



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:47 PM 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

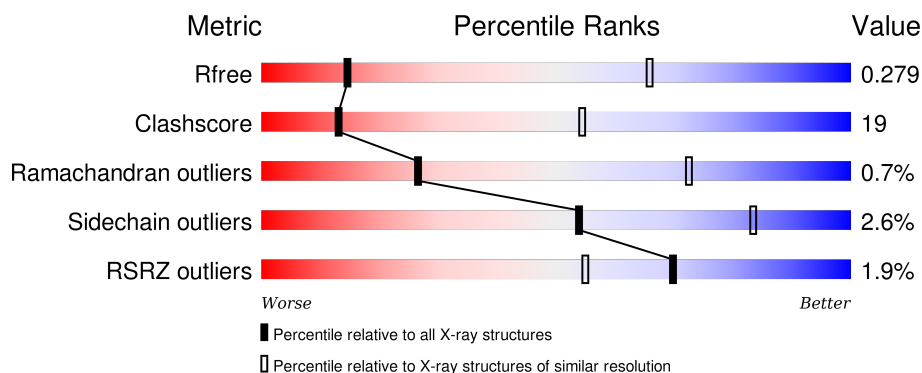
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (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%</div> <div>35%</div> <div>5%</div> </div>
1	B	617	<div> <div>2%</div> <div>58%</div> <div>36%</div> <div>5%</div> </div>
1	C	617	<div> <div>%</div> <div>58%</div> <div>36%</div> <div>5%</div> </div>
1	D	617	<div> <div>2%</div> <div>57%</div> <div>37%</div> <div>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			

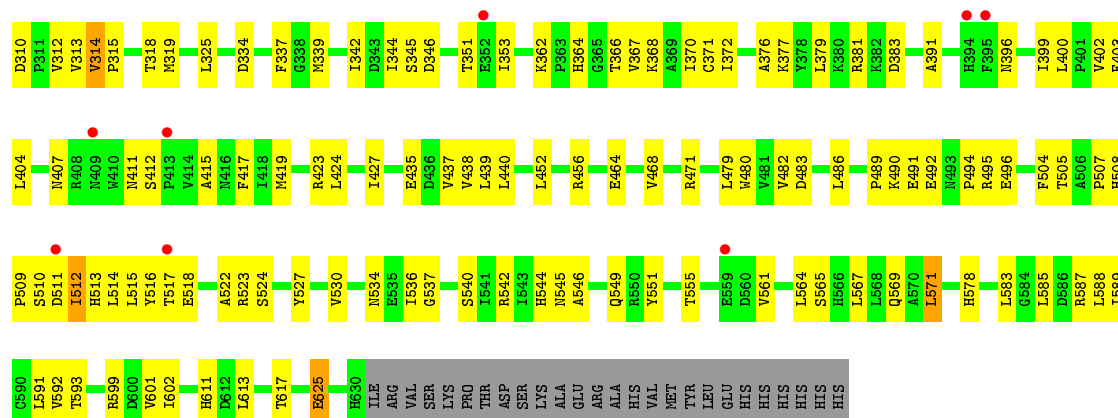
There are 48 discrepancies between the modelled and reference sequences:

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

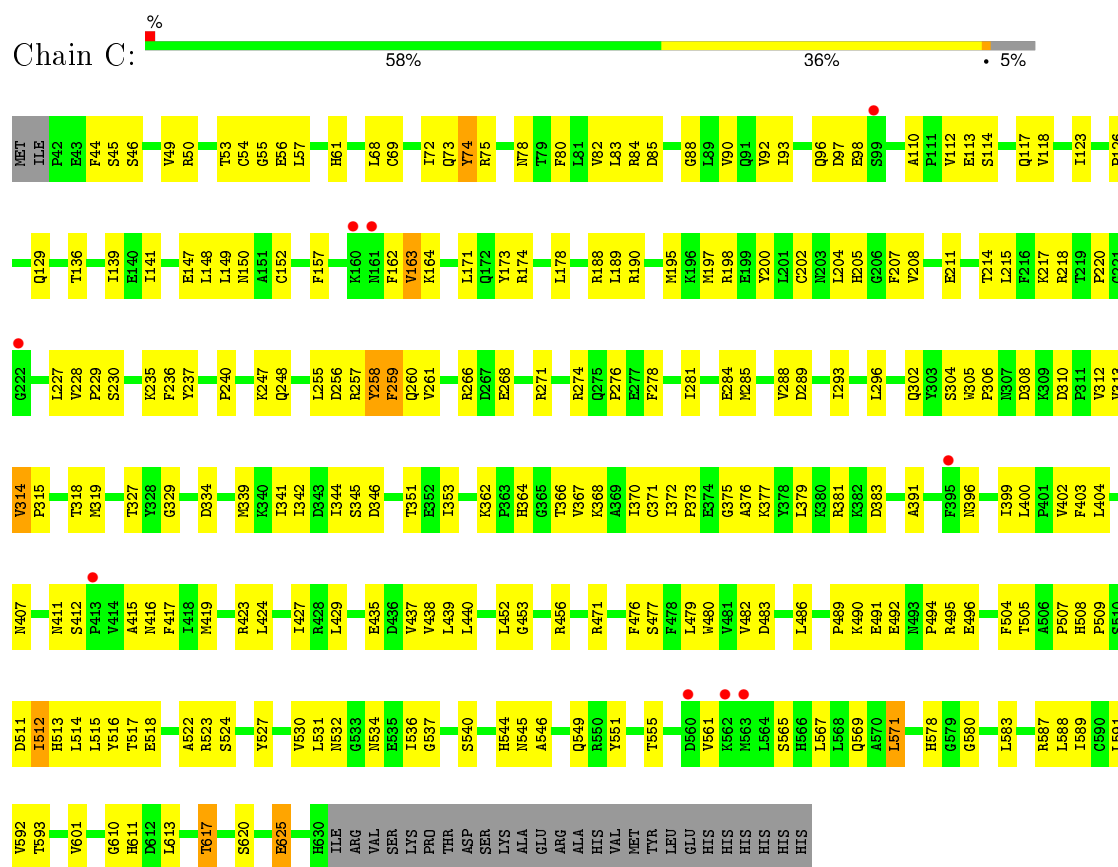
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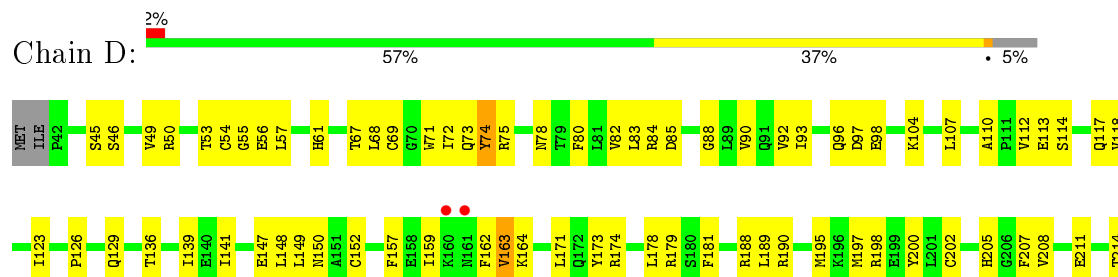
Chain	Residue	Modelled	Actual	Comment	Reference
B	654	HIS	-	EXPRESSION TAG	UNP Q6PI48
B	655	HIS	-	EXPRESSION TAG	UNP Q6PI48
B	656	HIS	-	EXPRESSION TAG	UNP Q6PI48
C	40	MET	-	EXPRESSION TAG	UNP Q6PI48
C	646	VAL	-	EXPRESSION TAG	UNP Q6PI48
C	647	MET	-	EXPRESSION TAG	UNP Q6PI48
C	648	TYR	-	EXPRESSION TAG	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



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C590	L591	V592	T593	V601	I602	H611	D612	L613	T617	E625	H630	ILE	ARG	VAL	SER	LYS	PRO	THR	ASP	SER	LYS	ALA	GLU	ARG	ALA	HIS	VAL	MET	TYR	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	H508	P509	S510	D511	I512	H513	L514	L515	Y516	T517	E518	A522	R523	S524	Y527	V530	L531	N534	E535	I536	G537	S540	I541	R542	I543	H544	N545	A546	E547	L548	Q549	R550	Y551	T555	K558	E559	S565	H566	L567	L568	Q569	A570	L571	H578	L583	G584	L585	L588	I589	I389	L400	P401	V402	F403	L404	M407	R408	N409	N410	N411	S412	F413	V414	A415	N416	F417	I418	M419	R423	L424	I427	E435	D436	V437	V438	L439	L440	L452	R456	F476	L479	W480	V481	V482	D483	L486	P489	K490	E491	E492	R493	P494	R495	E496	F504	T505	A506	P507	P306	H307	D308	K309	D310	P311	V312	V313	V314	P315	T318	M319	D334	T335	R336	M339	I342	D343	I344	S345	D346	T351	P352	I353	K362	P363	H364	T366	Q365	V367	K368	A369	I370	C371	I372	P373	E374	G375	A376	K377	Y378	L379	K380	R381	K382	D383	A391	A392	D393	H394	F395	N396	L215	F216	K217	R218	T219	P220	L227	V228	P229	S230	R231	E232	P233	G234	K235	F236	Y237	S238	L239	P240	K247	Q248	L255	D256	R257	Y258	F259	Q260	V261	Y265	R266	S270	R271	P272	Q275	P276	E277	F278	I281	E284	M285	V288	I293	L296	Q302	Y303	S304	W305
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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)	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
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 35688 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:198:ARG:CG	1:D:195:MET:CE	2.31	1.01
1:C:195:MET:CE	1:D:198:ARG:HG3	1.90	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:D:490:LYS:HB3	1:D:491:GLU:HA	1.54	0.88
1:A:490:LYS:HB3	1:A:491:GLU:HA	1.53	0.88
1:D:403:PHE:CE2	1:D:437:VAL:HG11	2.09	0.88
1:C:490:LYS:HB3	1:C:491:GLU:HA	1.54	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:C:314:VAL:HB	1:C:315:PRO:HD2	1.66	0.78
1:B:314:VAL:HB	1:B: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:B:504:PHE:CD1	1:B:549:GLN:NE2	2.62	0.67
1:A:486:LEU:HD23	1:A:515:LEU:HD21	1.75	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:C:207:PHE:CZ	1:C:296:LEU:HD11	2.29	0.67
1:B:258:TYR:HD2	1:B:284:GLU:HB2	1.58	0.67
1:B:207:PHE:CZ	1:B:296:LEU:HD11	2.30	0.66
1:D:403:PHE:CE2	1:D:437:VAL:CG1	2.77	0.66
1:D:113:GLU:O	1:D:152:CYS:SG	2.50	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:B:362:LYS:HG2	1:B:364:HIS:H	1.61	0.65
1:A:57:LEU:HB3	1:A:139:ILE:HD11	1.78	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:B:84:ARG:NH2	1:B:113:GLU:OE2	2.30	0.64
1:A:351:THR:HG22	1:A:353:ILE:HG22	1.78	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:D:517:THR:HG22	1:D:518:GLU:HG3	1.80	0.64
1:B:75:ARG:NH2	1:B:110:ALA:O	2.30	0.64
1:D:351:THR:HG22	1:D:353:ILE:HG22	1.80	0.64
1:B:587:ARG:O	1:B:591:LEU:HD13	1.98	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:46:SER:H	1:D:257:ARG:NH2	1.96	0.63
1:C:376:ALA:HB3	1:C:435:GLU:HB3	1.81	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:504:PHE:HD1	1:C:549:GLN:OE1	1.83	0.62
1:C:57:LEU:HB3	1:C:139:ILE:HD11	1.79	0.62
1:C:75:ARG:NH2	1:C:110:ALA:O	2.33	0.62
1:D:403:PHE:CD2	1:D:437:VAL:CG1	2.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ALA:HB3	1:A:435:GLU:HB3	1.81	0.62
1:A:516:TYR:HE1	1:A:551:TYR:CD2	2.17	0.62
1:A:372:ILE:HG23	1:A:437:VAL:CG1	2.30	0.62
1:A:75:ARG:NH2	1:A:110:ALA:O	2.33	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:D:516:TYR:HE1	1:D:551:TYR:CD2	2.18	0.61
1:C:351:THR:HG23	1:C:417:PHE:HE2	1.66	0.61
1:B:351:THR:HG22	1:B:353:ILE:HG22	1.81	0.61
1:B:534:ASN:HB2	1:B:591:LEU:HD21	1.82	0.61
1:B:376:ALA:HB3	1:B:435:GLU:HB3	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:C:516:TYR:HE1	1:C:551:TYR:CD2	2.19	0.60
1:B:504:PHE:CD1	1:B:549:GLN:CD	2.74	0.60
1:D:351:THR:HG23	1:D:417:PHE:HE2	1.66	0.60
1:D:248:GLN:OE1	1:D:578:HIS:NE2	2.30	0.60
1:B:302:GLN:HA	1:B:312:VAL:HG11	1.84	0.60
1:C:255:LEU:HA	1:D:188:ARG:HH22	1.66	0.60
1:B:54:CYS:HB2	1:B:85:ASP:HB2	1.83	0.60
1:C:372:ILE:HG23	1:C:437:VAL:CG2	2.31	0.60
1:A:46:SER:H	1:B:257:ARG:NH2	1.99	0.60
1:C:302:GLN:HA	1:C:312:VAL:HG11	1.84	0.60
1:C:504:PHE:HD1	1:C:549:GLN:CD	2.05	0.59
1:C:399:ILE:HD11	1:C:439:LEU:HB3	1.84	0.59
1:B:400:LEU:HD23	1:B:440:LEU:HD12	1.84	0.59
1:D:228:VAL:HG13	1:D:237:TYR:HB2	1.83	0.59
1:C:73:GLN:HB3	1:C:82:VAL:HG13	1.84	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: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:A:73:GLN:HB3	1:A:82:VAL:HG13	1.84	0.59
1:C:587:ARG:O	1:C:591:LEU:HD13	2.02	0.59
1:D:73:GLN:HB3	1:D:82:VAL:HG13	1.85	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:C:92:VAL:HG13	1:C:141:ILE:HG23	1.84	0.59
1:D:400:LEU:HD23	1:D:440:LEU:HD12	1.84	0.59
1:A:400:LEU:HD23	1:A:440:LEU:HD12	1.84	0.59
1:D:92:VAL:HG13	1:D:141:ILE:HG23	1.84	0.59
1:D:344:ILE:HD11	1:D:440:LEU:HD23	1.84	0.58
1:A:302:GLN:HA	1:A:312:VAL:HG11	1.85	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:344:ILE:HD11	1:B:440:LEU:HD23	1.84	0.58
1:B:270:SER:HA	1:B:272:PRO:HD3	1.85	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:C:611:HIS:HA	1:C:617:THR:O	2.04	0.58
1:B:399:ILE:HD11	1:B:439:LEU:HB3	1.84	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:D:208:VAL:HG21	1:D:255:LEU:HD22	1.85	0.57
1:C:344:ILE:HD11	1:C:440:LEU:HD23	1.86	0.57
1:B:92:VAL:HG13	1:B:141:ILE:HG23	1.85	0.57
1:A:611:HIS:HA	1:A:617:THR:O	2.04	0.57
1:A:198:ARG:CG	1:B:195:MET:CE	2.80	0.57
1:B:611:HIS:HA	1:B:617:THR:O	2.05	0.57
1:A:190:ARG:NH1	1:B:211:GLU:OE2	2.38	0.57
1:C:339:MET:O	1:C:456:ARG:NE	2.37	0.57
1:B:49:VAL:HG13	1:B:49:VAL:O	2.05	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:D:372:ILE:HG23	1:D:437:VAL:CG2	2.34	0.57
1:A:46:SER:O	1:B:257:ARG:NH2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:CYS:SG	1:D:68:LEU:HD13	2.44	0.57
1:A:211:GLU:OE2	1:B:190:ARG:NH1	2.38	0.57
1:B:208:VAL:HG21	1:B:255:LEU:HD22	1.87	0.57
1:C:248:GLN:OE1	1:C:578:HIS:NE2	2.30	0.56
1:A:49:VAL:HG13	1:A:49:VAL:O	2.04	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:A:608:PHE:HE2	1:D:414:VAL:HA	1.66	0.56
1:B:275:GLN:HE21	1:B:602:ILE:HD13	1.68	0.56
1:A:344:ILE:HD11	1:A:440:LEU:HD23	1.86	0.56
1:D:197:MET:HG3	1:D:304:SER:OG	2.05	0.56
1:D:214:THR:O	1:D:240:PRO:HD3	2.05	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:B:370:ILE:HG23	1:B:452:LEU:HD13	1.88	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: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:D:611:HIS:HA	1:D:617:THR:O	2.06	0.56
1:C:370:ILE:HG23	1:C:452:LEU:HD13	1.88	0.56
1:D:227:LEU:HD13	1:D:236:PHE:HE1	1.69	0.55
1:B:248:GLN:OE1	1:B:578:HIS:NE2	2.31	0.55
1:A:625:GLU:OE2	1:B:218:ARG:NH1	2.39	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: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:504:PHE:HD1	1:C:549:GLN:NE2	2.00	0.55
1:A:248:GLN:HB2	1:A:567:LEU:HD11	1.87	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:214:THR:O	1:C:240:PRO:HD3	2.07	0.55
1:C:126:PRO:HG2	1:C:129:GLN:HG3	1.89	0.55
1:D:189:LEU:HD13	1:D:593:THR:HG22	1.88	0.55
1:B:69:CYS:HB3	1:B:117:GLN:HG3	1.89	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:C:197:MET:HG3	1:C:304:SER:OG	2.08	0.53
1:A:534:ASN:HB2	1:A:591:LEU:HD21	1.90	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:C:402:VAL:HG22	1:C:415:ALA:HB1	1.90	0.53
1:B:339:MET:O	1:B:456:ARG:NE	2.40	0.53
1:D:402:VAL:HG22	1:D:415:ALA:HB1	1.90	0.53
1:A:546:ALA:HB2	1:A:571:LEU:HB3	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:D:534:ASN:HB2	1:D:591:LEU:HD21	1.91	0.53
1:C:391:ALA:O	1:C:396:ASN:HA	2.09	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:D:402:VAL:HB	1:D:438:VAL:HG23	1.90	0.53
1:C:329:GLY:HA3	1:C:453:GLY:HA3	1.91	0.53
1:B:379:LEU:HB3	1:B:383:ASP:OD1	2.08	0.53
1:B:400:LEU:HD11	1:B:415:ALA:HB2	1.91	0.53
1:B:247:LYS:HE2	1:B:284:GLU:HG2	1.89	0.53
1:D:514:LEU:HB2	1:D:522:ALA:HB2	1.91	0.53
1:D:247:LYS:HE2	1:D:284:GLU:HG2	1.90	0.53
1:D:126:PRO:HG2	1:D:129:GLN:HG3	1.90	0.53
1:D:486:LEU:HD22	1:D:507:PRO:HB3	1.91	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:C:400:LEU:HD11	1:C:415:ALA:HB2	1.90	0.53
1:B:504:PHE:HD1	1:B:549:GLN:OE1	1.92	0.53
1:A:514:LEU:HB2	1:A:522:ALA:HB2	1.91	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: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:379:LEU:HB3	1:A:383:ASP:OD1	2.09	0.52
1:A:198:ARG:HD3	1:A:259:PHE:CZ	2.44	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:A:197:MET:HG3	1:A:304:SER:OG	2.09	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: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:126:PRO:HG2	1:B:129:GLN:HG3	1.90	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:D:400:LEU:HD11	1:D:415:ALA:HB2	1.92	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:C:509:PRO:O	1:C:512:ILE:N	2.42	0.52
1:C:419:MET:O	1:C:423:ARG:HB2	2.09	0.52
1:D:174:ARG:O	1:D:178:LEU:HG	2.10	0.52
1:C:198:ARG:HD3	1:C:259:PHE:HZ	1.75	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:B:198:ARG:HD3	1:B:259:PHE:HZ	1.75	0.52
1:C:46:SER:O	1:D:257:ARG:NH2	2.39	0.51
1:C:247:LYS:HE2	1:C:284:GLU:HG2	1.92	0.51
1:D:423:ARG:O	1:D:427:ILE:HG12	2.10	0.51
1:B:93:ILE:HD11	1:B:123:ILE:HD11	1.92	0.51
1:A:195:MET:CE	1:B:198:ARG:HG2	2.34	0.51
1:D:198:ARG:HD3	1:D:259:PHE:CZ	2.46	0.51
1:C:113:GLU:O	1:C:152:CYS:SG	2.65	0.51
1:C:198:ARG:HD3	1:C:259:PHE:CZ	2.45	0.51
1:D:71:TRP:HE1	1:D:179:ARG:HH21	1.59	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:B:97:ASP:OD1	1:B:98:GLU:N	2.38	0.51
1:B:514:LEU:HB2	1:B:522:ALA:HB2	1.92	0.51
1:B:508:HIS:HB3	1:B:523:ARG:HG3	1.92	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:D:198:ARG:HD3	1:D:259:PHE:HZ	1.75	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:B:504:PHE:CD1	1:B:549:GLN:OE1	2.64	0.51
1:A:54:CYS:HB2	1:A:85:ASP:HB2	1.93	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: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:C:93:ILE:HD11	1:C:123:ILE:HD11	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: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:471:ARG:O	1:B:471:ARG:HG3	2.11	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:D:505:THR:HG23	1:D:540:SER:HB2	1.93	0.50
1:B:366:THR:HG21	1:B:368:LYS:HE2	1.94	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:C:174:ARG:O	1:C:178:LEU:HG	2.11	0.49
1:A:377:LYS:HG2	1:A:407:ASN:HD21	1.77	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:B:314:VAL:HB	1:B:315:PRO:CD	2.40	0.49
1:B:171:LEU:HB2	1:B:613:LEU:HD12	1.95	0.49
1:A:45:SER:OG	1:A:50:ARG:NH2	2.45	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: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:B:423:ARG:O	1:B:427:ILE:HG12	2.11	0.49
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: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:C:504:PHE:CE1	1:C:549:GLN:CD	2.85	0.49
1:B:74:TYR:O	1:B:82:VAL:HG12	2.13	0.49
1:B:505:THR:HG23	1:B:540:SER:HB2	1.94	0.49
1:D:312:VAL:HG22	1:D:313:VAL:H	1.77	0.49
1:A:93:ILE:HD11	1:A:123:ILE:HD11	1.95	0.49
1:A:55:GLY:HA3	1:A:88:GLY:HA3	1.95	0.49
1:B:117:GLN:HB2	1:B:149:LEU:HD11	1.94	0.49
1:A:293:ILE:HD11	1:A:527:TYR:CE1	2.47	0.49
1:D:366:THR:HG21	1:D:368:LYS:HE2	1.94	0.49
1:B:162:PHE:CE1	1:B:181:PHE:HB2	2.47	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:B:90:VAL:HG23	1:B:136:THR:HB	1.95	0.48
1:C:366:THR:HG21	1:C:368:LYS:HE2	1.94	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:D:171:LEU:HB2	1:D:613:LEU:HD12	1.95	0.48
1:C:505:THR:HG23	1:C:540:SER:HB2	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:B:55:GLY:HA3	1:B:88:GLY:HA3	1.96	0.48
1:A:90:VAL:HG23	1:A:136:THR:HB	1.95	0.48
1:D:314:VAL:HB	1:D:315:PRO:CD	2.40	0.48
1:D:275:GLN:NE2	1:D:602:ILE:HD12	2.29	0.48
1:D:293:ILE:HD11	1:D:527:TYR:CZ	2.49	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:D:551:TYR:O	1:D:555:THR:HG23	2.14	0.48
1:D:57:LEU:HA	1:D:61:HIS:ND1	2.29	0.48
1:A:74:TYR:O	1:A:82:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:LEU:HA	1:D:571:LEU:HD13	1.70	0.48
1:B:174:ARG:O	1:B:178:LEU:HG	2.14	0.48
1:D:589:ILE:HG23	1:D:601:VAL:HG21	1.95	0.48
1:C:266:ARG:HD2	1:C:278:PHE:CE1	2.49	0.48
1:A:229:PRO:HD2	1:B:227:LEU:O	2.14	0.48
1:B:312:VAL:HG22	1:B:313:VAL:H	1.79	0.48
1:A:617:THR:HB	1:B:217:LYS:HB3	1.94	0.48
1:A:117:GLN:HB2	1:A:149:LEU:HD11	1.95	0.48
1:D:504:PHE:CD1	1:D:549:GLN:NE2	2.82	0.48
1:D:163:VAL:HG12	1:D:164:LYS:HG2	1.96	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:C:171:LEU:HB2	1:C:613:LEU:HD12	1.95	0.47
1:B:171:LEU:HD23	1:B:174:ARG:HD3	1.96	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:293:ILE:HD11	1:D:527:TYR:CE1	2.48	0.47
1:D:319:MET:HB2	1:D:479:LEU:HD11	1.96	0.47
1:B:229:PRO:HA	1:B:236:PHE:HB3	1.96	0.47
1:C:274:ARG:CZ	1:C:587:ARG:HH21	2.27	0.47
1:A:171:LEU:HB2	1:A:613:LEU:HD12	1.96	0.47
1:A:589:ILE:HG23	1:A:601:VAL:HG21	1.95	0.47
1:B:489:PRO:HB2	1:B:494:PRO:HG3	1.97	0.47
1:C:511:ASP:OD2	1:C:513:HIS:HB3	2.15	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:314:VAL:HB	1:C:315:PRO:CD	2.39	0.47
1:C:551:TYR:O	1:C:555:THR:HG23	2.14	0.47
1:C:312:VAL:HG22	1:C:313:VAL:H	1.80	0.47
1:B:270:SER:HA	1:B:271:ARG:HA	1.64	0.47
1:A:163:VAL:HG12	1:A:164:LYS:HG2	1.96	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:A:489:PRO:HB2	1:A:494:PRO:HG3	1.97	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:D:113:GLU:OE1	1:D:159:ILE:HG13	2.14	0.47
1:A:306:PRO:C	1:A:308:ASP:H	2.17	0.47
1:B:215:LEU:CD1	1:B:237:TYR:CE2	2.98	0.47
1:C:229:PRO:HD2	1:D:227:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HD11	1:A:527:TYR:CZ	2.49	0.47
1:B:492:GLU:OE1	1:B:496:GLU:HG3	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:489:PRO:HB2	1:C:494:PRO:HG3	1.97	0.46
1:C:319:MET:HB2	1:C:479:LEU:HD11	1.98	0.46
1:D:494:PRO:HA	1:D:495:ARG:HA	1.42	0.46
1:D:305:TRP:HZ2	1:D:476:PHE:CD1	2.33	0.46
1:C:477:SER:N	1:C:532:ASN:OD1	2.34	0.46
1:C:492:GLU:OE1	1:C:496:GLU:HG3	2.15	0.46
1:A:227:LEU:O	1:B:229:PRO:HD2	2.14	0.46
1:B:45:SER:OG	1:B:50:ARG:NH2	2.48	0.46
1:B:163:VAL:HG12	1:B:164:LYS:HG2	1.97	0.46
1:B:157:PHE:CE1	1:B:173:TYR:HB2	2.51	0.46
1:A:424:LEU:HD12	1:A:424:LEU:H	1.81	0.46
1:B:510:SER:O	1:B:510:SER:OG	2.30	0.46
1:A:319:MET:HB2	1:A:479:LEU:HD11	1.97	0.46
1:D:489:PRO:HB2	1:D:494:PRO:HG3	1.96	0.46
1:D:318:THR:HA	1:D:480:TRP:HB2	1.97	0.46
1:A:536:ILE:HG13	1:A:588:LEU:HB2	1.97	0.46
1:D:492:GLU:OE1	1:D:496:GLU:HG3	2.15	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:171:LEU:HD23	1:D:174:ARG:HD3	1.96	0.46
1:A:494:PRO:HA	1:A:495:ARG:HA	1.43	0.46
1:A:164:LYS:HB2	1:D:396:ASN:ND2	2.31	0.46
1:D:71:TRP:HE1	1:D:179:ARG:NH2	2.13	0.46
1:A:261:VAL:HG12	1:A:281:ILE:HG12	1.98	0.46
1:D:306:PRO:C	1:D:308:ASP:H	2.18	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: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:D:114:SER:HB3	1:D:150:ASN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:THR:O	1:C:56:GLU:HG2	2.17	0.45
1:A:551:TYR:O	1:A:555:THR:HG23	2.16	0.45
1:B:511:ASP:OD2	1:B:513:HIS:HB3	2.16	0.45
1:A:57:LEU:HA	1:A:61:HIS:ND1	2.31	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:C:494:PRO:HA	1:C:495:ARG:HA	1.43	0.45
1:B:424:LEU:H	1:B:424:LEU:HD12	1.81	0.45
1:D:424:LEU:HD12	1:D:424:LEU:H	1.82	0.45
1:B:536:ILE:HG13	1:B:588:LEU:HB2	1.99	0.45
1:C:285:MET:HB2	1:C:288:VAL:HG11	1.99	0.45
1:C:339:MET:H	1:C:456:ARG:HH21	1.65	0.45
1:C:218:ARG:NE	1:C:220:PRO:HG3	2.32	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:A:475:LEU:HD12	1:A:476:PHE:H	1.82	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:D:275:GLN:NE2	1:D:602:ILE:CD1	2.80	0.45
1:A:492:GLU:OE1	1:A:496:GLU:HG3	2.16	0.45
1:C:258:TYR:CD2	1:C:284:GLU:HB2	2.46	0.45
1:B:339:MET:H	1:B:456:ARG:HH21	1.65	0.45
1:C:379:LEU:HD12	1:C:379:LEU:H	1.82	0.45
1:A:256:ASP:CG	1:B:50:ARG:HH22	2.20	0.45
1:C:147:GLU:HG2	1:C:148:LEU:N	2.32	0.45
1:B:266:ARG:HD2	1:B:278:PHE:HE2	1.82	0.45
1:C:198:ARG:HG2	1:D:195:MET:CE	2.36	0.44
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: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:C:198:ARG:C	1:D:195:MET:HE1	2.37	0.44
1:B:162:PHE:HE1	1:B:181:PHE:HB2	1.81	0.44
1:A:54:CYS:SG	1:A:68:LEU:HD13	2.58	0.44
1:B:379:LEU:H	1:B:379:LEU:HD12	1.81	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:B:72:ILE:O	1:B:113:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ARG:NE	1:D:220:PRO:HG3	2.32	0.44
1:B:218:ARG:NE	1:B:220:PRO:HG3	2.33	0.44
1:A:404:LEU:HA	1:A:419:MET:HG3	1.99	0.44
1:A:565:SER:O	1:A:569:GLN:HB2	2.18	0.44
1:C:544:HIS:O	1:C:545:ASN:ND2	2.51	0.44
1:C:371:CYS:HB2	1:C:438:VAL:HG12	1.99	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:C:72:ILE:O	1:C:113:GLU:HA	2.18	0.44
1:D:228:VAL:O	1:D:236:PHE:HB2	2.18	0.44
1:B:589:ILE:HA	1:B:592:VAL:HG12	2.00	0.44
1:D:589:ILE:HA	1:D:592:VAL:HG12	2.00	0.44
1:C:318:THR:HA	1:C:480:TRP:HB2	1.98	0.44
1:A:589:ILE:HA	1:A:592:VAL:HG12	1.99	0.44
1:A:345:SER:HA	1:A:367:VAL:HG13	2.00	0.44
1:D:261:VAL:HG12	1:D:281:ILE:HG12	2.00	0.44
1:D:319:MET:O	1:D:482:VAL:HG22	2.18	0.44
1:B:345:SER:HA	1:B:367:VAL:HG13	2.00	0.44
1:B:208:VAL:HG22	1:B:257:ARG:O	2.19	0.43
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: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:B:83:LEU:HG	1:B:92:VAL:HG21	2.01	0.43
1:A:147:GLU:HG2	1:A:148:LEU:N	2.33	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:A:318:THR:HA	1:A:480:TRP:HB2	1.99	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:516:TYR:CE1	1:A:551:TYR:CD2	3.04	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:A:92:VAL:HG11	1:A:118:VAL:HG11	2.00	0.43
1:D:339:MET:H	1:D:456:ARG:HH21	1.64	0.43
1:A:571:LEU:HD13	1:A:571:LEU:HA	1.71	0.43
1:D:305:TRP:HA	1:D:306:PRO:HD3	1.77	0.43
1:D:147:GLU:HG2	1:D:148:LEU:N	2.34	0.43
1:A:72:ILE:O	1:A:113:GLU:HA	2.19	0.43
1:C:412:SER:O	1:C:416:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:LEU:HD12	1:D:379:LEU:H	1.84	0.43
1:D:339:MET:HE2	1:D:373:PRO:HD2	2.01	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:A:285:MET:HB2	1:A:288:VAL:HG11	2.01	0.43
1:C:620:SER:N	1:D:235:LYS:HG2	2.33	0.43
1:A:471:ARG:HG3	1:A:471:ARG:O	2.19	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:D:72:ILE:O	1:D:113:GLU:HA	2.18	0.43
1:A:53:THR:O	1:A:56:GLU:HG2	2.18	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: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: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:571:LEU:HD13	1:B:571:LEU:HA	1.73	0.42
1:D:78:ASN:HB3	1:D:96:GLN:HE21	1.84	0.42
1:B:565:SER:O	1:B:569:GLN:HB2	2.19	0.42
1:D:107:LEU:HA	1:D:107:LEU:HD12	1.85	0.42
1:B:215:LEU:HD13	1:B:237:TYR:CZ	2.54	0.42
1:A:339:MET:H	1:A:456:ARG:HH21	1.65	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:C:92:VAL:HG11	1:C:118:VAL:HG11	2.01	0.42
1:B:147:GLU:HG2	1:B:148:LEU:N	2.34	0.42
1:C:513:HIS:CE1	1:C:516:TYR:HB2	2.54	0.42
1:B:534:ASN:CB	1:B:591:LEU:HD21	2.48	0.42
1:A:207:PHE:CG	1:A:257:ARG:HB3	2.54	0.42
1:D:230:SER:HB3	1:D:235:LYS:O	2.20	0.42
1:C:228:VAL:O	1:C:236:PHE:HB2	2.19	0.42
1:D:83:LEU:HG	1:D:92:VAL:HG21	2.01	0.42
1:A:164:LYS:NZ	1:D:392:ALA:HB1	2.34	0.42
1:D:531:LEU:HG	1:D:591:LEU:HD23	2.02	0.42
1:C:479:LEU:HB3	1:C:530:VAL:HG23	2.02	0.42
1:B:325:LEU:HA	1:B:325:LEU:HD12	1.85	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:D:504:PHE:CD1	1:D:549:GLN:CD	2.93	0.42
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:207:PHE:CG	1:D:257:ARG:HB3	2.55	0.42
1:B:504:PHE:HZ	1:B:564:LEU:HD13	1.85	0.42
1:A:399:ILE:HG13	1:A:439:LEU:HD12	2.01	0.42
1:A:207:PHE:CD2	1:A:257:ARG:HB3	2.55	0.42
1:D:372:ILE:CG2	1:D:437:VAL:HG23	2.44	0.42
1:B:247:LYS:NZ	1:B:542:ARG:HH21	2.17	0.42
1:A:531:LEU:HG	1:A:591:LEU:HD23	2.02	0.42
1:C:402:VAL:HG22	1:C:415:ALA:CB	2.50	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:D:404:LEU:HA	1:D:419:MET:HG3	2.02	0.42
1:B:265:TYR:CD1	1:B:277:GLU:HB3	2.55	0.42
1:D:157:PHE:CZ	1:D:173:TYR:HB2	2.55	0.42
1:A:620:SER:N	1:B:235:LYS:HG2	2.34	0.42
1:D:232:GLU:HA	1:D:233:PRO:HD3	1.86	0.42
1:C:204:LEU:HA	1:C:204:LEU:HD12	1.90	0.42
1:C:207:PHE:CG	1:C:257:ARG:HB3	2.55	0.42
1:A:247:LYS:HZ3	1:A:542:ARG:HH21	1.68	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:C:78:ASN:HB3	1:C:96:GLN:HE21	1.85	0.42
1:C:345:SER:HA	1:C:367:VAL:HG13	2.02	0.42
1:D:479:LEU:HB3	1:D:530:VAL:HG23	2.02	0.41
1:B:207:PHE:CD2	1:B:257:ARG:HB3	2.56	0.41
1:B:207:PHE:CG	1:B:257:ARG:HB3	2.55	0.41
1:D:399:ILE:HG13	1:D:439:LEU:HD12	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:C:490:LYS:CB	1:C:491:GLU:HA	2.35	0.41
1:C:207:PHE:CD2	1:C:257:ARG:HB3	2.55	0.41
1:C:208:VAL:HG22	1:C:257:ARG:O	2.21	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:A:83:LEU:HG	1:A:92:VAL:HG21	2.01	0.41
1:B:585:LEU:O	1:B:589:ILE:HG22	2.20	0.41
1:A:585:LEU:O	1:A:589:ILE:HG22	2.21	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:A:325:LEU:HA	1:A:325:LEU:HD12	1.86	0.41
1:A:195:MET:HE2	1:B:198:ARG:CG	2.28	0.41
1:D:544:HIS:O	1:D:545:ASN:ND2	2.53	0.41
1:A:510:SER:O	1:A:510:SER:OG	2.32	0.41
1:C:381:ARG:HD2	1:C:411:ASN:OD1	2.21	0.41
1:B:78:ASN:HB3	1:B:96:GLN:HE21	1.85	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:C:258:TYR:OH	1:C:260:GLN:NE2	2.51	0.41
1:A:265:TYR:HE2	1:B:214:THR:HG1	1.69	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:C:372:ILE:CG2	1:C:437:VAL:HG23	2.41	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:A:258:TYR:OH	1:A:260:GLN:NE2	2.51	0.41
1:B:229:PRO:HA	1:B:236:PHE:CB	2.51	0.41
1:D:229:PRO:HA	1:D:236:PHE:CB	2.51	0.41
1:A:68:LEU:CD1	1:A:83:LEU:HD12	2.50	0.41
1:D:265:TYR:CD1	1:D:277:GLU:HB3	2.54	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:A:373:PRO:C	1:A:375:GLY:H	2.24	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:B:107:LEU:HD12	1:B:107:LEU:HA	1.85	0.41
1:B:275:GLN:HE22	1:B:602:ILE:HD12	1.80	0.41
1:D:513:HIS:CE1	1:D:516:TYR:HB2	2.55	0.41
1:C:319:MET:O	1:C:482:VAL:HG22	2.21	0.41
1:B:464:GLU:HA	1:B:468:VAL:O	2.21	0.41
1:B:198:ARG:HH22	1:B:261:VAL:HG21	1.87	0.40
1:D:49:VAL:O	1:D:49:VAL:CG1	2.69	0.40
1:D:373:PRO:C	1:D:375:GLY:H	2.24	0.40
1:C:561:VAL:O	1:C:565:SER:HB2	2.21	0.40
1:B:381:ARG:HD2	1:B:411:ASN:OD1	2.21	0.40
1:B:404:LEU:H	1:B:404:LEU:HD23	1.86	0.40
1:D:412:SER:O	1:D:416:ASN:HB2	2.21	0.40
1:B:504:PHE:HD1	1:B:549:GLN:CD	2.20	0.40
1:C:44:PHE:HB3	1:C:45:SER:H	1.72	0.40
1:B:96:GLN:HG2	1:B:104:LYS:NZ	2.37	0.40

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

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	587/617 (95%)	512 (87%)	71 (12%)	4 (1%)	26	72
1	B	587/617 (95%)	510 (87%)	73 (12%)	4 (1%)	26	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	587/617 (95%)	512 (87%)	71 (12%)	4 (1%)	26	72
1	D	587/617 (95%)	511 (87%)	72 (12%)	4 (1%)	26	72
All	All	2348/2468 (95%)	2045 (87%)	287 (12%)	16 (1%)	26	72

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%)	48	81
1	B	525/551 (95%)	514 (98%)	11 (2%)	61	86
1	C	525/551 (95%)	510 (97%)	15 (3%)	50	81
1	D	525/551 (95%)	512 (98%)	13 (2%)	55	84
All	All	2100/2204 (95%)	2045 (97%)	55 (3%)	54	83

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%)	-0.18	12 (2%) 68 53	55, 102, 161, 211	0
1	B	589/617 (95%)	-0.13	12 (2%) 68 53	54, 104, 163, 205	0
1	C	589/617 (95%)	-0.11	9 (1%) 76 62	53, 104, 162, 204	0
1	D	589/617 (95%)	-0.19	12 (2%) 68 53	53, 101, 160, 199	0
All	All	2356/2468 (95%)	-0.15	45 (1%) 70 55	53, 103, 162, 211	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	LYS	5.5
1	D	409	ASN	4.9
1	B	409	ASN	4.6
1	D	558	LYS	4.1
1	A	222	GLY	3.9
1	C	560	ASP	3.7
1	B	517	THR	3.6
1	D	160	LYS	3.5
1	D	271	ARG	3.4
1	B	161	ASN	3.4
1	B	559	GLU	3.3
1	B	352	GLU	3.3
1	A	395	PHE	3.2
1	B	220	PRO	3.2
1	D	394	HIS	3.1
1	D	517	THR	3.1
1	A	559	GLU	3.0
1	B	394	HIS	3.0
1	A	560	ASP	3.0
1	A	558	LYS	3.0
1	C	413	PRO	2.9

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

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

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

6.3 Carbohydrates [i](#)

There are no 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.