



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:52 pm BST

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

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : 2.11
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) : 2.11

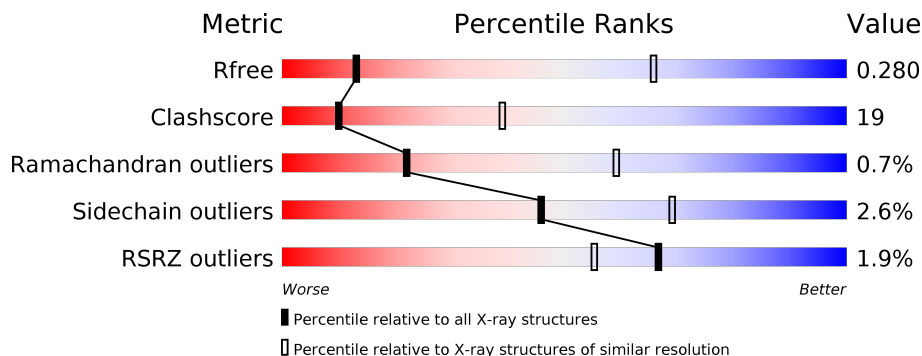
1 Overall quality at a glance

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}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	617	
1	B	617	
1	C	617	
1	D	617	

2 Entry composition i

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
			Total	C	N	O	S			
1	A	589	4710	3007	813	867	23	0	0	0
1	B	589	4710	3007	813	867	23	0	0	0
1	C	589	4710	3007	813	867	23	0	0	0
1	D	589	4710	3007	813	867	23	0	0	0

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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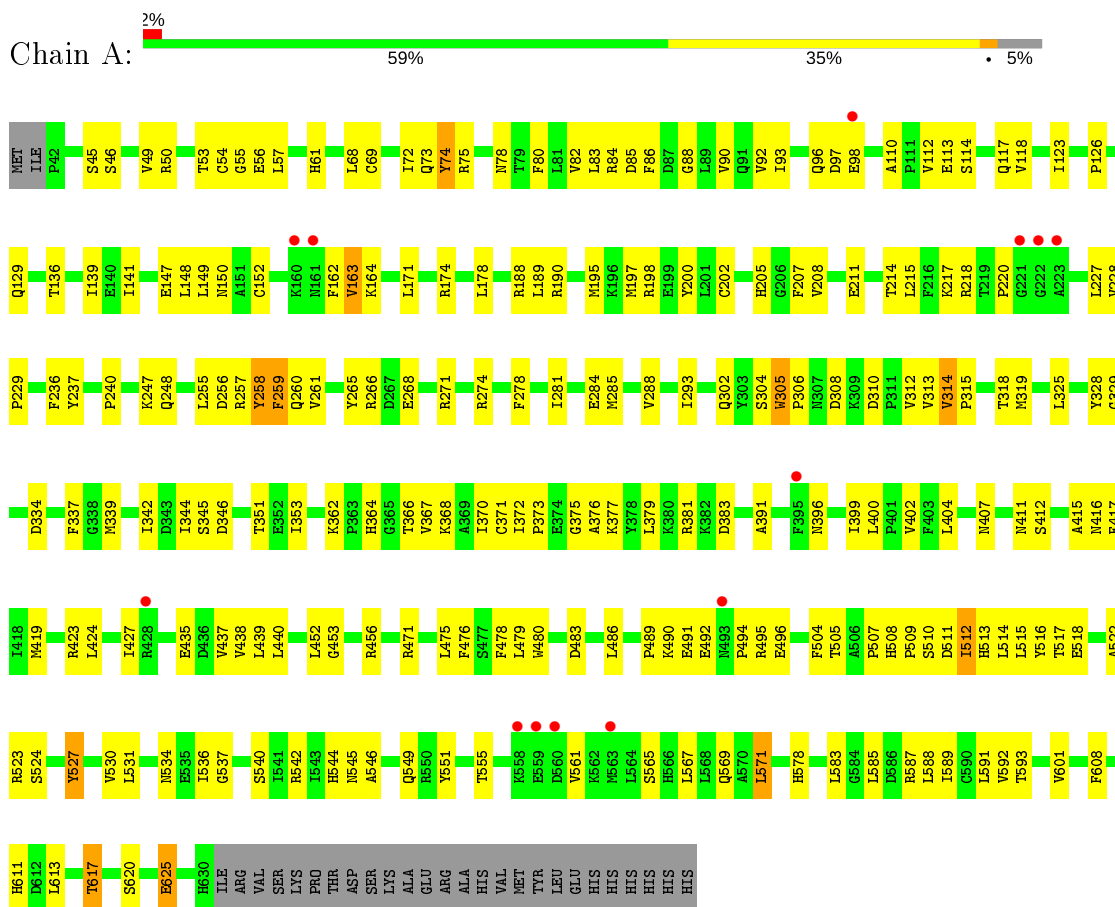
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Chain	Residue	Modelled	Actual	Comment	Reference
B	654	HIS	-	expression tag	UNP Q6PI48
B	655	HIS	-	expression tag	UNP Q6PI48
B	656	HIS	-	expression tag	UNP Q6PI48
C	40	MET	-	expression tag	UNP Q6PI48
C	646	VAL	-	expression tag	UNP Q6PI48
C	647	MET	-	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

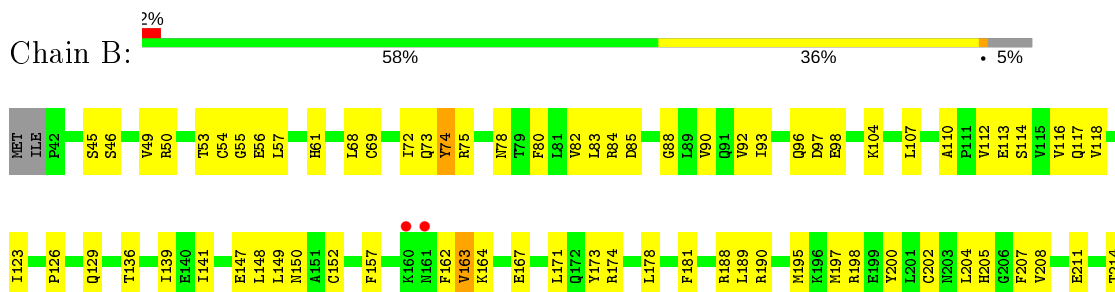
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: ASPARTATE-TRNA LIGASE, MITOCHONDRIAL



- Molecule 1: ASPARTATE-TRNA LIGASE, MITOCHONDRIAL



HIS	L589	H508	I399	P306	L215	MET
CYS	G590	P509	L400	R507	F216	ILE
V592	L591	S510	P401	D308	R217	P42
T593	V592	D511	V402	R309	R218	S45
V601	T593	I512	F403	D310	T219	S46
I602	L514	H513	L404	P311	P220	V49
H611	L515	L514	M407	V312	T136	R50
D612	Y516	Y516	R408	V313	L227	T53
L613	T517	E518	M409	V314	V228	C54
T617	E518	E518	M410	P315	P229	G55
E625	K524	K524	M411	T318	S230	E56
H630	A522	A522	S412	R319	R232	L57
ILE	R523	R523	P413	M318	F233	H61
ARG	S524	S524	V414	D334	G234	T87
ARG	S524	S524	A415	T335	K235	L68
VAL	Y527	Y527	M416	R336	F236	C69
VAL	V530	V530	F417	R339	Y237	W71
VAL	L531	L531	I418	M339	S238	I72
VAL	M534	M534	M419	I342	L239	Q73
PRO	E535	E535	R423	D343	L255	Y74
THR	I536	I536	L424	I344	R256	R75
ASP	G537	G537	I427	S345	R257	N78
SER	S540	S540	E435	D346	L285	I79
LYS	I541	I541	D436	T351	D256	F80
GLU	R542	R542	V437	E352	R257	L81
ARG	I543	I543	V438	I353	Y258	N88
ALA	H544	H544	L439	K362	F259	F80
HIS	N545	N545	L440	P363	Y261	L83
VAL	A546	A546	L452	H364	Y265	V82
MET	E547	E547	L456	G365	R266	L83
TYR	L548	L548	R456	V367	Y265	R34
LEU	Q549	Q549	F476	K368	S270	D85
GLU	R550	R550	L479	A369	R271	G88
HIS	Y551	Y551	L486	I370	F272	L89
HIS	T555	T555	L486	C371	P275	V90
HIS	K558	K558	L488	L372	Q275	Q91
HIS	E559	E559	L488	P373	P276	V92
HIS	S565	S565	L488	E374	E277	I93
HIS	H566	H566	L488	G375	F278	Q96
HIS	L567	L567	P489	A376	I281	D97
HIS	L568	L568	K490	Y378	L281	D97
HIS	Q569	Q569	K490	L379	E284	E98
HIS	A570	A570	E491	K380	M285	K104
HIS	L571	L571	E492	R381	Y288	L107
HIS	H578	H578	M493	K382	V288	L107
HIS	L583	L583	P494	D383	I283	A110
HIS	G584	G584	R495	A391	L283	P111
HIS	L585	L585	E496	A392	L296	V112
HIS	L588	L588	F504	H393	Q302	E113
HIS	L588	L588	T505	H394	S303	S114
HIS	L588	L588	A506	F395	W304	Q117
HIS	L588	L588	P507	M396	W305	V118

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.40 Å 82.60 Å 146.30 Å 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 3.75 Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.219 , 0.280 0.224 , 0.280	Depositor DCC
R_{free} test set	1782 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	88.0	Xtrriage
Anisotropy	0.622	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.044 for l,-k,h	Xtrriage
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

Xtrriage'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%)	22 59
1	B	587/617 (95%)	510 (87%)	73 (12%)	4 (1%)	22 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	587/617 (95%)	512 (87%)	71 (12%)	4 (1%)	22	59
1	D	587/617 (95%)	511 (87%)	72 (12%)	4 (1%)	22	59
All	All	2348/2468 (95%)	2045 (87%)	287 (12%)	16 (1%)	22	59

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 [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	525/551 (95%)	509 (97%)	16 (3%)	41	66
1	B	525/551 (95%)	514 (98%)	11 (2%)	53	74
1	C	525/551 (95%)	510 (97%)	15 (3%)	42	66
1	D	525/551 (95%)	512 (98%)	13 (2%)	47	70
All	All	2100/2204 (95%)	2045 (97%)	55 (3%)	46	69

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	13 (2%) 62 50	55, 102, 161, 211	0
1	B	589/617 (95%)	-0.16	12 (2%) 65 53	54, 104, 163, 205	0
1	C	589/617 (95%)	-0.14	8 (1%) 75 64	53, 104, 162, 204	0
1	D	589/617 (95%)	-0.22	12 (2%) 65 53	53, 101, 160, 199	0
All	All	2356/2468 (95%)	-0.18	45 (1%) 66 55	53, 103, 162, 211	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	LYS	5.6
1	D	409	ASN	4.7
1	B	409	ASN	4.7
1	D	558	LYS	4.2
1	A	222	GLY	3.9
1	C	560	ASP	3.6
1	D	160	LYS	3.5
1	D	271	ARG	3.5
1	B	517	THR	3.5
1	B	161	ASN	3.3
1	A	395	PHE	3.3
1	B	220	PRO	3.2
1	B	352	GLU	3.2
1	B	559	GLU	3.2
1	A	558	LYS	3.2
1	D	394	HIS	3.1
1	B	394	HIS	3.1
1	D	517	THR	3.0
1	A	559	GLU	3.0
1	A	560	ASP	3.0
1	C	413	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	222	GLY	2.8
1	C	562	LYS	2.8
1	D	161	ASN	2.8
1	C	395	PHE	2.7
1	C	161	ASN	2.6
1	A	493	ASN	2.5
1	B	395	PHE	2.5
1	D	559	GLU	2.4
1	D	395	PHE	2.4
1	B	271	ARG	2.4
1	A	221	GLY	2.4
1	B	413	PRO	2.3
1	C	563	MET	2.3
1	D	511	ASP	2.2
1	D	363	PRO	2.2
1	C	160	LYS	2.2
1	A	223	ALA	2.1
1	A	428	ARG	2.1
1	A	563	MET	2.1
1	A	98	GLU	2.1
1	A	160	LYS	2.1
1	B	511	ASP	2.1
1	A	161	ASN	2.0
1	D	521	LYS	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 [i](#)

There are no such residues in this entry.