C:544:HIS:O	1:C:545:ASN:ND2	2.51	0.44
1:D:218:ARG:NE	1:D:220:PRO:HG3	2.32	0.44
1:B:589:ILE:HA	1:B:592:VAL:HG12	2.00	0.44
1:C:72:ILE:O	1:C:113:GLU:HA	2.18	0.44
1:C:371:CYS:HB2	1:C:438:VAL:HG12	1.99	0.44
1:C:318:THR:HA	1:C:480:TRP:HB2	1.98	0.44
1:D:228:VAL:O	1:D:236:PHE:HB2	2.18	0.44
1:D:247:LYS:NZ	1:D:542:ARG:HH21	2.16	0.44
1:D:511:ASP:OD2	1:D:513:HIS:HB3	2.18	0.44
1:D:589:ILE:HA	1:D:592:VAL:HG12	2.00	0.44
1:A:345:SER:HA	1:A:367:VAL:HG13	2.00	0.44
1:A:589:ILE:HA	1:A:592:VAL:HG12	1.99	0.44
1:D:261:VAL:HG12	1:D:281:ILE:HG12	2.00	0.44
1:B:345:SER:HA	1:B:367:VAL:HG13	2.00	0.44
1:D:319:MET:O	1:D:482:VAL:HG22	2.18	0.44
1:A:371:CYS:HB2	1:A:438:VAL:HG12	2.00	0.43
1:B:92:VAL:HG11	1:B:118:VAL:HG11	2.00	0.43
1:B:208:VAL:HG22	1:B:257:ARG:O	2.19	0.43
1:C:261:VAL:HG12	1:C:281:ILE:HG12	1.99	0.43
1:D:537:GLY:HA3	1:D:583:LEU:HD12	1.98	0.43
1:A:147:GLU:HG2	1:A:148:LEU:N	2.33	0.43
1:B:83:LEU:HG	1:B:92:VAL:HG21	2.01	0.43
1:A:318:THR:HA	1:A:480:TRP:HB2	1.99	0.43
1:B:261:VAL:HG12	1:B:281:ILE:HG12	1.99	0.43
1:C:516:TYR:CE1	1:C:551:TYR:CD2	3.05	0.43
1:C:83:LEU:HG	1:C:92:VAL:HG21	2.01	0.43
1:D:345:SER:HA	1:D:367:VAL:HG13	2.00	0.43
1:B:371:CYS:HB2	1:B:438:VAL:HG12	2.01	0.43
1:A:92:VAL:HG11	1:A:118:VAL:HG11	2.00	0.43
1:A:516:TYR:CE1	1:A:551:TYR:CD2	3.04	0.43
1:A:571:LEU:HA	1:A:571:LEU:HD13	1.71	0.43
1:B:258:TYR:OH	1:B:260:GLN:NE2	2.50	0.43
1:C:399:ILE:HG13	1:C:439:LEU:HD12	2.01	0.43
1:D:147:GLU:HG2	1:D:148:LEU:N	2.34	0.43
1:D:305:TRP:HA	1:D:306:PRO:HD3	1.77	0.43
1:D:339:MET:H	1:D:456:ARG:HH21	1.64	0.43
1:A:285:MET:HB2	1:A:288:VAL:HG11	2.01	0.43
1:A:471:ARG:HG3	1:A:471:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:O	1:A:113:GLU:HA	2.19	0.43
1:A:50:ARG:HH22	1:B:256:ASP:CG	2.22	0.43
1:B:319:MET:O	1:B:482:VAL:HG22	2.18	0.43
1:C:412:SER:O	1:C:416:ASN:HB2	2.19	0.43
1:C:620:SER:N	1:D:235:LYS:HG2	2.33	0.43
1:D:339:MET:HE2	1:D:373:PRO:HD2	2.01	0.43
1:D:379:LEU:HD12	1:D:379:LEU:H	1.84	0.43
1:D:565:SER:O	1:D:569:GLN:HB2	2.19	0.43
1:D:92:VAL:HG11	1:D:118:VAL:HG11	2.00	0.43
1:D:157:PHE:CE1	1:D:173:TYR:HB2	2.53	0.43
1:D:53:THR:O	1:D:56:GLU:HG2	2.18	0.43
1:A:53:THR:O	1:A:56:GLU:HG2	2.18	0.43
1:D:72:ILE:O	1:D:113:GLU:HA	2.18	0.43
1:A:328:TYR:O	1:A:453:GLY:HA2	2.19	0.43
1:B:230:SER:HB3	1:B:235:LYS:O	2.19	0.43
1:B:372:ILE:CG2	1:B:437:VAL:HG23	2.42	0.43
1:C:404:LEU:HA	1:C:419:MET:HG3	1.99	0.43
1:D:536:ILE:HG13	1:D:588:LEU:HB2	2.01	0.43
1:B:285:MET:HB2	1:B:288:VAL:HG11	2.01	0.42
1:B:565:SER:O	1:B:569:GLN:HB2	2.19	0.42
1:B:571:LEU:HA	1:B:571:LEU:HD13	1.73	0.42
1:D:107:LEU:HA	1:D:107:LEU:HD12	1.85	0.42
1:D:78:ASN:HB3	1:D:96:GLN:HE21	1.84	0.42
1:A:339:MET:H	1:A:456:ARG:HH21	1.65	0.42
1:B:215:LEU:HD13	1:B:237:TYR:CZ	2.54	0.42
1:B:494:PRO:HA	1:B:495:ARG:HA	1.44	0.42
1:A:258:TYR:CD2	1:A:284:GLU:HB2	2.47	0.42
1:B:147:GLU:HG2	1:B:148:LEU:N	2.34	0.42
1:C:92:VAL:HG11	1:C:118:VAL:HG11	2.01	0.42
1:A:207:PHE:CG	1:A:257:ARG:HB3	2.54	0.42
1:B:534:ASN:CB	1:B:591:LEU:HD21	2.48	0.42
1:C:513:HIS:CE1	1:C:516:TYR:HB2	2.54	0.42
1:D:230:SER:HB3	1:D:235:LYS:O	2.20	0.42
1:A:164:LYS:NZ	1:D:392:ALA:HB1	2.34	0.42
1:B:325:LEU:HA	1:B:325:LEU:HD12	1.85	0.42
1:C:228:VAL:O	1:C:236:PHE:HB2	2.19	0.42
1:C:479:LEU:HB3	1:C:530:VAL:HG23	2.02	0.42
1:D:531:LEU:HG	1:D:591:LEU:HD23	2.02	0.42
1:D:83:LEU:HG	1:D:92:VAL:HG21	2.01	0.42
1:A:228:VAL:O	1:A:236:PHE:HB2	2.19	0.42
1:A:379:LEU:H	1:A:379:LEU:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:HD2	1:A:411:ASN:OD1	2.20	0.42
1:A:78:ASN:HB3	1:A:96:GLN:HE21	1.84	0.42
1:D:504:PHE:CD1	1:D:549:GLN:CD	2.93	0.42
1:A:207:PHE:CD2	1:A:257:ARG:HB3	2.55	0.42
1:A:399:ILE:HG13	1:A:439:LEU:HD12	2.01	0.42
1:B:504:PHE:HZ	1:B:564:LEU:HD13	1.85	0.42
1:D:207:PHE:CG	1:D:257:ARG:HB3	2.55	0.42
1:A:531:LEU:HG	1:A:591:LEU:HD23	2.02	0.42
1:B:247:LYS:NZ	1:B:542:ARG:HH21	2.17	0.42
1:D:372:ILE:CG2	1:D:437:VAL:HG23	2.44	0.42
1:A:337:PHE:CZ	1:A:339:MET:HE3	2.55	0.42
1:A:478:PHE:CE1	1:A:531:LEU:HD13	2.54	0.42
1:A:620:SER:N	1:B:235:LYS:HG2	2.34	0.42
1:B:265:TYR:CD1	1:B:277:GLU:HB3	2.55	0.42
1:C:204:LEU:HA	1:C:204:LEU:HD12	1.90	0.42
1:C:402:VAL:HG22	1:C:415:ALA:CB	2.50	0.42
1:D:157:PHE:CZ	1:D:173:TYR:HB2	2.55	0.42
1:D:232:GLU:HA	1:D:233:PRO:HD3	1.86	0.42
1:D:404:LEU:HA	1:D:419:MET:HG3	2.02	0.42
1:A:247:LYS:HZ3	1:A:542:ARG:HH21	1.68	0.42
1:C:207:PHE:CG	1:C:257:ARG:HB3	2.55	0.42
1:C:345:SER:HA	1:C:367:VAL:HG13	2.02	0.42
1:C:78:ASN:HB3	1:C:96:GLN:HE21	1.85	0.42
1:C:55:GLY:HA3	1:C:88:GLY:CA	2.50	0.42
1:D:585:LEU:O	1:D:589:ILE:HG22	2.20	0.42
1:D:479:LEU:HB3	1:D:530:VAL:HG23	2.02	0.41
1:A:561:VAL:O	1:A:565:SER:HB2	2.20	0.41
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.91	0.41
1:B:207:PHE:CG	1:B:257:ARG:HB3	2.55	0.41
1:B:207:PHE:CD2	1:B:257:ARG:HB3	2.56	0.41
1:D:399:ILE:HG13	1:D:439:LEU:HD12	2.02	0.41
1:A:305:TRP:HA	1:A:306:PRO:HD3	1.77	0.41
1:A:479:LEU:HB3	1:A:530:VAL:HG23	2.02	0.41
1:B:266:ARG:HD2	1:B:278:PHE:CE2	2.56	0.41
1:C:208:VAL:HG22	1:C:257:ARG:O	2.21	0.41
1:C:207:PHE:CD2	1:C:257:ARG:HB3	2.55	0.41
1:C:490:LYS:CB	1:C:491:GLU:HA	2.35	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD12	1.86	0.41
1:A:585:LEU:O	1:A:589:ILE:HG22	2.21	0.41
1:A:83:LEU:HG	1:A:92:VAL:HG21	2.01	0.41
1:B:561:VAL:O	1:B:565:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:LEU:O	1:B:589:ILE:HG22	2.20	0.41
1:A:510:SER:O	1:A:510:SER:OG	2.32	0.41
1:A:195:MET:HE2	1:B:198:ARG:CG	2.28	0.41
1:B:78:ASN:HB3	1:B:96:GLN:HE21	1.85	0.41
1:C:381:ARG:HD2	1:C:411:ASN:OD1	2.21	0.41
1:D:544:HIS:O	1:D:545:ASN:ND2	2.53	0.41
1:A:544:HIS:O	1:A:545:ASN:ND2	2.53	0.41
1:C:373:PRO:C	1:C:375:GLY:H	2.24	0.41
1:A:265:TYR:HE2	1:B:214:THR:HG1	1.69	0.41
1:C:258:TYR:OH	1:C:260:GLN:NE2	2.51	0.41
1:D:239:LEU:HB3	1:D:265:TYR:CD2	2.56	0.41
1:A:513:HIS:CE1	1:A:516:TYR:HB2	2.54	0.41
1:A:258:TYR:OH	1:A:260:GLN:NE2	2.51	0.41
1:A:373:PRO:C	1:A:375:GLY:H	2.24	0.41
1:A:68:LEU:CD1	1:A:83:LEU:HD12	2.50	0.41
1:B:229:PRO:HA	1:B:236:PHE:CB	2.51	0.41
1:B:479:LEU:HB3	1:B:530:VAL:HG23	2.03	0.41
1:C:230:SER:HB3	1:C:235:LYS:O	2.20	0.41
1:C:276:PRO:HG2	1:C:610:GLY:HA2	2.03	0.41
1:C:289:ASP:N	1:C:289:ASP:OD1	2.49	0.41
1:C:372:ILE:CG2	1:C:437:VAL:HG23	2.41	0.41
1:D:265:TYR:CD1	1:D:277:GLU:HB3	2.54	0.41
1:D:371:CYS:HB2	1:D:438:VAL:HG12	2.02	0.41
1:A:402:VAL:HG22	1:A:415:ALA:CB	2.50	0.41
1:A:412:SER:O	1:A:416:ASN:HB2	2.21	0.41
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.85	0.41
1:D:229:PRO:HA	1:D:236:PHE:CB	2.51	0.41
1:B:464:GLU:HA	1:B:468:VAL:O	2.21	0.41
1:B:275:GLN:HE22	1:B:602:ILE:HD12	1.80	0.41
1:C:319:MET:O	1:C:482:VAL:HG22	2.21	0.41
1:D:513:HIS:CE1	1:D:516:TYR:HB2	2.55	0.41
1:B:198:ARG:HH22	1:B:261:VAL:HG21	1.87	0.40
1:B:404:LEU:H	1:B:404:LEU:HD23	1.86	0.40
1:B:381:ARG:HD2	1:B:411:ASN:OD1	2.21	0.40
1:C:561:VAL:O	1:C:565:SER:HB2	2.21	0.40
1:D:373:PRO:C	1:D:375:GLY:H	2.24	0.40
1:D:49:VAL:O	1:D:49:VAL:CG1	2.69	0.40
1:B:504:PHE:HD1	1:B:549:GLN:CD	2.20	0.40
1:B:96:GLN:HG2	1:B:104:LYS:NZ	2.37	0.40
1:C:44:PHE:HB3	1:C:45:SER:H	1.72	0.40
1:D:412:SER:O	1:D:416:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:MET:SD	1:B:296:LEU:CD1	3.10	0.40
1:D:208:VAL:HG22	1:D:257:ARG:O	2.21	0.40
1:D:266:ARG:HD2	1:D:278:PHE:CE2	2.56	0.40
1:D:381:ARG:HD2	1:D:411:ASN:OD1	2.21	0.40
1:D:402:VAL:HG22	1:D:415:ALA:CB	2.51	0.40
1:A:198:ARG:HH22	1:A:261:VAL:HG21	1.85	0.40
1:B:116:VAL:HG23	1:B:147:GLU:O	2.22	0.40
1:B:167:GLU:CD	1:B:599:ARG:HD2	2.42	0.40
1:C:327:THR:HA	1:C:341:ILE:HB	2.04	0.40
1:C:476:PHE:HB3	1:C:531:LEU:HD11	2.04	0.40
1:C:571:LEU:HA	1:C:571:LEU:HD13	1.71	0.40
1:D:258:TYR:CD2	1:D:284:GLU:HB2	2.47	0.40
1:D:490:LYS:CB	1:D:491:GLU:HA	2.35	0.40
1:A:248:GLN:HE22	1:A:542:ARG:HB3	1.86	0.40
1:B:513:HIS:CE1	1:B:516:TYR:HB2	2.57	0.40
1:B:247:LYS:HZ3	1:B:542:ARG:HH21	1.69	0.40
1:B:516:TYR:CE1	1:B:551:TYR:CD2	3.04	0.40
1:D:96:GLN:HG2	1:D:104:LYS:NZ	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:THR:OG1	1:D:547:GLU:OE2[1_545]	2.18	0.02

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	587/617 (95%)	512 (87%)	71 (12%)	4 (1%)	25	68
1	B	587/617 (95%)	510 (87%)	73 (12%)	4 (1%)	25	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	587/617 (95%)	512 (87%)	71 (12%)	4 (1%)	25	68
1	D	587/617 (95%)	511 (87%)	72 (12%)	4 (1%)	25	68
All	All	2348/2468 (95%)	2045 (87%)	287 (12%)	16 (1%)	25	68

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	ILE
1	B	512	ILE
1	C	512	ILE
1	D	512	ILE
1	A	163	VAL
1	B	163	VAL
1	C	163	VAL
1	D	163	VAL
1	A	112	VAL
1	B	112	VAL
1	C	112	VAL
1	D	112	VAL
1	C	314	VAL
1	D	314	VAL
1	A	314	VAL
1	B	314	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/551 (95%)	509 (97%)	16 (3%)	46	78
1	B	525/551 (95%)	514 (98%)	11 (2%)	59	84
1	C	525/551 (95%)	510 (97%)	15 (3%)	48	78
1	D	525/551 (95%)	512 (98%)	13 (2%)	53	81
All	All	2100/2204 (95%)	2045 (97%)	55 (3%)	51	80

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	TYR
1	A	80	PHE
1	A	162	PHE
1	A	215	LEU
1	A	258	TYR
1	A	259	PHE
1	A	305	TRP
1	A	310	ASP
1	A	334	ASP
1	A	342	ILE
1	A	346	ASP
1	A	483	ASP
1	A	527	TYR
1	A	571	LEU
1	A	617	THR
1	A	625	GLU
1	B	74	TYR
1	B	80	PHE
1	B	258	TYR
1	B	259	PHE
1	B	310	ASP
1	B	334	ASP
1	B	342	ILE
1	B	346	ASP
1	B	483	ASP
1	B	571	LEU
1	B	625	GLU
1	C	74	TYR
1	C	80	PHE
1	C	162	PHE
1	C	215	LEU
1	C	258	TYR
1	C	259	PHE
1	C	305	TRP
1	C	310	ASP
1	C	334	ASP
1	C	342	ILE
1	C	346	ASP
1	C	483	ASP
1	C	571	LEU
1	C	617	THR
1	C	625	GLU

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Mol	Chain	Res	Type
1	D	67	THR
1	D	74	TYR
1	D	80	PHE
1	D	215	LEU
1	D	258	TYR
1	D	259	PHE
1	D	310	ASP
1	D	334	ASP
1	D	342	ILE
1	D	346	ASP
1	D	483	ASP
1	D	571	LEU
1	D	625	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	78	ASN
1	A	96	GLN
1	A	205	HIS
1	A	260	GLN
1	A	290	GLN
1	A	307	ASN
1	A	422	GLN
1	A	544	HIS
1	A	545	ASN
1	B	73	GLN
1	B	78	ASN
1	B	96	GLN
1	B	205	HIS
1	B	260	GLN
1	B	290	GLN
1	B	307	ASN
1	B	422	GLN
1	B	544	HIS
1	B	545	ASN
1	C	73	GLN
1	C	78	ASN
1	C	96	GLN
1	C	205	HIS
1	C	260	GLN

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Mol	Chain	Res	Type
1	C	290	GLN
1	C	422	GLN
1	C	544	HIS
1	C	545	ASN
1	D	73	GLN
1	D	78	ASN
1	D	96	GLN
1	D	205	HIS
1	D	260	GLN
1	D	290	GLN
1	D	422	GLN
1	D	544	HIS
1	D	545	ASN

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 carbohydrates 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	589/617 (95%)	-0.21	12 (2%) 65 53	55, 102, 161, 211	0
1	B	589/617 (95%)	-0.15	12 (2%) 65 53	54, 104, 163, 205	0
1	C	589/617 (95%)	-0.14	9 (1%) 74 62	53, 104, 162, 204	0
1	D	589/617 (95%)	-0.21	13 (2%) 62 49	53, 101, 160, 199	0
All	All	2356/2468 (95%)	-0.18	46 (1%) 65 53	53, 103, 162, 211	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	LYS	5.6
1	D	409	ASN	4.8
1	B	409	ASN	4.6
1	D	558	LYS	4.2
1	A	222	GLY	4.0
1	C	560	ASP	3.6
1	B	517	THR	3.6
1	D	160	LYS	3.5
1	D	271	ARG	3.5
1	B	161	ASN	3.4
1	B	559	GLU	3.2
1	A	395	PHE	3.2
1	B	352	GLU	3.2
1	B	220	PRO	3.2
1	D	394	HIS	3.2
1	B	394	HIS	3.1
1	A	558	LYS	3.0
1	D	517	THR	3.0
1	A	559	GLU	3.0
1	A	560	ASP	2.9
1	C	413	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	222	GLY	2.9
1	C	562	LYS	2.8
1	D	161	ASN	2.7
1	C	161	ASN	2.7
1	C	395	PHE	2.7
1	A	493	ASN	2.6
1	B	271	ARG	2.5
1	B	395	PHE	2.5
1	A	221	GLY	2.4
1	D	395	PHE	2.4
1	D	511	ASP	2.4
1	D	559	GLU	2.4
1	C	563	MET	2.3
1	B	413	PRO	2.3
1	A	223	ALA	2.2
1	A	428	ARG	2.1
1	C	160	LYS	2.1
1	B	511	ASP	2.1
1	A	563	MET	2.1
1	A	98	GLU	2.1
1	D	410	TRP	2.1
1	D	363	PRO	2.0
1	D	521	LYS	2.0
1	C	99	SER	2.0
1	A	161	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.