



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 AM GMT

PDB ID : 3H0L
Title : Structure of trna-dependent amidotransferase gatcab from aquifex aeolicus
Authors : Wu, J.; Bu, W.; Sheppard, K.; Kitabatake, M.; Soll, D.; Smith, J.L.
Deposited on : 2009-04-09
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

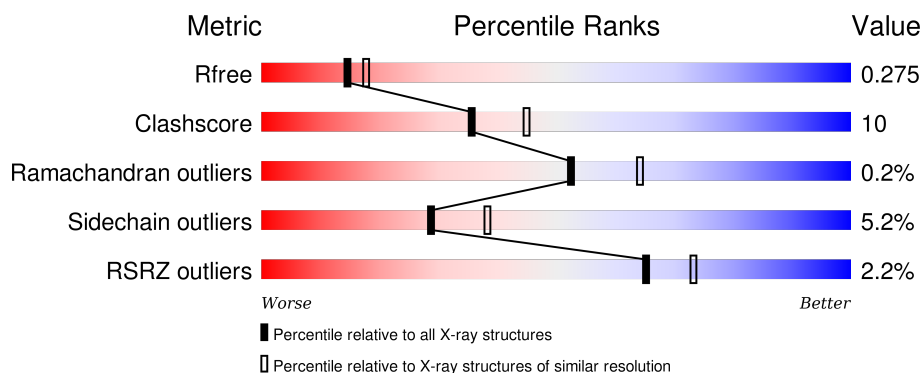
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.













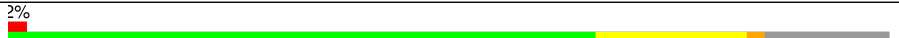


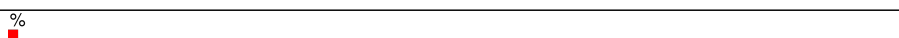
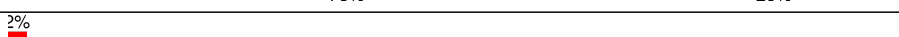
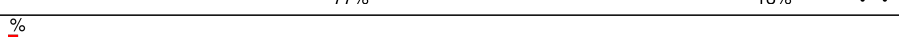



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	478	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	D	478	<div> <div>2%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	G	478	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	J	478	<div> <div>%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	M	478	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	P	478	
1	S	478	
1	V	478	
2	B	478	
2	E	478	
2	H	478	
2	K	478	
2	N	478	
2	Q	478	
2	T	478	
2	W	478	
3	C	94	
3	F	94	
3	I	94	
3	L	94	
3	O	94	
3	R	94	
3	U	94	
3	X	94	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	B	801	-	-	-	X
5	MG	H	803	-	-	-	X
5	MG	N	805	-	-	-	X
5	MG	Q	806	-	-	-	X
5	MG	T	807	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	W	808	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 63144 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	D	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	G	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	J	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	M	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	P	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	S	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	V	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	E	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	H	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	K	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	N	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	Q	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

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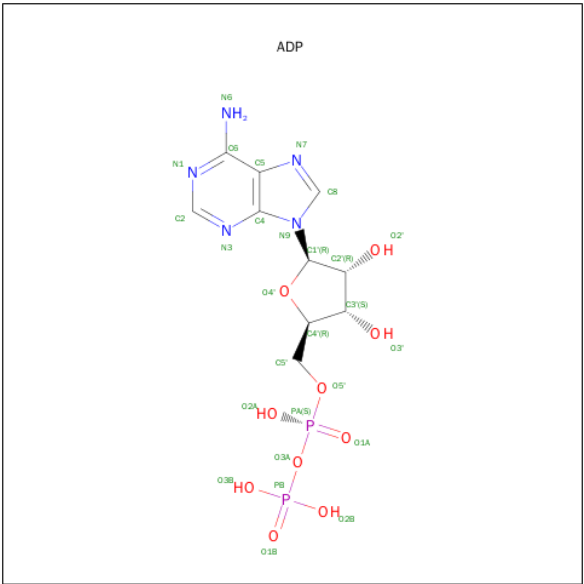
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	W	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	F	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	I	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	L	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	O	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	R	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	U	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	X	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	W	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Q	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	W	1	Total	Mg	0	0
			1	1		
5	T	1	Total	Mg	0	0
			1	1		
5	N	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

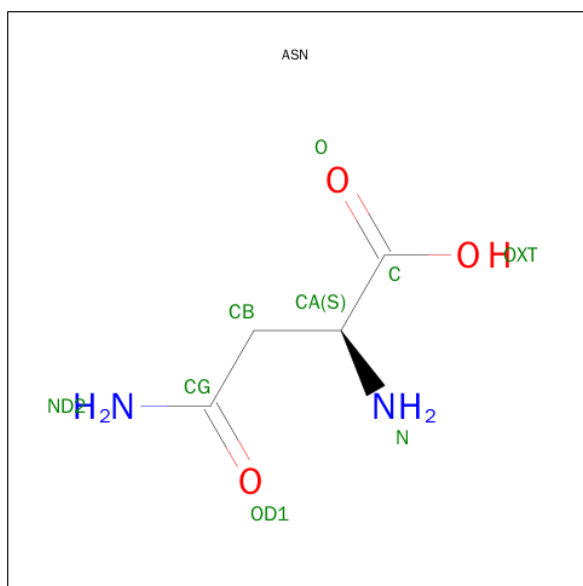
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Q	1	Total	Zn	0	0
			1	1		
6	K	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	Zn	0	0
			1	1		
6	H	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		
6	W	1	Total	Zn	0	0
			1	1		
6	T	1	Total	Zn	0	0
			1	1		
6	N	1	Total	Zn	0	0
			1	1		

- Molecule 7 is ASPARAGINE (three-letter code: ASN) (formula: $C_4H_8N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		
7	G	1	Total	C	N	O	0	0
			8	4	1	3		
7	J	1	Total	C	N	O	0	0
			8	4	1	3		
7	M	1	Total	C	N	O	0	0
			8	4	1	3		

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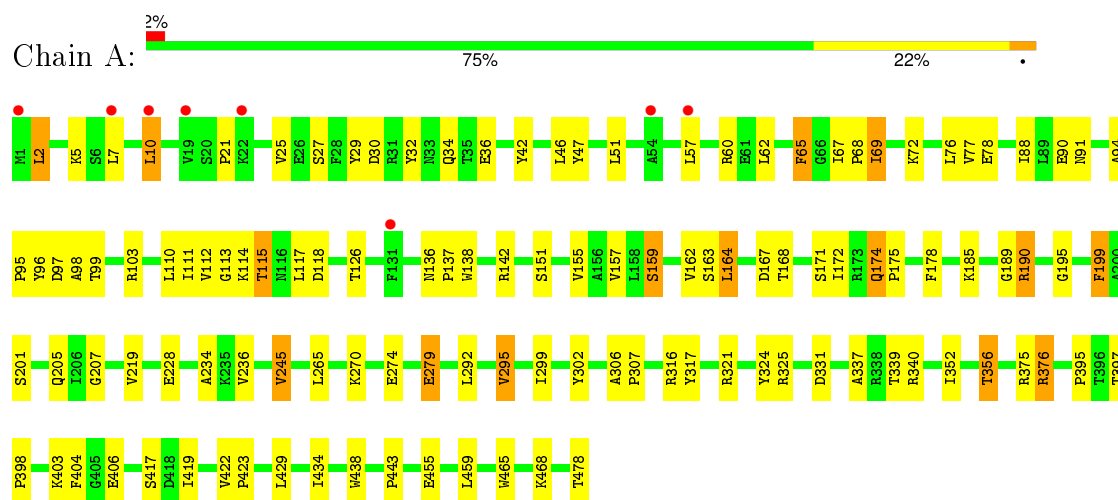
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	P	1	Total	C	N	O	0	0
			8	4	1	3		
7	S	1	Total	C	N	O	0	0
			8	4	1	3		
7	V	1	Total	C	N	O	0	0
			8	4	1	3		

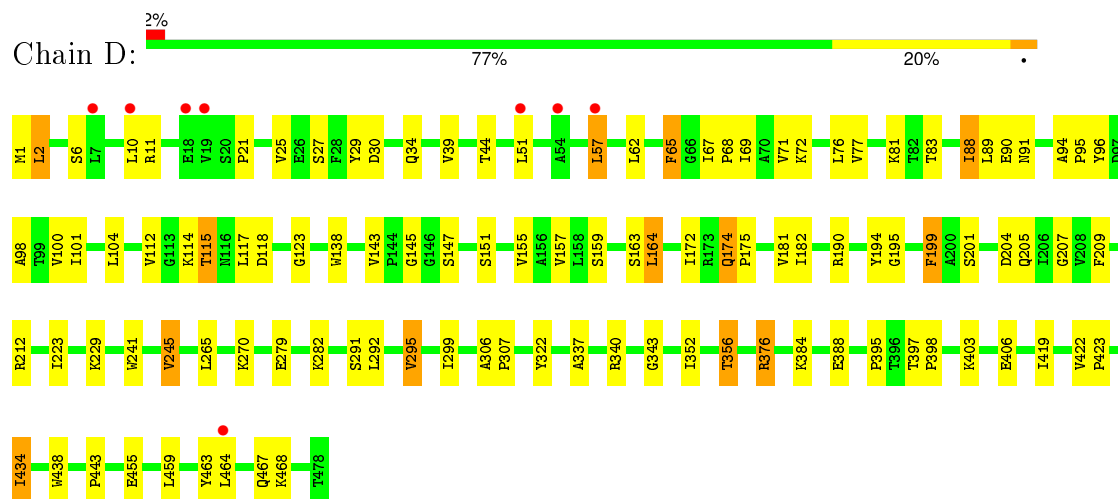
3 Residue-property plots

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

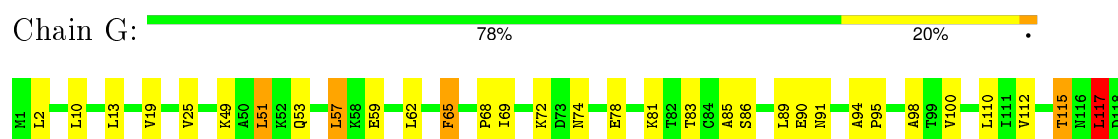
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

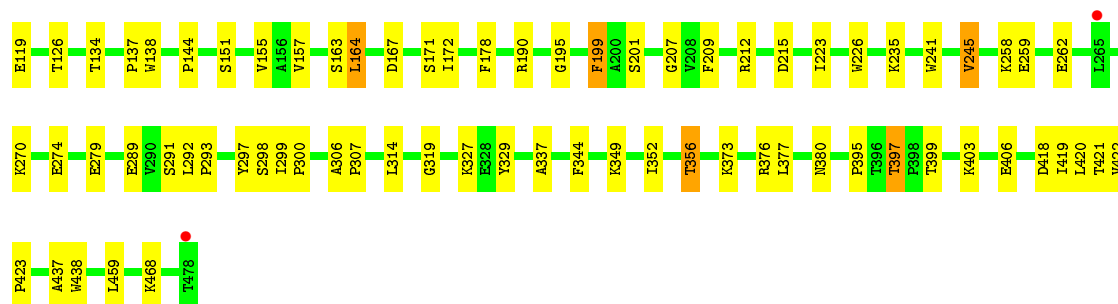


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

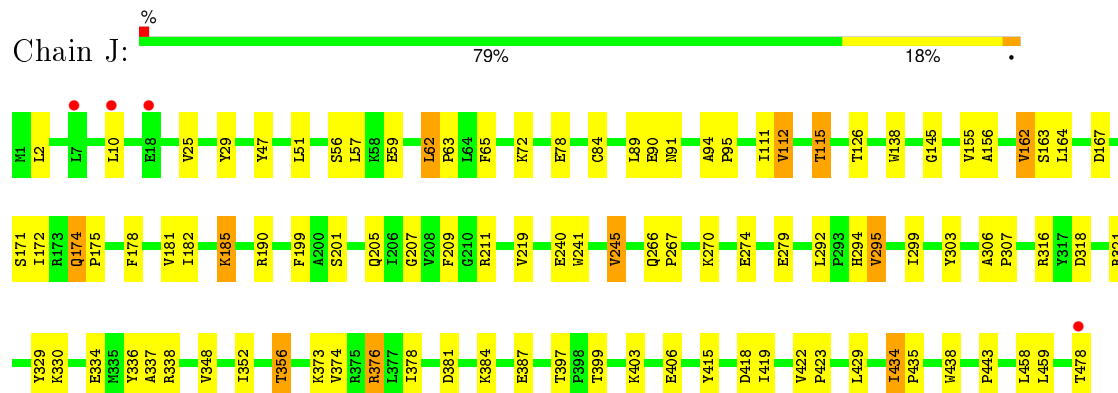


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

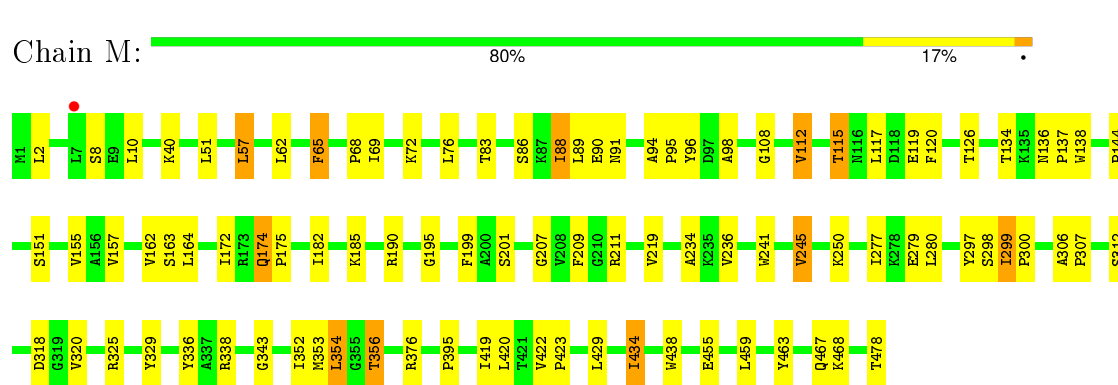




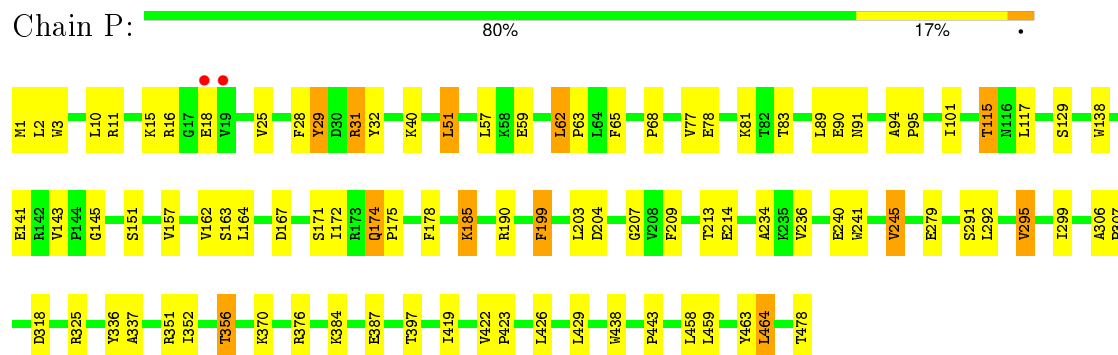
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



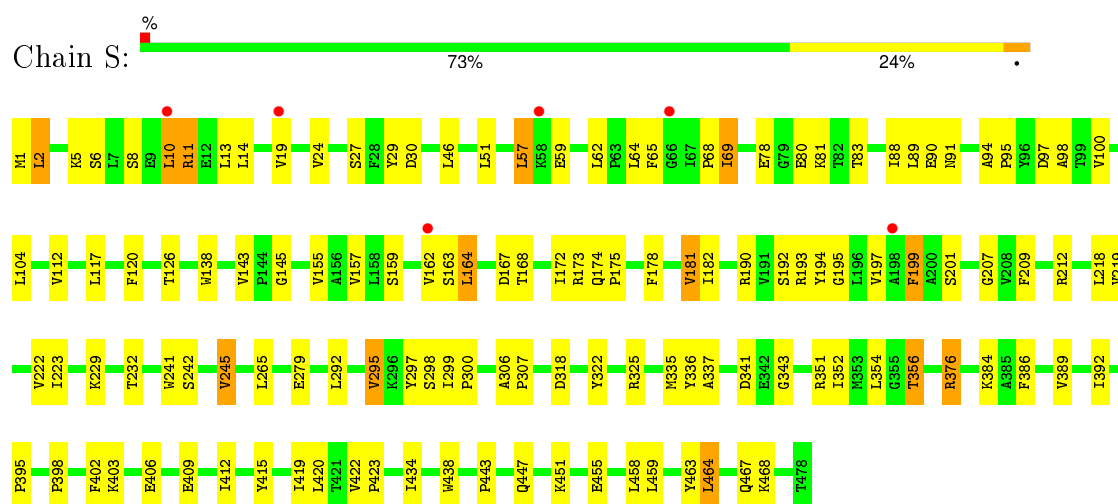
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



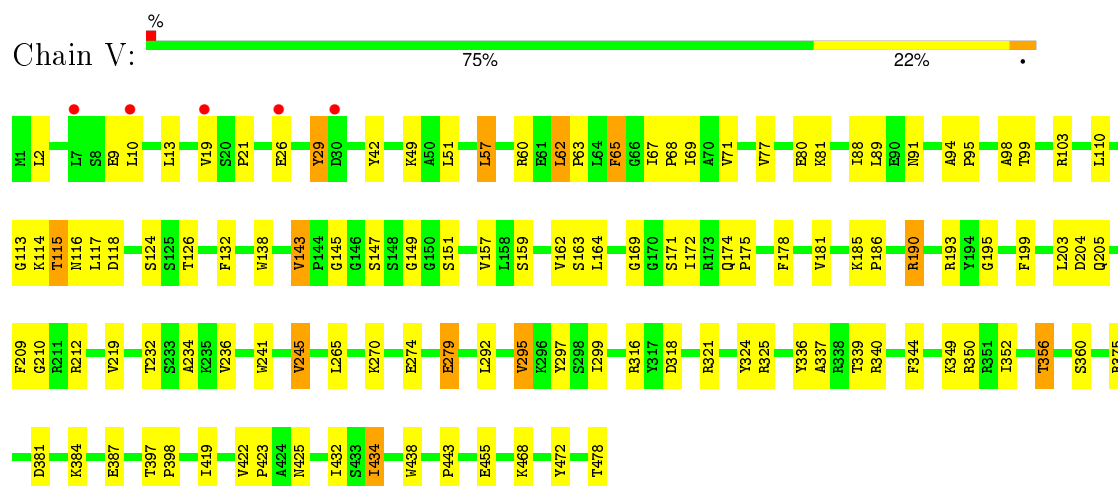
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



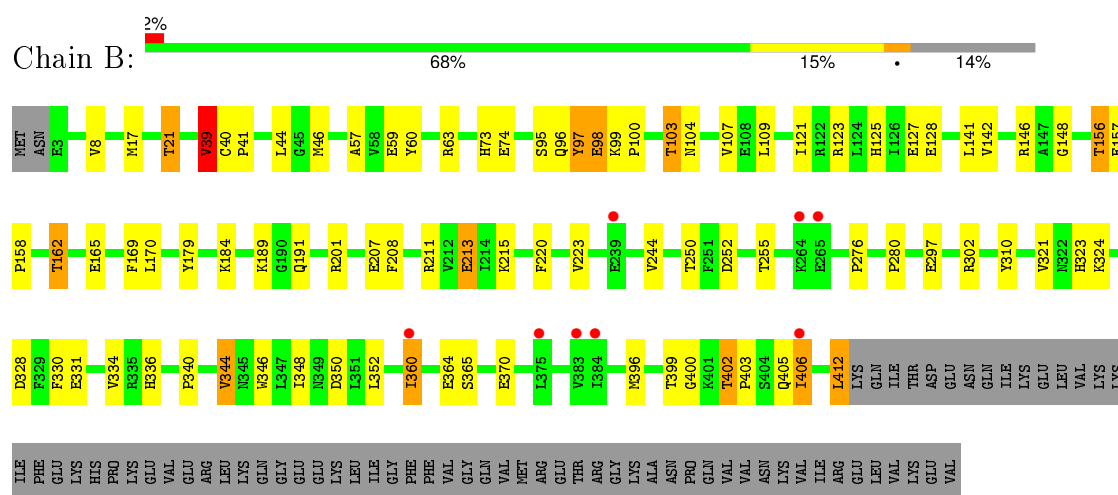
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

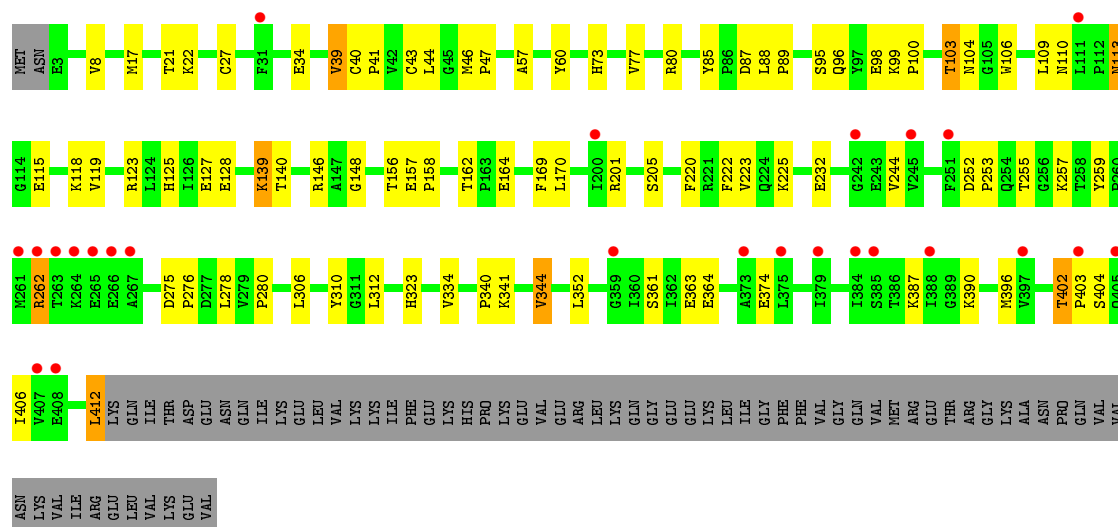


- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

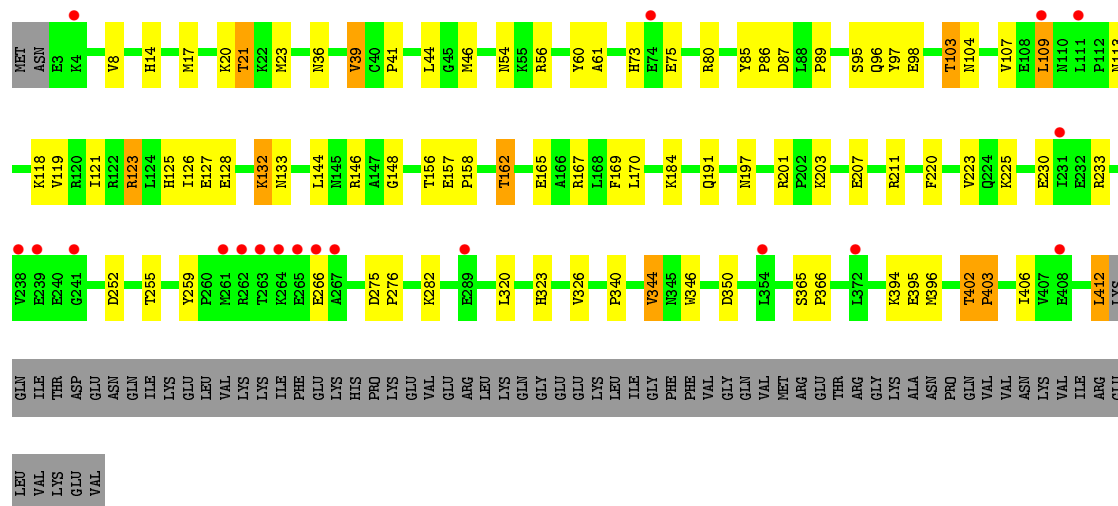


- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

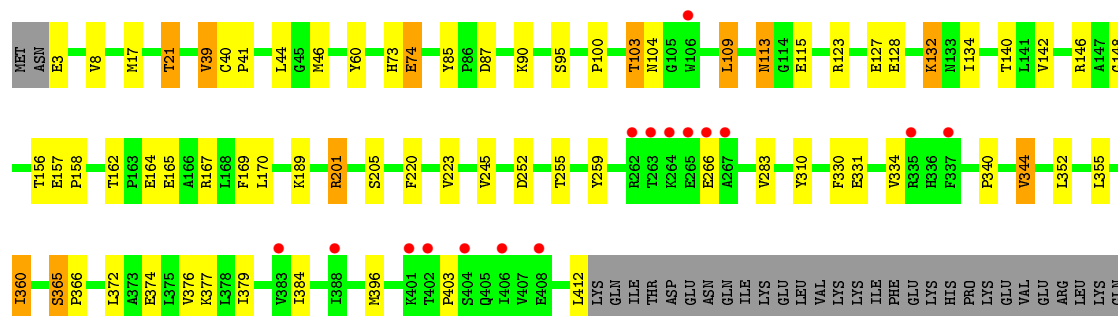




• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



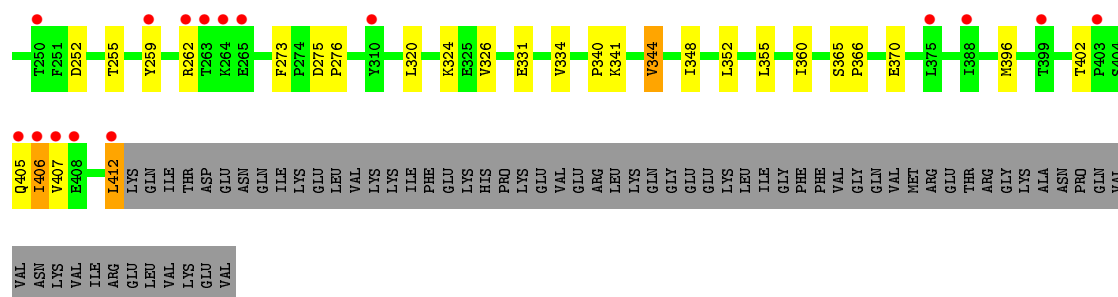
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



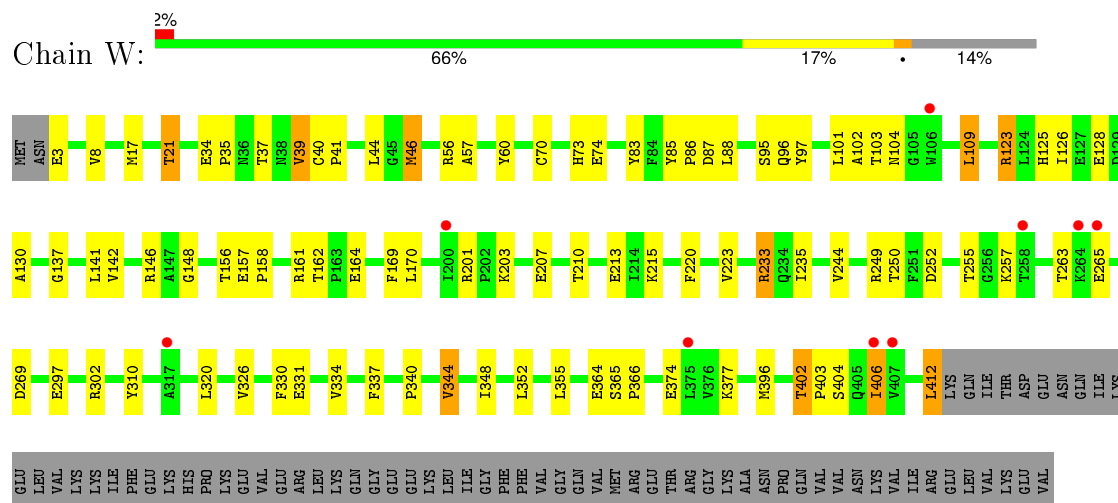
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LYS	V407	K264	R124	ASN	ME2
VAL	E408	E265	H125	ASN	ME3
ILE		E266	H126	ASN	ME4
ARG	L412	A267	E127	ASN	ME5
GLU	LYS		E128	ASN	ME6
LEU	GLN	D275		ASN	ME7
VAL	ILE	P276		ASN	ME8
LYS	THR		I134	ASN	ME9
GLU	ASP	K282		ASN	ME10
VAL	GLU	V283	L141	ASN	ME11
VAL	ASN			ASN	ME12
	ASN	R302	R146	ASN	ME13
	ILE		A147	ASN	ME14
	LYS	V321	G148	ASN	ME15
	GLU	N322		ASN	ME16
	LEU	H323	T156	ASN	ME17
	VAL		E157	ASN	ME18
	LYS	P340	P158	ASN	ME19
	LYS			ASN	ME20
	ILE	V344	T162	ASN	ME21
	PHE	N345		ASN	ME22
	GLU	K346	E165	ASN	ME23
	LYS	L347	A166	ASN	ME24
	LYS	I348	R167	ASN	ME25
	PRO	N349	L168	ASN	ME26
	LYS	D350	F169	ASN	ME27
	GLU	L351	L170	ASN	ME28
	VAL	L352		ASN	ME29
	GLU		K184	ASN	ME30
	ARG	L355		ASN	ME31
	LEU		Q191	ASN	ME32
	LYS	K358	N197	ASN	ME33
	GLN	G359		ASN	ME34
	GLY	I360		ASN	ME35
	GLU		R201	ASN	ME36
	GLU	E364	P202	ASN	ME37
	LYS	S365	K203	ASN	ME38
	LEU		G204	ASN	ME39
	LEU	K368	G205	ASN	ME40
	ILE	P369	K206	ASN	ME41
	GLY		E207	ASN	ME42
	PHE	E370		ASN	ME43
	PHE			ASN	ME44
	VAL	I384	R211	ASN	ME45
	GLN			ASN	ME46
	GLN	K387	V217	ASN	ME47
	VAL			ASN	ME48
	ARG	K390	F220	ASN	ME49
	GLU	E391		ASN	ME50
	GLU		V223	ASN	ME51
	THR	K394		ASN	ME52
	ARG	E395	E232	ASN	ME53
	GLY	N396		ASN	ME54
	LYS	V397	G241	ASN	ME55
	ALA	E398		ASN	ME56
	ASN		V244	ASN	ME57
	PRO	T402		ASN	ME58
	GLN	P403	T250	ASN	ME59
	VAL	S404		ASN	ME60
	VAL	D405	G252	ASN	ME61

HIS	P940	R146	ASN	MT
PRO	V944	A147	ASN	E3
GLU	N945	G148		M17
VAL	I346			
GLU	L347	T156		T21
ARG	N949	E157		
LEU	D350			C25
GLN	I351	T162		
GLY	L352	P163		V39
GLU		E164		C40
GLU	L355	E165		P41
LEU		F169		V42
LEU	I360	L170		C43
ILE				L44
GLY	S365	R201		G45
PHE	P366			M46
PHE		S205		N54
VAL	L372	T210		Y60
GLN	A373			A64
GLY	E374	E213		
VAL	L375	T214		L68
MET	V376	K215		
ARG	K377			H73
GLU	L378	F220		E74
THR	L379	V223		Y83
ARG	I384	E230		F84
LYS	M396	R233		Y85
ALA		P403		P86
ASN	T402	V245		D87
PRO	Q403			L88
GLN	S404	D252		S95
VAL	Q405	V407		T103
VAL	A406	T256		
ASN	V407			W106
LYS	E408			L109
ILE				R120
ARG	L412	R262		R123
GLU	LYS	T263		L124
LEU	GLN	K264		I125
VAL	ILE	E265		I126
VAL	THR	E266		E127
LYS	ASP			E128
GLU	GLU	D269		D129
VAL	ASN	V283		K132
	GLN			G137
	ILE			T140
	LYS	R302		
	LYS	R305		
	LEU			
	VAL	Y310		
	LYS	H323		
	ILE			
	PHE	V334		
	GLU			
	LYS			

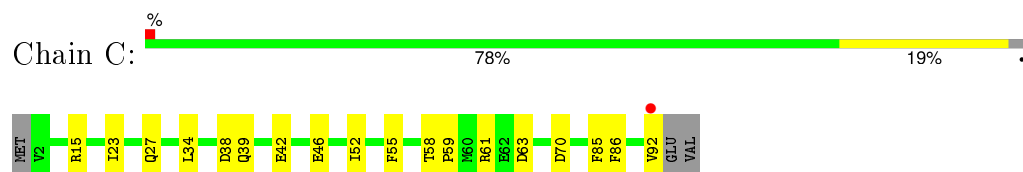
M10	M110	M111	M112	M113	M114	M115	M116	M117	M118	M119	M120	M121	M122	M123	M124	M125	M126	M127	M128	M129	M130	M131	M132	M133	M134	M135	M136	M137	M138	M139	M140	M141	M142	M143	M144	M145	M146	M147	M148	M149	M150	M151	M152	M153	M154	M155	M156	M157	M158	M159	M160	M161	M162	M163	M164	M165	M166	M167	M168	M169	M170	M171	M172	M173	M174	M175	M176	M177	M178	M179	M180	M181	M182	M183	M184	M185	M186	M187	M188	M189	M190	M191	M192	M193	M194	M195	M196	M197	M198	M199	M200	M201	M202	M203	M204	M205	M206	M207	M208	M209	M210	M211	M212	M213	M214	M215	M216	M217	M218	M219	M220	M221	M222	M223	M224	M225	M226	M227	M228	M229	M230	M231	M232	M233	M234	M235	M236	M237	M238	M239	M240	M241	M242	M243	M244	M245	M246	M247	M248	M249	M250	M251	M252	M253	M254	M255	M256	M257	M258	M259	M260	M261	M262	M263	M264	M265	M266	M267	M268	M269	M270	M271	M272	M273	M274	M275	M276	M277	M278	M279	M280	M281	M282	M283	M284	M285	M286	M287	M288	M289	M290	M291	M292	M293	M294	M295	M296	M297	M298	M299	M300	M301	M302	M303	M304	M305	M306	M307	M308	M309	M310	M311	M312	M313	M314	M315	M316	M317	M318	M319	M320	M321	M322	M323	M324	M325	M326	M327	M328	M329	M330	M331	M332	M333	M334	M335	M336	M337	M338	M339	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353	M354	M355	M356	M357	M358	M359	M360	M361	M362	M363	M364	M365	M366	M367	M368	M369	M370	M371	M372	M373	M374	M375	M376	M377	M378	M379	M380	M381	M382	M383	M384	M385	M386	M387	M388	M389	M390	M391	M392	M393	M394	M395	M396	M397	M398	M399	M400	M401	M402	M403	M404	M405	M406	M407	M408	M409	M410	M411	M412	M413	M414	M415	M416	M417	M418	M419	M420	M421	M422	M423	M424	M425	M426	M427	M428	M429	M430	M431	M432	M433	M434	M435	M436	M437	M438	M439	M440	M441	M442	M443	M444	M445	M446	M447	M448	M449	M450	M451	M452	M453	M454	M455	M456	M457	M458	M459	M460	M461	M462	M463	M464	M465	M466	M467	M468	M469	M470	M471	M472	M473	M474	M475	M476	M477	M478	M479	M480	M481	M482	M483	M484	M485	M486	M487	M488	M489	M490	M491	M492	M493	M494	M495	M496	M497	M498	M499	M500	M501	M502	M503	M504	M505	M506	M507	M508	M509	M510	M511	M512	M513	M514	M515	M516	M517	M518	M519	M520	M521	M522	M523	M524	M525	M526	M527	M528	M529	M530	M531	M532	M533	M534	M535	M536	M537	M538	M539	M540	M541	M542	M543	M544	M545	M546	M547	M548	M549	M550	M551	M552	M553	M554	M555	M556	M557	M558	M559	M560	M561	M562	M563	M564	M565	M566	M567	M568	M569	M570	M571	M572	M573	M574	M575	M576	M577	M578	M579	M580	M581	M582	M583	M584	M585	M586	M587	M588	M589	M590	M591	M592	M593	M594	M595	M596	M597	M598	M599	M600	M601	M602	M603	M604	M605	M606	M607	M608	M609	M610	M611	M612	M613	M614	M615	M616	M617	M618	M619	M620
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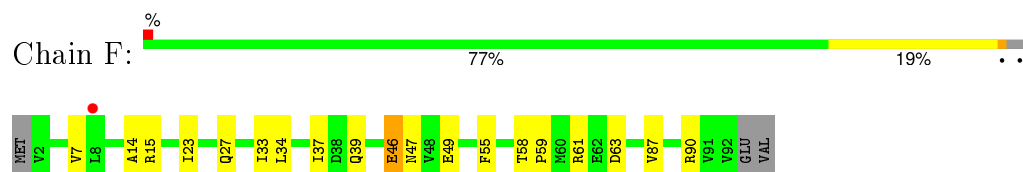
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



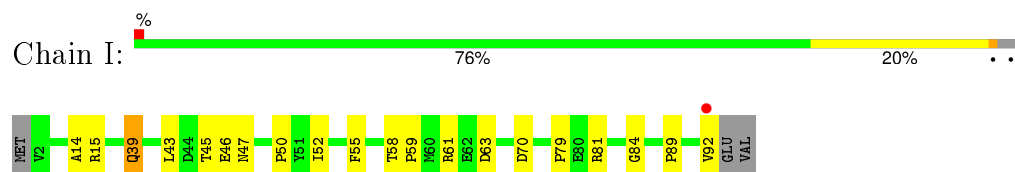
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



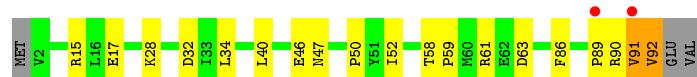
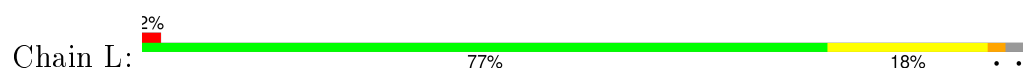
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



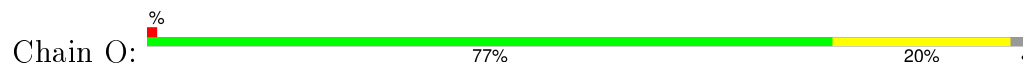
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



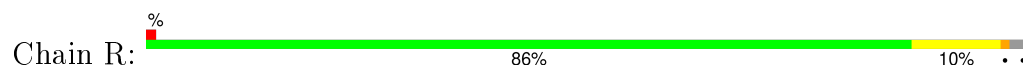
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



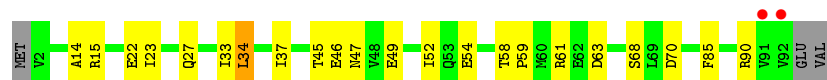
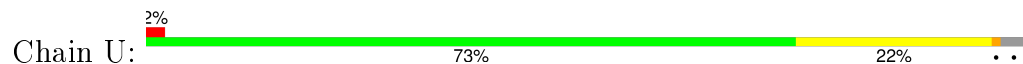
- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



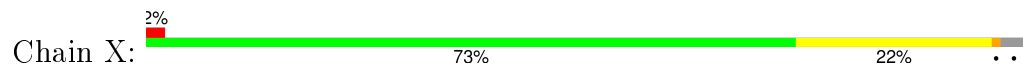
- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	127.48Å 131.01Å 154.67Å 90.02° 90.00° 89.91°	Depositor
Resolution (Å)	40.50 – 2.30 40.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.7 (40.50-2.30) 91.4 (40.51-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.273 0.251 , 0.275	Depositor DCC
R_{free} test set	20322 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	1.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.1	EDS
Estimated twinning fraction	0.000 for -k,h,l 0.000 for k,-h,l 0.146 for h,-k,-l 0.459 for -h,k,-l 0.146 for -h,-k,l 0.000 for -k,-h,-l 0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 405875 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	63144	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.50 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.2482e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ADP

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	0.64	0/3874	0.73	4/5244 (0.1%)
1	D	0.62	0/3874	0.71	0/5244
1	G	0.60	0/3874	0.70	1/5244 (0.0%)
1	J	0.62	1/3874 (0.0%)	0.70	0/5244
1	M	0.59	0/3874	0.69	1/5244 (0.0%)
1	P	0.59	0/3874	0.71	2/5244 (0.0%)
1	S	0.63	0/3874	0.71	0/5244
1	V	0.65	0/3874	0.72	1/5244 (0.0%)
2	B	0.56	0/3371	0.65	1/4541 (0.0%)
2	E	0.62	2/3371 (0.1%)	0.66	1/4541 (0.0%)
2	H	0.57	0/3371	0.66	1/4541 (0.0%)
2	K	0.58	0/3371	0.67	0/4541
2	N	0.57	0/3371	0.67	2/4541 (0.0%)
2	Q	0.56	0/3371	0.69	2/4541 (0.0%)
2	T	0.61	1/3371 (0.0%)	0.66	1/4541 (0.0%)
2	W	0.58	0/3371	0.65	1/4541 (0.0%)
3	C	0.67	0/778	0.72	0/1050
3	F	0.59	0/778	0.69	0/1050
3	I	0.64	0/778	0.66	0/1050
3	L	0.59	0/778	0.69	0/1050
3	O	0.61	0/778	0.67	0/1050
3	R	0.60	0/778	0.69	0/1050
3	U	0.57	0/778	0.65	0/1050
3	X	0.61	0/778	0.70	0/1050
All	All	0.60	4/64184 (0.0%)	0.69	18/86680 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	I	0	1
3	O	0	1
3	U	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	43	CYS	CB-SG	-5.55	1.72	1.81
2	T	43	CYS	CB-SG	-5.48	1.72	1.81
1	J	84	CYS	CB-SG	-5.26	1.73	1.81
2	E	110	ASN	CG-OD1	5.14	1.35	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	412	LEU	CA-CB-CG	5.84	128.74	115.30
1	G	117	LEU	CA-CB-CG	5.79	128.60	115.30
1	A	375	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	E	412	LEU	CA-CB-CG	5.67	128.34	115.30
1	P	464	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	316	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	N	120	ARG	NE-CZ-NH2	-5.49	117.56	120.30
2	W	412	LEU	CA-CB-CG	5.46	127.86	115.30
2	H	412	LEU	CA-CB-CG	5.46	127.85	115.30
2	B	412	LEU	CA-CB-CG	5.38	127.68	115.30
2	Q	120	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	M	354	LEU	CA-CB-CG	5.31	127.51	115.30
1	P	204	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	331	ASP	CB-CG-OD2	5.20	122.98	118.30
2	Q	269	ASP	CB-CG-OD1	5.20	122.98	118.30
2	N	120	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	376	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	V	381	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	39	VAL	Peptide
2	B	97	TYR	Peptide

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Mol	Chain	Res	Type	Group
3	I	45	THR	Peptide
3	O	45	THR	Peptide
3	U	45	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	0	3816	92	0
1	D	3784	0	3816	79	0
1	G	3784	0	3816	90	0
1	J	3784	0	3816	70	0
1	M	3784	0	3816	71	0
1	P	3784	0	3816	76	0
1	S	3784	0	3816	91	0
1	V	3784	0	3816	97	0
2	B	3308	0	3354	80	0
2	E	3308	0	3353	72	0
2	H	3308	0	3353	78	0
2	K	3308	0	3353	62	0
2	N	3308	0	3353	65	0
2	Q	3308	0	3353	61	0
2	T	3308	0	3353	72	0
2	W	3308	0	3353	71	0
3	C	764	0	755	11	0
3	F	764	0	755	16	0
3	I	764	0	755	17	0
3	L	764	0	755	21	0
3	O	764	0	755	15	0
3	R	764	0	755	14	0
3	U	764	0	755	15	0
3	X	764	0	755	17	0
4	B	27	0	12	1	0
4	E	27	0	12	0	0
4	H	27	0	12	0	0
4	K	27	0	12	0	0
4	N	27	0	12	0	0
4	Q	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	27	0	12	1	0
4	W	27	0	12	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
5	N	1	0	0	0	0
5	Q	1	0	0	0	0
5	T	1	0	0	0	0
5	W	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	H	1	0	0	0	0
6	K	1	0	0	0	0
6	N	1	0	0	0	0
6	Q	1	0	0	0	0
6	T	1	0	0	0	0
6	W	1	0	0	0	0
7	A	8	0	3	1	0
7	D	8	0	3	1	0
7	G	8	0	3	0	0
7	J	8	0	3	0	0
7	M	8	0	3	0	0
7	P	8	0	3	1	0
7	S	8	0	3	1	0
7	V	8	0	3	0	0
All	All	63144	0	63513	1225	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1225) 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:190:ARG:HG3	1:A:190:ARG:HH11	1.05	1.16
1:V:77:VAL:HG21	1:V:114:LYS:NZ	1.61	1.13
1:A:47:TYR:O	1:A:51:LEU:HD13	1.54	1.07
1:V:190:ARG:HH11	1:V:190:ARG:HG3	1.10	1.06
1:P:31:ARG:CG	1:P:31:ARG:HH11	1.69	1.05
3:L:92:VAL:HG22	3:L:92:VAL:O	1.58	1.04
1:V:77:VAL:HG21	1:V:114:LYS:HZ1	1.08	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ARG:HD3	1:D:241:TRP:HH2	1.20	1.03
1:M:88:ILE:HG23	1:M:343:GLY:HA3	1.40	1.03
1:S:376:ARG:HH11	1:S:376:ARG:HG3	1.24	1.02
1:V:77:VAL:CG2	1:V:114:LYS:HZ1	1.72	1.02
2:N:21:THR:HG21	3:O:61:ARG:HH12	1.24	1.01
2:B:21:THR:HB	3:C:63:ASP:OD1	1.61	1.01
1:V:336:TYR:O	1:V:339:THR:HG22	1.61	1.00
2:B:21:THR:HG21	3:C:61:ARG:HH12	1.25	1.00
2:E:21:THR:HG21	3:F:61:ARG:HH12	1.23	1.00
1:V:77:VAL:CG2	1:V:114:LYS:NZ	2.23	0.99
1:D:376:ARG:HG3	1:D:376:ARG:HH11	1.25	0.98
2:T:21:THR:HG21	3:U:61:ARG:HH12	1.26	0.97
2:H:21:THR:HG21	3:I:61:ARG:HH12	1.26	0.97
1:P:190:ARG:HD3	1:P:241:TRP:HH2	1.27	0.97
1:J:376:ARG:HG3	1:J:376:ARG:HH11	1.26	0.96
2:K:360:ILE:HD11	2:K:365:SER:HA	1.45	0.96
1:A:47:TYR:CE2	1:A:112:VAL:CG1	2.48	0.96
1:D:138:TRP:CE2	1:D:438:TRP:HH2	1.81	0.96
1:A:47:TYR:CE2	1:A:112:VAL:HG11	2.00	0.95
2:E:17:MET:HE2	2:E:57:ALA:HA	1.47	0.95
1:P:352:ILE:O	1:P:356:THR:HG22	1.66	0.94
2:T:21:THR:HB	3:U:63:ASP:OD1	1.65	0.94
2:K:100:PRO:HB3	2:K:123:ARG:HH21	1.32	0.94
1:S:155:VAL:HG12	1:S:181:VAL:HG21	1.48	0.94
1:J:190:ARG:HD3	1:J:241:TRP:HH2	1.32	0.93
1:M:352:ILE:O	1:M:356:THR:HG22	1.67	0.93
1:D:138:TRP:CE2	1:D:438:TRP:CH2	2.56	0.93
2:W:17:MET:CE	2:W:60:TYR:HB2	1.99	0.93
2:Q:360:ILE:HD11	2:Q:365:SER:HA	1.52	0.91
1:G:85:ALA:HB2	1:G:117:LEU:HD13	1.53	0.91
1:D:72:LYS:HA	1:D:115:THR:HG22	1.50	0.90
2:W:252:ASP:HB3	2:W:255:THR:HG22	1.54	0.90
2:B:162:THR:HG22	2:B:165:GLU:H	1.33	0.90
2:K:156:THR:HG22	2:K:157:GLU:O	1.70	0.90
2:H:252:ASP:HB3	2:H:255:THR:HG22	1.53	0.89
2:B:100:PRO:HB3	2:B:123:ARG:HH21	1.35	0.89
2:W:103:THR:HG22	2:W:104:ASN:OD1	1.73	0.88
1:P:31:ARG:HG2	1:P:31:ARG:HH11	1.36	0.88
2:B:17:MET:HE2	2:B:57:ALA:HA	1.55	0.88
1:S:386:PHE:HB3	1:S:451:LYS:HE2	1.54	0.88
1:V:190:ARG:HG3	1:V:190:ARG:NH1	1.84	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:370:LYS:HZ2	3:R:45:THR:HB	1.37	0.88
1:A:68:PRO:HB3	1:A:112:VAL:HG21	1.55	0.87
2:H:252:ASP:HB3	2:H:255:THR:CG2	2.05	0.85
2:E:17:MET:CE	2:E:60:TYR:HB2	2.06	0.85
2:B:40:CYS:O	2:B:44:LEU:HB2	1.76	0.85
2:W:34:GLU:O	2:W:37:THR:HG22	1.77	0.85
2:W:39:VAL:HG13	2:W:44:LEU:HD11	1.57	0.85
2:E:252:ASP:HB3	2:E:255:THR:HG22	1.57	0.84
2:N:21:THR:CG2	3:O:61:ARG:HH12	1.90	0.84
1:M:190:ARG:HD3	1:M:241:TRP:HH2	1.43	0.84
1:A:47:TYR:CD2	1:A:112:VAL:CG1	2.61	0.84
1:M:88:ILE:HD11	1:M:120:PHE:CE2	2.11	0.83
2:T:156:THR:HG22	2:T:157:GLU:O	1.78	0.83
1:A:190:ARG:HG3	1:A:190:ARG:NH1	1.84	0.83
1:V:71:VAL:HB	1:V:114:LYS:HZ3	1.42	0.83
2:E:17:MET:HE1	2:E:60:TYR:HB2	1.60	0.83
2:B:21:THR:CG2	3:C:61:ARG:HH12	1.92	0.83
2:W:17:MET:HE2	2:W:57:ALA:HA	1.60	0.82
1:A:95:PRO:HG2	2:B:46:MET:HE1	1.61	0.82
1:G:422:VAL:N	1:G:423:PRO:CD	2.43	0.82
2:T:103:THR:HG22	2:T:104:ASN:OD1	1.78	0.81
1:D:190:ARG:HD3	1:D:241:TRP:CH2	2.12	0.81
1:A:279:GLU:HG3	1:A:468:LYS:NZ	1.94	0.81
1:A:138:TRP:CE2	1:A:438:TRP:HH2	1.98	0.81
2:Q:21:THR:CG2	3:R:61:ARG:HH12	1.94	0.80
1:A:47:TYR:CD2	1:A:112:VAL:HG13	2.17	0.80
1:M:88:ILE:HD11	1:M:120:PHE:CZ	2.16	0.80
1:G:85:ALA:CB	1:G:117:LEU:HD13	2.11	0.80
1:S:376:ARG:HG3	1:S:376:ARG:NH1	1.97	0.80
2:W:17:MET:HE1	2:W:60:TYR:HB2	1.62	0.80
1:G:190:ARG:HD3	1:G:241:TRP:HH2	1.44	0.80
2:B:39:VAL:HG13	2:B:44:LEU:HD11	1.64	0.80
1:A:138:TRP:CE2	1:A:438:TRP:CH2	2.70	0.80
3:L:92:VAL:CG2	3:L:92:VAL:O	2.30	0.79
1:P:31:ARG:HH11	1:P:31:ARG:HG3	1.47	0.79
2:N:162:THR:HG22	2:N:165:GLU:H	1.45	0.79
1:S:81:LYS:HE2	1:S:91:ASN:HA	1.64	0.79
1:D:77:VAL:HG23	1:D:114:LYS:NZ	1.98	0.79
2:T:17:MET:HE2	2:T:57:ALA:HA	1.64	0.79
2:K:21:THR:HG21	3:L:61:ARG:HH12	1.46	0.78
2:E:17:MET:CE	2:E:57:ALA:HA	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:190:ARG:HD3	1:P:241:TRP:CH2	2.17	0.78
1:G:352:ILE:O	1:G:356:THR:HG23	1.84	0.78
1:J:352:ILE:O	1:J:356:THR:HG22	1.84	0.78
2:B:17:MET:CE	2:B:57:ALA:HA	2.14	0.77
1:D:194:TYR:CD1	1:D:229:LYS:HB3	2.19	0.77
1:V:190:ARG:HH11	1:V:190:ARG:CG	1.95	0.77
1:P:31:ARG:HG2	1:P:31:ARG:NH1	1.97	0.77
2:N:21:THR:HB	3:O:63:ASP:OD1	1.85	0.76
2:T:85:TYR:HD2	2:T:87:ASP:OD1	1.69	0.76
2:Q:17:MET:CE	2:Q:60:TYR:HB2	2.15	0.76
2:Q:17:MET:HE2	2:Q:60:TYR:HB2	1.66	0.76
1:A:190:ARG:CG	1:A:190:ARG:HH11	1.94	0.76
2:K:21:THR:CG2	3:L:61:ARG:HH12	1.97	0.76
1:M:95:PRO:HG2	2:N:46:MET:CE	2.16	0.76
2:Q:156:THR:HG22	2:Q:157:GLU:O	1.84	0.76
2:B:17:MET:CE	2:B:60:TYR:HB2	2.16	0.75
1:S:190:ARG:HD3	1:S:241:TRP:HH2	1.51	0.75
2:Q:109:LEU:HD11	2:Q:169:PHE:HA	1.68	0.75
2:B:21:THR:HG21	3:C:61:ARG:NH1	2.00	0.75
1:D:352:ILE:O	1:D:356:THR:HG23	1.86	0.75
2:E:21:THR:HB	3:F:63:ASP:OD1	1.87	0.75
2:H:17:MET:HE2	2:H:60:TYR:HB3	1.69	0.75
2:H:17:MET:CE	2:H:60:TYR:HB3	2.17	0.74
1:V:279:GLU:HG3	1:V:468:LYS:NZ	2.03	0.74
1:J:174:GLN:HG3	1:J:175:PRO:HD3	1.70	0.74
2:W:21:THR:CG2	3:X:61:ARG:HH12	1.99	0.73
2:N:109:LEU:HD11	2:N:169:PHE:HA	1.70	0.73
2:H:21:THR:CG2	3:I:61:ARG:HH12	1.99	0.73
2:H:103:THR:CG2	2:H:104:ASN:OD1	2.36	0.73
2:W:252:ASP:HB3	2:W:255:THR:CG2	2.17	0.73
1:J:352:ILE:O	1:J:356:THR:CG2	2.35	0.73
1:P:306:ALA:HB3	1:P:307:PRO:HD3	1.70	0.73
2:K:109:LEU:HD11	2:K:169:PHE:HA	1.71	0.73
1:M:138:TRP:CE2	1:M:438:TRP:CH2	2.77	0.73
1:V:193:ARG:NH1	1:V:232:THR:OG1	2.22	0.72
2:W:97:TYR:O	2:W:123:ARG:NH2	2.22	0.72
2:W:21:THR:HG21	3:X:61:ARG:HH12	1.53	0.72
2:H:17:MET:HE1	2:H:60:TYR:CB	2.20	0.72
2:B:213:GLU:OE1	2:B:215:LYS:HE3	1.89	0.72
2:B:252:ASP:HB3	2:B:255:THR:HG22	1.71	0.72
2:B:156:THR:HG22	2:B:157:GLU:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:185:LYS:NZ	1:M:429:LEU:O	2.24	0.71
2:H:20:LYS:HE2	2:H:56:ARG:HH12	1.55	0.71
1:A:110:LEU:O	1:A:112:VAL:HG23	1.90	0.71
2:B:39:VAL:CG1	2:B:44:LEU:HD11	2.21	0.71
2:T:17:MET:CE	2:T:57:ALA:HA	2.20	0.71
1:D:138:TRP:CZ2	1:D:438:TRP:CH2	2.78	0.71
2:N:156:THR:HG22	2:N:157:GLU:O	1.90	0.71
1:D:182:ILE:HG12	1:D:434:ILE:HD12	1.71	0.71
2:N:17:MET:HE1	2:N:60:TYR:HB2	1.73	0.71
1:V:352:ILE:O	1:V:356:THR:HG23	1.89	0.71
2:N:21:THR:HG21	3:O:61:ARG:NH1	2.04	0.70
2:B:17:MET:HE1	2:B:57:ALA:O	1.90	0.70
1:A:47:TYR:O	1:A:51:LEU:CD1	2.37	0.70
2:T:21:THR:CG2	3:U:61:ARG:HH12	2.00	0.70
1:P:31:ARG:CG	1:P:31:ARG:NH1	2.40	0.70
1:D:115:THR:HG21	1:D:151:SER:OG	1.90	0.70
2:N:360:ILE:HD11	2:N:365:SER:HA	1.74	0.70
3:L:46:GLU:O	3:L:47:ASN:HB2	1.91	0.70
1:G:270:LYS:HE3	1:G:274:GLU:OE2	1.91	0.70
3:F:23:ILE:O	3:F:27:GLN:HG3	1.92	0.69
2:H:17:MET:CE	2:H:60:TYR:CB	2.70	0.69
2:W:123:ARG:NH1	2:W:125:HIS:ND1	2.40	0.69
1:J:190:ARG:HD3	1:J:241:TRP:CH2	2.23	0.69
2:Q:17:MET:CE	2:Q:60:TYR:CB	2.70	0.69
2:W:402:THR:HG22	2:W:403:PRO:HD2	1.74	0.69
2:E:21:THR:HG21	3:F:61:ARG:NH1	2.03	0.69
2:W:17:MET:CE	2:W:57:ALA:HA	2.22	0.69
1:S:182:ILE:HG12	1:S:434:ILE:HD12	1.74	0.69
2:E:156:THR:HG22	2:E:157:GLU:O	1.91	0.69
1:G:190:ARG:HD3	1:G:241:TRP:CH2	2.26	0.69
2:T:402:THR:OG1	2:T:405:GLN:HB2	1.93	0.69
2:H:95:SER:HB3	2:H:127:GLU:HB3	1.73	0.69
1:G:13:LEU:HB3	1:G:19:VAL:HG12	1.75	0.69
2:H:109:LEU:HD11	2:H:169:PHE:HA	1.74	0.69
1:V:204:ASP:O	1:V:205:GLN:HG2	1.93	0.69
1:M:95:PRO:HG2	2:N:46:MET:HE1	1.75	0.68
2:T:17:MET:CE	2:T:60:TYR:HB2	2.24	0.68
2:E:103:THR:HG22	2:E:104:ASN:OD1	1.93	0.68
1:M:115:THR:HG21	1:M:151:SER:OG	1.93	0.68
2:K:85:TYR:OH	3:L:91:VAL:HG11	1.92	0.68
1:D:376:ARG:NH1	1:D:376:ARG:HG3	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:17:MET:HE1	2:T:57:ALA:O	1.93	0.68
2:H:97:TYR:O	2:H:123:ARG:NH2	2.27	0.68
2:T:255:THR:HG21	2:T:259:TYR:OH	1.92	0.68
2:K:95:SER:CB	2:K:127:GLU:HB3	2.23	0.68
1:M:190:ARG:HD3	1:M:241:TRP:CH2	2.28	0.68
1:M:90:GLU:O	1:M:91:ASN:HB2	1.92	0.68
1:S:155:VAL:CG1	1:S:181:VAL:HG21	2.24	0.68
1:G:306:ALA:HB3	1:G:307:PRO:HD3	1.75	0.68
1:V:336:TYR:O	1:V:339:THR:CG2	2.41	0.67
2:E:310:TYR:CE1	2:E:334:VAL:HG11	2.28	0.67
2:K:3:GLU:OE1	2:K:3:GLU:HA	1.93	0.67
1:V:138:TRP:CE2	1:V:438:TRP:CH2	2.81	0.67
2:W:156:THR:HG22	2:W:157:GLU:O	1.94	0.67
2:Q:21:THR:HG21	3:R:61:ARG:HH12	1.59	0.67
1:M:69:ILE:HD11	1:M:164:LEU:HD13	1.76	0.67
2:Q:162:THR:HG22	2:Q:165:GLU:H	1.59	0.67
2:K:74:GLU:HG2	2:K:283:VAL:O	1.95	0.67
1:V:77:VAL:HG21	1:V:114:LYS:CE	2.24	0.67
2:H:17:MET:HE1	2:H:60:TYR:HB2	1.77	0.67
2:N:17:MET:HE1	2:N:60:TYR:CB	2.24	0.67
1:G:422:VAL:HG22	1:G:423:PRO:HD3	1.75	0.67
1:S:83:THR:HG22	1:S:90:GLU:HA	1.77	0.67
2:T:252:ASP:HB3	2:T:255:THR:HG22	1.77	0.67
1:V:71:VAL:CB	1:V:114:LYS:HZ3	2.07	0.67
1:G:85:ALA:HB2	1:G:117:LEU:CD1	2.23	0.67
1:A:279:GLU:HG3	1:A:468:LYS:HZ3	1.55	0.67
1:G:115:THR:HG21	1:G:151:SER:OG	1.95	0.67
1:A:352:ILE:O	1:A:356:THR:HG23	1.94	0.67
2:B:156:THR:CG2	2:B:157:GLU:O	2.42	0.66
1:M:163:SER:HB3	1:M:209:PHE:HB2	1.77	0.66
2:B:402:THR:HG22	2:B:403:PRO:HD2	1.77	0.66
1:S:167:ASP:HB2	1:S:172:ILE:HD12	1.76	0.66
2:B:39:VAL:HG13	2:B:44:LEU:CD1	2.24	0.66
1:A:438:TRP:CH2	1:A:443:PRO:HG3	2.31	0.66
2:W:213:GLU:OE2	2:W:215:LYS:HE3	1.95	0.66
2:K:17:MET:CE	2:K:60:TYR:CB	2.73	0.66
2:E:252:ASP:HB3	2:E:255:THR:CG2	2.24	0.66
1:D:174:GLN:HG3	1:D:175:PRO:HD3	1.77	0.66
3:U:46:GLU:O	3:U:47:ASN:HB2	1.95	0.66
1:S:190:ARG:HD3	1:S:241:TRP:CH2	2.29	0.66
1:M:155:VAL:CG2	1:M:163:SER:HB2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:376:ARG:NH1	1:J:376:ARG:HG3	1.94	0.66
1:M:174:GLN:HG3	1:M:175:PRO:HD3	1.78	0.66
2:E:103:THR:CG2	2:E:104:ASN:OD1	2.44	0.66
2:K:95:SER:HB2	2:K:127:GLU:HB3	1.76	0.66
2:B:103:THR:CG2	2:B:104:ASN:OD1	2.44	0.66
2:T:21:THR:HG21	3:U:61:ARG:NH1	2.07	0.65
1:M:138:TRP:CE2	1:M:438:TRP:HH2	2.13	0.65
1:D:292:LEU:O	1:D:295:VAL:HG22	1.97	0.65
2:B:17:MET:HE1	2:B:60:TYR:HB2	1.78	0.65
1:P:299:ILE:HG13	1:P:419:ILE:HG22	1.78	0.65
1:D:69:ILE:HD11	1:D:164:LEU:HD13	1.77	0.65
2:B:73:HIS:NE2	2:B:103:THR:HB	2.12	0.65
1:S:143:VAL:HG12	1:S:145:GLY:H	1.60	0.65
1:V:77:VAL:CG2	1:V:114:LYS:HZ2	2.07	0.65
2:W:103:THR:CG2	2:W:104:ASN:OD1	2.44	0.65
2:E:17:MET:HE1	2:E:57:ALA:O	1.97	0.65
1:J:178:PHE:HE1	1:J:397:THR:HG21	1.62	0.65
1:S:299:ILE:HG13	1:S:419:ILE:HG22	1.79	0.64
2:Q:95:SER:HB3	2:Q:127:GLU:CB	2.26	0.64
2:B:302:ARG:HD3	2:B:321:VAL:HG22	1.80	0.64
1:P:95:PRO:HG2	2:Q:46:MET:CE	2.27	0.64
2:T:103:THR:CG2	2:T:104:ASN:OD1	2.45	0.64
3:X:23:ILE:O	3:X:27:GLN:HG3	1.96	0.64
2:N:103:THR:HG23	2:N:104:ASN:OD1	1.98	0.64
1:M:86:SER:OG	1:M:88:ILE:HG13	1.98	0.64
1:D:77:VAL:HG23	1:D:114:LYS:HZ1	1.60	0.64
2:K:17:MET:HE1	2:K:60:TYR:HB2	1.80	0.64
1:J:306:ALA:HB3	1:J:307:PRO:HD3	1.80	0.64
1:G:422:VAL:CG2	1:G:423:PRO:HD3	2.28	0.64
1:G:300:PRO:HG2	3:I:39:GLN:HG3	1.80	0.64
2:H:220:PHE:O	2:H:223:VAL:HG22	1.97	0.64
1:J:138:TRP:CE2	1:J:438:TRP:CH2	2.86	0.64
2:N:100:PRO:HB3	2:N:123:ARG:NH2	2.13	0.63
1:D:2:LEU:HD23	1:D:27:SER:HB2	1.79	0.63
1:M:376:ARG:HG3	1:M:376:ARG:HH11	1.62	0.63
1:S:352:ILE:O	1:S:356:THR:HG23	1.97	0.63
1:G:90:GLU:O	1:G:91:ASN:HB2	1.98	0.63
2:Q:213:GLU:OE2	2:Q:215:LYS:HE3	1.98	0.63
1:J:90:GLU:O	1:J:91:ASN:HB2	1.98	0.63
2:N:39:VAL:HG13	2:N:44:LEU:HD11	1.79	0.63
1:P:174:GLN:HG3	1:P:175:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:115:THR:HG21	1:V:151:SER:OG	1.99	0.63
1:V:95:PRO:HG2	2:W:46:MET:HE3	1.80	0.63
1:P:185:LYS:NZ	1:P:429:LEU:O	2.30	0.63
2:E:21:THR:CG2	3:F:61:ARG:HH12	2.07	0.63
1:V:292:LEU:HB2	1:V:295:VAL:HG22	1.79	0.63
2:Q:95:SER:HB3	2:Q:127:GLU:HB2	1.81	0.63
2:K:170:LEU:CD1	2:K:223:VAL:HG21	2.29	0.63
1:V:190:ARG:HD2	1:V:455:GLU:OE2	1.99	0.62
2:B:330:PHE:CE1	2:B:344:VAL:HG13	2.34	0.62
1:J:163:SER:HB3	1:J:209:PHE:HB2	1.81	0.62
1:G:95:PRO:HG2	2:H:46:MET:CE	2.30	0.62
2:H:23:MET:CE	2:H:126:ILE:HG21	2.29	0.62
2:E:39:VAL:HG22	2:E:44:LEU:HG	1.81	0.62
2:B:40:CYS:O	2:B:44:LEU:CB	2.47	0.62
1:V:350:ARG:NH1	3:X:29:GLN:OE1	2.33	0.62
1:V:118:ASP:OD2	1:V:147:SER:HA	2.00	0.62
2:B:109:LEU:HD11	2:B:169:PHE:HA	1.82	0.62
1:P:138:TRP:CE2	1:P:438:TRP:CH2	2.87	0.62
1:G:299:ILE:HG13	1:G:419:ILE:HG22	1.81	0.62
2:E:170:LEU:HD12	2:E:223:VAL:HG21	1.80	0.62
2:B:97:TYR:O	2:B:123:ARG:NH2	2.33	0.62
1:S:306:ALA:HB3	1:S:307:PRO:HD3	1.81	0.61
2:K:17:MET:CE	2:K:60:TYR:HB3	2.29	0.61
1:A:30:ASP:O	1:A:34:GLN:HG3	2.00	0.61
1:P:31:ARG:NE	1:P:157:VAL:O	2.32	0.61
2:H:103:THR:HG22	2:H:104:ASN:OD1	2.00	0.61
2:N:17:MET:CE	2:N:60:TYR:CB	2.79	0.61
3:R:46:GLU:O	3:R:47:ASN:HB2	2.00	0.61
2:K:17:MET:CE	2:K:60:TYR:HB2	2.31	0.61
2:H:162:THR:HG22	2:H:165:GLU:H	1.65	0.61
2:B:146:ARG:HH11	2:B:146:ARG:HG2	1.66	0.61
1:G:262:GLU:HA	1:G:262:GLU:OE1	2.01	0.61
1:A:78:GLU:N	1:A:97:ASP:OD1	2.24	0.61
2:H:201:ARG:HD2	2:H:207:GLU:O	2.00	0.61
1:M:138:TRP:CD2	1:M:438:TRP:HZ3	2.18	0.61
1:M:299:ILE:N	1:M:300:PRO:HD2	2.15	0.61
1:P:3:TRP:CE3	1:P:31:ARG:HD2	2.36	0.61
2:W:17:MET:HE1	2:W:57:ALA:O	2.00	0.61
3:C:23:ILE:O	3:C:27:GLN:HG3	2.01	0.61
2:N:17:MET:CE	2:N:60:TYR:HB3	2.30	0.61
1:V:81:LYS:HE2	1:V:91:ASN:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:HG13	2:B:40:CYS:N	2.15	0.60
2:E:310:TYR:HE1	2:E:334:VAL:HG11	1.66	0.60
1:S:376:ARG:HD2	3:U:49:GLU:O	2.02	0.60
2:B:8:VAL:HG12	2:B:158:PRO:HB2	1.84	0.60
2:W:109:LEU:HD11	2:W:169:PHE:HA	1.82	0.60
1:S:13:LEU:HB3	1:S:19:VAL:HG12	1.83	0.60
1:M:279:GLU:HG3	1:M:468:LYS:NZ	2.16	0.60
2:K:220:PHE:O	2:K:223:VAL:HG22	2.01	0.60
2:N:220:PHE:O	2:N:223:VAL:HG22	2.00	0.60
1:D:88:ILE:HG13	1:D:343:GLY:HA3	1.82	0.60
2:H:21:THR:HB	3:I:63:ASP:OD1	2.02	0.60
2:H:73:HIS:NE2	2:H:103:THR:HB	2.16	0.60
1:A:2:LEU:HD23	1:A:27:SER:HB2	1.83	0.60
1:G:421:THR:C	1:G:423:PRO:HD2	2.22	0.60
2:H:320:LEU:HD22	2:H:326:VAL:HG12	1.83	0.60
1:V:270:LYS:O	1:V:274:GLU:HG3	2.01	0.60
2:Q:17:MET:HE2	2:Q:60:TYR:CB	2.32	0.60
1:M:88:ILE:HD11	1:M:120:PHE:HE2	1.63	0.60
2:K:17:MET:HE2	2:K:60:TYR:HB3	1.82	0.60
1:D:138:TRP:NE1	1:D:438:TRP:HH2	1.99	0.59
1:D:352:ILE:O	1:D:356:THR:CG2	2.49	0.59
2:T:396:MET:HG3	2:T:406:ILE:HD11	1.84	0.59
2:N:346:TRP:O	2:N:350:ASP:HB2	2.02	0.59
1:G:422:VAL:N	1:G:423:PRO:HD2	2.16	0.59
1:G:81:LYS:HE2	1:G:91:ASN:HA	1.83	0.59
1:D:68:PRO:HB3	1:D:112:VAL:HG11	1.84	0.59
3:O:46:GLU:O	3:O:47:ASN:HB2	2.03	0.59
2:W:17:MET:HE3	2:W:60:TYR:HB2	1.82	0.59
2:Q:156:THR:CG2	2:Q:157:GLU:O	2.50	0.59
1:G:69:ILE:HD11	1:G:164:LEU:HD13	1.84	0.59
1:S:297:TYR:O	1:S:300:PRO:HD2	2.01	0.59
1:M:138:TRP:CZ2	1:M:438:TRP:CH2	2.90	0.59
2:T:340:PRO:O	2:T:344:VAL:HG22	2.02	0.59
2:K:201:ARG:HG3	2:K:205:SER:OG	2.03	0.59
2:B:103:THR:HG22	2:B:104:ASN:OD1	2.03	0.59
2:K:90:LYS:NZ	2:K:128:GLU:OE2	2.31	0.59
1:D:245:VAL:HG12	1:D:459:LEU:HB3	1.84	0.59
2:K:360:ILE:HD11	2:K:366:PRO:HD3	1.84	0.59
1:A:95:PRO:CG	2:B:46:MET:HE1	2.32	0.59
1:D:356:THR:HG21	3:F:14:ALA:HB2	1.85	0.59
2:H:346:TRP:O	2:H:350:ASP:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:140:THR:OG1	3:L:90:ARG:HA	2.02	0.58
1:J:299:ILE:HG13	1:J:419:ILE:HG22	1.85	0.58
2:K:103:THR:CG2	2:K:104:ASN:OD1	2.51	0.58
2:B:297:GLU:OE2	2:B:302:ARG:HA	2.02	0.58
2:E:41:PRO:HB3	2:E:46:MET:HE2	1.85	0.58
1:V:438:TRP:CZ3	1:V:443:PRO:HG3	2.38	0.58
1:A:25:VAL:CG1	1:A:51:LEU:HD12	2.34	0.58
1:S:190:ARG:HH11	1:S:190:ARG:HG3	1.68	0.58
2:W:21:THR:HB	3:X:63:ASP:OD1	2.03	0.58
1:V:172:ILE:O	1:V:175:PRO:HD2	2.03	0.58
2:E:100:PRO:HB3	2:E:123:ARG:NH2	2.18	0.58
1:A:306:ALA:HB3	1:A:307:PRO:HD3	1.84	0.58
2:W:170:LEU:HD12	2:W:223:VAL:HG21	1.86	0.58
2:K:170:LEU:HD12	2:K:223:VAL:HG21	1.85	0.58
2:W:17:MET:HE3	2:W:60:TYR:CB	2.34	0.58
1:D:143:VAL:CG1	1:D:145:GLY:H	2.17	0.58
1:S:194:TYR:CD1	1:S:229:LYS:HB3	2.39	0.57
2:H:95:SER:CB	2:H:127:GLU:HB3	2.34	0.57
2:H:95:SER:HB3	2:H:127:GLU:CB	2.33	0.57
1:G:72:LYS:HA	1:G:115:THR:HG22	1.86	0.57
2:N:14:HIS:CD2	2:N:127:GLU:OE2	2.57	0.57
1:S:163:SER:HB3	1:S:209:PHE:HB2	1.84	0.57
1:M:306:ALA:HB3	1:M:307:PRO:HD3	1.86	0.57
1:G:397:THR:HG23	1:G:399:THR:O	2.03	0.57
2:T:355:LEU:HD21	2:T:365:SER:HB2	1.86	0.57
2:K:360:ILE:CD1	2:K:366:PRO:HD3	2.34	0.57
1:D:201:SER:HB2	2:E:276:PRO:HG2	1.87	0.57
1:D:83:THR:HG22	1:D:90:GLU:HA	1.87	0.57
2:W:17:MET:CE	2:W:60:TYR:CB	2.79	0.57
1:M:395:PRO:O	1:M:420:LEU:HD13	2.04	0.57
1:G:138:TRP:CE2	1:G:438:TRP:CZ3	2.92	0.57
1:J:138:TRP:CE2	1:J:438:TRP:CZ3	2.92	0.57
1:P:438:TRP:CH2	1:P:443:PRO:HG3	2.39	0.57
1:S:193:ARG:NH1	1:S:232:THR:OG1	2.38	0.57
1:S:138:TRP:CE2	1:S:438:TRP:CH2	2.93	0.57
2:T:170:LEU:CD1	2:T:223:VAL:HG21	2.34	0.57
3:F:46:GLU:O	3:F:47:ASN:HB2	2.05	0.57
2:W:130:ALA:O	2:W:146:ARG:HG2	2.05	0.57
2:W:252:ASP:CB	2:W:255:THR:HG22	2.30	0.57
2:K:374:GLU:O	2:K:377:LYS:HB3	2.05	0.57
2:E:118:LYS:NZ	1:G:291:SER:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:17:MET:HE2	2:K:60:TYR:CB	2.33	0.57
1:G:329:TYR:CE2	3:I:89:PRO:HG3	2.40	0.57
1:J:72:LYS:HA	1:J:115:THR:HG22	1.87	0.57
1:A:292:LEU:O	1:A:295:VAL:HG22	2.04	0.57
2:N:394:LYS:HE2	1:P:141:GLU:OE2	2.05	0.56
1:J:292:LEU:HB2	1:J:295:VAL:HG22	1.86	0.56
2:Q:137:GLY:O	3:R:90:ARG:NH1	2.36	0.56
2:B:98:GLU:HG3	2:B:98:GLU:O	2.05	0.56
1:V:138:TRP:CZ2	1:V:438:TRP:CH2	2.93	0.56
2:W:156:THR:CG2	2:W:157:GLU:O	2.53	0.56
1:D:204:ASP:O	1:D:205:GLN:HG2	2.06	0.56
2:E:17:MET:HE3	2:E:60:TYR:HB2	1.85	0.56
1:D:77:VAL:HG23	1:D:114:LYS:HZ2	1.71	0.56
1:S:143:VAL:CG1	1:S:145:GLY:H	2.19	0.56
1:J:397:THR:HG22	1:J:399:THR:H	1.70	0.56
1:S:138:TRP:CZ2	1:S:438:TRP:CH2	2.94	0.56
2:B:201:ARG:HD2	2:B:207:GLU:O	2.05	0.56
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.69	0.56
1:V:190:ARG:HD3	1:V:241:TRP:HH2	1.69	0.56
1:M:299:ILE:HG13	1:M:419:ILE:HG22	1.88	0.56
2:Q:252:ASP:HB3	2:Q:255:THR:HG23	1.87	0.56
1:G:376:ARG:HG3	1:G:376:ARG:HH11	1.71	0.56
2:Q:95:SER:CB	2:Q:127:GLU:HB3	2.35	0.56
1:P:172:ILE:HD13	1:P:207:GLY:HA3	1.88	0.56
2:K:128:GLU:HB2	2:K:148:GLY:HA2	1.88	0.56
2:Q:340:PRO:O	2:Q:344:VAL:HG22	2.04	0.56
1:M:245:VAL:HG12	1:M:459:LEU:HB3	1.87	0.56
2:T:128:GLU:HB2	2:T:148:GLY:HA2	1.86	0.56
1:P:163:SER:HB3	1:P:209:PHE:HB2	1.87	0.56
1:V:138:TRP:CE2	1:V:438:TRP:CZ3	2.93	0.56
1:P:438:TRP:CZ3	1:P:443:PRO:HG3	2.40	0.56
1:D:104:LEU:HD11	1:D:164:LEU:HD21	1.86	0.56
1:G:138:TRP:CD2	1:G:438:TRP:HZ3	2.23	0.56
1:M:245:VAL:CG1	1:M:459:LEU:HB3	2.36	0.56
1:V:299:ILE:HG13	1:V:419:ILE:HG22	1.87	0.56
1:V:162:VAL:HG21	1:V:219:VAL:HG21	1.88	0.56
2:B:17:MET:HE3	2:B:60:TYR:HB2	1.87	0.56
1:D:77:VAL:CG2	1:D:114:LYS:NZ	2.67	0.56
1:V:138:TRP:CD2	1:V:438:TRP:HZ3	2.24	0.56
1:S:351:ARG:NH1	7:S:907:ASN:O	2.26	0.56
1:P:178:PHE:HE1	1:P:397:THR:HG21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:MET:HE1	2:H:126:ILE:HG21	1.88	0.56
1:M:182:ILE:HG12	1:M:434:ILE:HD12	1.87	0.56
2:T:156:THR:CG2	2:T:157:GLU:O	2.51	0.55
2:E:109:LEU:HD11	2:E:169:PHE:HA	1.88	0.55
1:S:292:LEU:O	1:S:295:VAL:HG22	2.06	0.55
1:D:376:ARG:HD2	3:F:49:GLU:O	2.06	0.55
2:T:17:MET:HE1	2:T:60:TYR:HB2	1.89	0.55
2:E:220:PHE:O	2:E:223:VAL:HG22	2.07	0.55
2:T:109:LEU:HD11	2:T:169:PHE:HA	1.88	0.55
2:Q:21:THR:HB	3:R:63:ASP:OD1	2.07	0.55
1:V:26:GLU:HG3	1:V:51:LEU:HD11	1.89	0.55
1:V:138:TRP:CE2	1:V:438:TRP:HH2	2.25	0.55
3:U:23:ILE:O	3:U:27:GLN:HG3	2.07	0.55
2:W:73:HIS:NE2	2:W:103:THR:HB	2.21	0.55
2:N:201:ARG:HD2	2:N:207:GLU:O	2.07	0.55
2:T:140:THR:OG1	3:U:90:ARG:HA	2.05	0.55
2:Q:21:THR:HG21	3:R:61:ARG:NH1	2.21	0.55
1:P:138:TRP:CE2	1:P:438:TRP:CZ3	2.95	0.55
1:D:291:SER:HB3	2:H:118:LYS:HZ2	1.72	0.55
2:K:21:THR:HG21	3:L:61:ARG:NH1	2.17	0.55
1:A:299:ILE:HG13	1:A:419:ILE:HG22	1.89	0.55
2:H:156:THR:HG22	2:H:157:GLU:N	2.21	0.55
2:E:21:THR:HG22	2:E:22:LYS:O	2.07	0.55
1:P:352:ILE:O	1:P:356:THR:CG2	2.50	0.55
1:P:143:VAL:HG13	1:P:145:GLY:H	1.70	0.55
1:D:81:LYS:HE2	1:D:91:ASN:HA	1.89	0.55
1:G:138:TRP:CZ2	1:G:438:TRP:CH2	2.95	0.55
3:X:33:ILE:O	3:X:37:ILE:HG12	2.07	0.55
1:D:57:LEU:HD22	1:D:65:PHE:CE1	2.42	0.55
1:S:1:MET:O	1:S:1:MET:HG2	2.06	0.55
2:W:252:ASP:OD2	2:W:255:THR:HG22	2.07	0.54
1:G:138:TRP:CE2	1:G:438:TRP:CH2	2.95	0.54
2:K:255:THR:HG21	2:K:259:TYR:OH	2.07	0.54
2:Q:230:GLU:OE2	2:Q:233:ARG:NH1	2.40	0.54
1:V:172:ILE:C	1:V:175:PRO:HD2	2.28	0.54
2:W:162:THR:HG22	2:W:164:GLU:H	1.72	0.54
1:G:356:THR:HG21	3:I:14:ALA:HB2	1.88	0.54
1:M:138:TRP:CE2	1:M:438:TRP:CZ3	2.96	0.54
2:E:40:CYS:O	2:E:44:LEU:HB2	2.07	0.54
1:A:174:GLN:CB	1:A:175:PRO:HD3	2.37	0.54
1:V:143:VAL:HG13	1:V:145:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:162:THR:HG22	2:E:164:GLU:H	1.72	0.54
2:H:255:THR:HG21	2:H:259:TYR:OH	2.07	0.54
2:W:8:VAL:HG12	2:W:158:PRO:HB2	1.89	0.54
2:T:162:THR:HG22	2:T:164:GLU:H	1.73	0.54
2:B:310:TYR:CE1	2:B:334:VAL:HG11	2.43	0.54
1:A:115:THR:HG21	1:A:151:SER:OG	2.06	0.54
3:C:39:GLN:O	3:C:42:GLU:HG3	2.08	0.54
2:E:139:LYS:HG2	3:F:87:VAL:CG1	2.38	0.54
1:J:138:TRP:CD2	1:J:438:TRP:HZ3	2.25	0.54
1:V:185:LYS:NZ	1:V:186:PRO:O	2.39	0.54
1:G:126:THR:HG22	1:G:126:THR:O	2.07	0.54
1:A:25:VAL:HG11	1:A:51:LEU:HD12	1.89	0.54
1:P:3:TRP:CZ3	1:P:31:ARG:HD2	2.43	0.54
2:N:80:ARG:HE	2:N:275:ASP:CG	2.10	0.54
2:N:17:MET:HE2	2:N:60:TYR:HB3	1.88	0.54
2:K:39:VAL:HG13	2:K:44:LEU:HD11	1.88	0.54
2:E:96:GLN:HB2	2:E:125:HIS:HB2	1.90	0.54
1:D:104:LEU:HD11	1:D:164:LEU:CD2	2.38	0.54
2:E:128:GLU:HB2	2:E:148:GLY:HA2	1.90	0.54
2:Q:220:PHE:O	2:Q:223:VAL:HG22	2.07	0.54
2:Q:374:GLU:OE1	2:Q:402:THR:HG22	2.08	0.54
1:S:322:TYR:CZ	2:T:47:PRO:HD3	2.43	0.54
1:V:60:ARG:HA	1:V:65:PHE:CD1	2.43	0.54
1:G:100:VAL:HG12	1:G:223:ILE:HB	1.90	0.54
1:A:142:ARG:NH2	1:A:403:LYS:HE3	2.23	0.54
1:A:185:LYS:NZ	1:A:429:LEU:O	2.42	0.53
2:Q:85:TYR:HD2	2:Q:87:ASP:OD1	1.91	0.53
2:W:128:GLU:HB2	2:W:148:GLY:HA2	1.91	0.53
1:P:81:LYS:HE2	1:P:91:ASN:HA	1.89	0.53
2:E:113:ASN:ND2	2:E:115:GLU:HG2	2.23	0.53
2:B:40:CYS:SG	2:B:41:PRO:HD2	2.48	0.53
1:P:174:GLN:HG3	1:P:175:PRO:CD	2.38	0.53
1:D:245:VAL:CG1	1:D:459:LEU:HB3	2.39	0.53
2:T:95:SER:HB3	2:T:127:GLU:OE1	2.09	0.53
2:Q:21:THR:HG23	3:R:61:ARG:HH12	1.72	0.53
1:V:163:SER:HB3	1:V:209:PHE:HB2	1.91	0.53
2:T:146:ARG:HH11	2:T:146:ARG:HG2	1.73	0.53
2:B:360:ILE:HD11	2:B:365:SER:HA	1.90	0.53
1:P:16:ARG:HB2	1:P:18:GLU:OE2	2.08	0.53
1:A:138:TRP:NE1	1:A:438:TRP:HH2	2.06	0.53
1:P:90:GLU:O	1:P:91:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:8:SER:HA	1:S:11:ARG:HH21	1.73	0.53
1:S:69:ILE:HD11	1:S:164:LEU:HD13	1.90	0.53
1:S:69:ILE:HD12	1:S:162:VAL:HG13	1.91	0.53
2:T:8:VAL:HG12	2:T:158:PRO:HB2	1.90	0.53
2:K:252:ASP:HB3	2:K:255:THR:CG2	2.38	0.53
2:W:337:PHE:CE2	2:W:377:LYS:HA	2.44	0.53
1:A:60:ARG:HA	1:A:65:PHE:CD1	2.44	0.53
1:S:64:LEU:HD21	1:S:218:LEU:HG	1.90	0.53
2:W:348:ILE:HA	2:W:352:LEU:HD22	1.90	0.53
1:M:90:GLU:O	1:M:91:ASN:CB	2.57	0.53
1:G:418:ASP:HB3	1:G:422:VAL:HG13	1.91	0.53
1:G:418:ASP:O	1:G:422:VAL:HG13	2.09	0.53
2:T:17:MET:HE3	2:T:60:TYR:HB2	1.90	0.53
2:K:85:TYR:OH	3:L:91:VAL:CG1	2.57	0.53
2:K:17:MET:HE1	2:K:60:TYR:CB	2.37	0.53
1:P:178:PHE:CE1	1:P:397:THR:HG21	2.43	0.53
2:W:162:THR:HG22	2:W:164:GLU:N	2.24	0.53
2:N:396:MET:HE1	2:N:403:PRO:HB3	1.91	0.53
1:S:201:SER:HB2	2:T:276:PRO:HG2	1.90	0.53
1:A:118:ASP:OD1	1:A:126:THR:HA	2.09	0.53
1:D:322:TYR:CZ	2:E:47:PRO:HD3	2.43	0.52
2:Q:128:GLU:HB2	2:Q:148:GLY:HA2	1.90	0.52
2:E:77:VAL:HG23	2:E:99:LYS:HD2	1.91	0.52
2:B:184:LYS:HB2	2:B:191:GLN:OE1	2.09	0.52
2:E:252:ASP:CB	2:E:255:THR:HG22	2.35	0.52
2:W:220:PHE:O	2:W:223:VAL:HG22	2.09	0.52
1:M:338:ARG:HG3	3:O:17:GLU:OE1	2.09	0.52
2:T:96:GLN:HB2	2:T:125:HIS:HB2	1.90	0.52
2:N:167:ARG:HG3	2:N:220:PHE:HB3	1.92	0.52
2:H:85:TYR:HD2	2:H:87:ASP:OD1	1.92	0.52
2:B:170:LEU:HD12	2:B:223:VAL:HG21	1.91	0.52
2:W:396:MET:HG3	2:W:406:ILE:HD11	1.92	0.52
2:N:74:GLU:HG2	2:N:283:VAL:O	2.08	0.52
1:V:339:THR:HG23	1:V:340:ARG:N	2.24	0.52
1:S:138:TRP:CE2	1:S:438:TRP:CZ3	2.97	0.52
3:X:21:GLU:O	3:X:25:VAL:HG23	2.10	0.52
2:K:73:HIS:NE2	2:K:103:THR:HB	2.25	0.52
1:D:90:GLU:O	1:D:91:ASN:HB2	2.10	0.52
2:Q:170:LEU:CD1	2:Q:223:VAL:HG21	2.38	0.52
1:A:46:LEU:HG	1:A:113:GLY:HA2	1.90	0.52
2:E:85:TYR:HD2	2:E:87:ASP:OD1	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:17:MET:HE3	2:E:60:TYR:CB	2.39	0.52
2:W:96:GLN:HB2	2:W:125:HIS:HB2	1.92	0.52
2:K:372:LEU:O	2:K:376:VAL:HG23	2.10	0.52
3:L:28:LYS:NZ	3:L:32:ASP:OD2	2.43	0.52
1:S:463:TYR:O	1:S:467:GLN:HG2	2.09	0.52
2:H:146:ARG:HG2	2:H:146:ARG:HH11	1.75	0.52
2:B:252:ASP:OD2	2:B:255:THR:HG22	2.09	0.52
2:H:123:ARG:NH1	2:H:125:HIS:CE1	2.77	0.52
2:Q:140:THR:OG1	3:R:90:ARG:HA	2.10	0.52
2:B:310:TYR:HE1	2:B:334:VAL:HG11	1.74	0.52
2:B:396:MET:HG3	2:B:406:ILE:HD11	1.90	0.52
2:E:222:PHE:CZ	2:E:253:PRO:HB3	2.45	0.52
1:J:292:LEU:CB	1:J:295:VAL:HG22	2.40	0.52
1:V:181:VAL:HG13	1:V:210:GLY:O	2.09	0.52
1:A:167:ASP:HB2	1:A:172:ILE:HD12	1.92	0.52
2:H:14:HIS:CD2	2:H:127:GLU:OE2	2.63	0.52
1:J:178:PHE:CE1	1:J:397:THR:HG21	2.45	0.52
2:Q:95:SER:HB3	2:Q:127:GLU:HB3	1.91	0.52
1:V:292:LEU:HB2	1:V:295:VAL:CG2	2.40	0.52
1:A:98:ALA:HA	1:A:195:GLY:HA3	1.92	0.52
2:B:211:ARG:HD3	4:B:701:ADP:C5	2.45	0.52
2:T:252:ASP:OD2	2:T:255:THR:HG22	2.10	0.52
1:V:292:LEU:O	1:V:295:VAL:HG22	2.10	0.52
1:M:422:VAL:N	1:M:423:PRO:CD	2.73	0.52
1:D:299:ILE:HG13	1:D:419:ILE:HG22	1.90	0.52
2:E:95:SER:CB	2:E:127:GLU:HB3	2.39	0.52
2:Q:17:MET:CE	2:Q:60:TYR:HB3	2.38	0.51
2:K:85:TYR:HD2	2:K:87:ASP:OD1	1.93	0.51
1:J:438:TRP:CZ3	1:J:443:PRO:HG3	2.46	0.51
2:T:170:LEU:HD12	2:T:223:VAL:HG21	1.90	0.51
2:K:252:ASP:HB3	2:K:255:THR:HG22	1.91	0.51
2:E:146:ARG:HH11	2:E:146:ARG:HG2	1.74	0.51
1:V:203:LEU:HD23	1:V:375:ARG:NH2	2.25	0.51
1:J:90:GLU:O	1:J:91:ASN:CB	2.58	0.51
2:T:360:ILE:HD11	2:T:365:SER:HA	1.91	0.51
2:E:396:MET:HG3	2:E:406:ILE:HD11	1.92	0.51
2:B:128:GLU:HB2	2:B:148:GLY:HA2	1.92	0.51
2:Q:74:GLU:HG2	2:Q:283:VAL:O	2.09	0.51
2:Q:201:ARG:HG3	2:Q:205:SER:OG	2.10	0.51
2:H:80:ARG:HE	2:H:275:ASP:CG	2.13	0.51
1:D:422:VAL:N	1:D:423:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HG2	2:B:46:MET:CE	2.38	0.51
1:D:71:VAL:HG11	1:D:101:ILE:HD11	1.93	0.51
2:N:128:GLU:HB2	2:N:148:GLY:HA2	1.93	0.51
2:H:39:VAL:HG13	2:H:44:LEU:HD11	1.93	0.51
1:V:190:ARG:HD3	1:V:241:TRP:CH2	2.46	0.51
2:B:98:GLU:O	2:B:99:LYS:HB2	2.11	0.51
2:B:252:ASP:HB3	2:B:255:THR:CG2	2.38	0.51
1:A:155:VAL:HG21	1:A:163:SER:HB3	1.93	0.51
1:J:47:TYR:CD2	1:J:112:VAL:HG22	2.45	0.51
1:D:306:ALA:HB3	1:D:307:PRO:HD3	1.93	0.51
1:S:100:VAL:HG12	1:S:223:ILE:HB	1.93	0.51
2:N:282:LYS:HD3	3:O:55:PHE:CZ	2.46	0.51
1:J:374:VAL:O	1:J:378:ILE:HG13	2.11	0.51
2:N:302:ARG:HD3	2:N:321:VAL:HG22	1.93	0.51
1:V:292:LEU:CB	1:V:295:VAL:HG22	2.41	0.51
3:F:7:VAL:HG21	3:F:27:GLN:HG2	1.93	0.51
2:E:170:LEU:CD1	2:E:223:VAL:HG21	2.40	0.51
2:B:142:VAL:HB	3:C:86:PHE:HB2	1.92	0.51
2:W:263:THR:HB	2:W:265:GLU:HG3	1.92	0.51
2:E:21:THR:CG2	2:E:22:LYS:N	2.74	0.50
1:D:138:TRP:CD2	1:D:438:TRP:CZ3	2.99	0.50
1:V:279:GLU:HG3	1:V:468:LYS:HZ3	1.75	0.50
2:E:340:PRO:O	2:E:344:VAL:HG22	2.11	0.50
2:K:162:THR:HG22	2:K:165:GLU:H	1.77	0.50
2:T:106:TRP:CD1	2:T:118:LYS:HE2	2.46	0.50
2:T:100:PRO:HB3	2:T:123:ARG:NH1	2.26	0.50
1:V:71:VAL:CG1	1:V:114:LYS:HZ3	2.24	0.50
2:E:156:THR:HG22	2:E:157:GLU:N	2.26	0.50
2:T:22:LYS:HD2	2:T:27:CYS:HB2	1.92	0.50
1:G:72:LYS:HD3	1:G:74:ASN:OD1	2.12	0.50
1:S:104:LEU:HD11	1:S:164:LEU:HD21	1.93	0.50
1:D:265:LEU:HD11	1:D:395:PRO:HG2	1.93	0.50
1:G:422:VAL:N	1:G:423:PRO:HD3	2.25	0.50
1:M:86:SER:HB2	1:M:119:GLU:HG3	1.93	0.50
1:S:90:GLU:O	1:S:91:ASN:HB2	2.12	0.50
1:M:138:TRP:CD2	1:M:438:TRP:CZ3	2.98	0.50
1:A:151:SER:HB3	1:A:163:SER:OG	2.11	0.50
1:A:403:LYS:O	1:A:406:GLU:HB2	2.12	0.50
1:V:384:LYS:O	1:V:387:GLU:HB2	2.12	0.50
1:V:360:SER:HA	2:W:269:ASP:OD2	2.12	0.50
1:D:123:GLY:N	7:D:902:ASN:OXT	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:438:TRP:CH2	1:J:443:PRO:HG3	2.46	0.50
1:G:178:PHE:HE1	1:G:397:THR:HG21	1.76	0.50
2:K:40:CYS:HB2	2:K:41:PRO:HD2	1.93	0.50
1:P:167:ASP:HA	1:P:171:SER:HB2	1.94	0.50
1:S:298:SER:HB3	1:S:422:VAL:HG23	1.94	0.50
1:M:329:TYR:CE2	3:O:89:PRO:HG3	2.46	0.50
2:T:77:VAL:HG23	2:T:99:LYS:HD2	1.94	0.50
1:S:190:ARG:NH1	1:S:190:ARG:HG3	2.27	0.50
1:V:279:GLU:HG3	1:V:468:LYS:HZ1	1.76	0.50
2:E:119:VAL:HG12	2:E:156:THR:HG23	1.93	0.50
2:T:167:ARG:HG3	2:T:220:PHE:HB3	1.92	0.50
2:N:96:GLN:HB2	2:N:125:HIS:HB2	1.94	0.49
1:J:162:VAL:HG11	1:J:219:VAL:HG21	1.94	0.49
2:B:59:GLU:OE2	2:B:63:ARG:NH2	2.44	0.49
1:A:118:ASP:OD1	1:A:126:THR:CA	2.60	0.49
2:T:77:VAL:CG2	2:T:99:LYS:HD2	2.42	0.49
1:S:245:VAL:CG1	1:S:459:LEU:HB3	2.42	0.49
2:Q:73:HIS:NE2	2:Q:103:THR:HB	2.27	0.49
2:T:39:VAL:HG13	2:T:44:LEU:HD11	1.93	0.49
1:J:167:ASP:HA	1:J:171:SER:HB2	1.94	0.49
2:E:118:LYS:HZ3	1:G:291:SER:HB3	1.76	0.49
1:D:291:SER:HB3	2:H:118:LYS:NZ	2.27	0.49
2:N:197:ASN:HB3	2:N:211:ARG:HD2	1.95	0.49
1:D:463:TYR:O	1:D:467:GLN:HG2	2.12	0.49
2:H:128:GLU:HB2	2:H:148:GLY:HA2	1.93	0.49
2:K:340:PRO:O	2:K:344:VAL:HG22	2.12	0.49
2:E:280:PRO:HD2	3:F:55:PHE:CZ	2.47	0.49
1:D:279:GLU:HG3	1:D:468:LYS:NZ	2.27	0.49
1:G:376:ARG:HG3	1:G:376:ARG:NH1	2.26	0.49
1:G:373:LYS:HE2	3:I:50:PRO:HD3	1.93	0.49
2:E:21:THR:HG22	2:E:22:LYS:N	2.27	0.49
2:E:22:LYS:HD2	2:E:27:CYS:HB2	1.95	0.49
1:S:81:LYS:HE2	1:S:91:ASN:CA	2.38	0.49
2:K:85:TYR:CZ	3:L:91:VAL:HG11	2.48	0.49
1:J:172:ILE:HD13	1:J:207:GLY:HA3	1.95	0.49
3:X:46:GLU:O	3:X:47:ASN:HB2	2.13	0.49
1:V:116:ASN:ND2	1:V:132:PHE:O	2.45	0.49
1:V:318:ASP:HB2	1:V:336:TYR:HE1	1.78	0.49
1:A:138:TRP:CZ2	1:A:438:TRP:CH2	3.01	0.49
2:T:95:SER:CB	2:T:127:GLU:HB3	2.42	0.49
1:A:7:LEU:HD22	1:A:67:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:197:ASN:HB3	2:H:211:ARG:HD2	1.95	0.49
1:S:464:LEU:HD12	1:S:464:LEU:O	2.13	0.49
1:A:190:ARG:HD2	1:A:455:GLU:OE2	2.13	0.49
2:Q:360:ILE:CD1	2:Q:366:PRO:HD3	2.43	0.49
2:B:280:PRO:HD2	3:C:55:PHE:CZ	2.48	0.49
2:N:156:THR:HG22	2:N:157:GLU:N	2.27	0.49
1:M:298:SER:HB3	1:M:422:VAL:HG23	1.94	0.49
1:S:395:PRO:O	1:S:420:LEU:HD13	2.12	0.49
1:P:384:LYS:O	1:P:387:GLU:HB2	2.13	0.49
1:M:201:SER:HB2	2:N:276:PRO:HG2	1.95	0.49
1:V:432:ILE:HG12	1:V:434:ILE:HD13	1.93	0.49
2:E:140:THR:OG1	3:F:90:ARG:HA	2.13	0.49
1:J:329:TYR:CE2	3:L:89:PRO:HG3	2.47	0.49
1:M:88:ILE:HD11	1:M:120:PHE:HZ	1.75	0.49
2:W:56:ARG:HD2	3:X:63:ASP:OD2	2.13	0.49
1:J:156:ALA:O	1:J:211:ARG:NH1	2.46	0.49
2:H:340:PRO:O	2:H:344:VAL:HG22	2.12	0.49
2:K:21:THR:HB	3:L:63:ASP:OD1	2.12	0.48
2:B:220:PHE:O	2:B:223:VAL:HG22	2.13	0.48
2:H:17:MET:CE	2:H:60:TYR:HB2	2.38	0.48
1:P:138:TRP:CD2	1:P:438:TRP:HZ3	2.31	0.48
1:D:143:VAL:HG13	1:D:145:GLY:H	1.79	0.48
2:E:402:THR:HG22	2:E:403:PRO:HD2	1.95	0.48
1:A:397:THR:HG22	1:A:398:PRO:HD2	1.95	0.48
1:V:162:VAL:HG22	1:V:163:SER:H	1.77	0.48
2:Q:170:LEU:HD12	2:Q:223:VAL:HG21	1.94	0.48
2:N:22:LYS:HD2	2:N:27:CYS:HB2	1.94	0.48
2:H:170:LEU:HD12	2:H:223:VAL:HG21	1.95	0.48
1:P:167:ASP:HB3	1:P:185:LYS:HG3	1.94	0.48
2:T:8:VAL:HG13	2:T:161:ARG:HH12	1.79	0.48
1:A:172:ILE:HD13	1:A:207:GLY:HA3	1.95	0.48
2:N:83:TYR:CZ	2:N:88:LEU:HD22	2.48	0.48
2:T:348:ILE:HA	2:T:352:LEU:HD22	1.96	0.48
1:S:172:ILE:HD13	1:S:207:GLY:HA3	1.95	0.48
2:H:167:ARG:HG3	2:H:220:PHE:HB3	1.93	0.48
1:M:279:GLU:HG3	1:M:468:LYS:HZ1	1.76	0.48
2:N:282:LYS:HD3	3:O:55:PHE:CE2	2.49	0.48
2:Q:39:VAL:HG13	2:Q:44:LEU:HD11	1.94	0.48
1:D:403:LYS:O	1:D:406:GLU:HB2	2.14	0.48
1:A:321:ARG:HD2	2:B:44:LEU:O	2.14	0.48
2:H:96:GLN:HB2	2:H:125:HIS:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:138:TRP:CE2	1:P:438:TRP:HH2	2.32	0.48
2:Q:372:LEU:O	2:Q:376:VAL:HG23	2.13	0.48
1:A:5:LYS:HB2	1:A:10:LEU:HD13	1.94	0.48
1:V:88:ILE:HA	1:V:324:TYR:HB3	1.95	0.48
2:W:142:VAL:HB	3:X:86:PHE:HB2	1.95	0.48
1:D:157:VAL:HG23	1:D:159:SER:H	1.77	0.48
1:M:376:ARG:HG3	1:M:376:ARG:NH1	2.24	0.48
2:K:167:ARG:HG3	2:K:220:PHE:HB3	1.96	0.48
1:S:2:LEU:HB3	1:S:27:SER:OG	2.13	0.48
1:V:98:ALA:HA	1:V:195:GLY:HA3	1.95	0.48
2:N:8:VAL:HG12	2:N:158:PRO:HB2	1.94	0.48
1:D:163:SER:HB3	1:D:209:PHE:HB2	1.95	0.48
1:D:199:PHE:C	1:D:199:PHE:CD1	2.87	0.48
2:T:370:GLU:CD	2:T:370:GLU:H	2.17	0.48
1:P:28:PHE:CD2	1:P:68:PRO:HG2	2.49	0.48
2:Q:360:ILE:HD11	2:Q:366:PRO:HD3	1.95	0.48
2:B:100:PRO:CB	2:B:123:ARG:HH21	2.18	0.47
2:B:39:VAL:HG13	2:B:40:CYS:H	1.76	0.47
1:S:245:VAL:HG12	1:S:459:LEU:HB3	1.95	0.47
2:H:230:GLU:OE2	2:H:233:ARG:NH1	2.47	0.47
1:M:297:TYR:CE2	3:O:43:LEU:HD21	2.48	0.47
2:B:17:MET:HE3	2:B:60:TYR:CB	2.44	0.47
1:S:190:ARG:HD2	1:S:455:GLU:OE2	2.13	0.47
2:Q:355:LEU:HD21	2:Q:365:SER:HB2	1.96	0.47
2:N:85:TYR:HD2	2:N:87:ASP:OD1	1.97	0.47
2:H:8:VAL:CG1	2:H:158:PRO:HB2	2.44	0.47
2:W:233:ARG:HD2	2:W:249:ARG:NH2	2.29	0.47
3:O:36:PHE:O	3:O:39:GLN:NE2	2.43	0.47
2:N:170:LEU:HB3	2:N:220:PHE:CE1	2.48	0.47
2:T:220:PHE:O	2:T:223:VAL:HG22	2.15	0.47
2:Q:374:GLU:O	2:Q:377:LYS:HB3	2.14	0.47
1:D:398:PRO:HG3	1:D:419:ILE:HD11	1.97	0.47
1:G:163:SER:HB3	1:G:209:PHE:HB2	1.96	0.47
2:N:41:PRO:HB3	2:N:46:MET:HE2	1.96	0.47
2:K:40:CYS:HB2	2:K:41:PRO:CD	2.44	0.47
2:W:331:GLU:O	2:W:334:VAL:HG12	2.13	0.47
1:G:418:ASP:HB3	1:G:422:VAL:CG1	2.44	0.47
1:V:138:TRP:CD2	1:V:438:TRP:CZ3	3.02	0.47
1:P:138:TRP:NE1	1:P:438:TRP:HH2	2.12	0.47
2:B:8:VAL:HG11	2:B:208:PHE:HE1	1.80	0.47
1:S:138:TRP:CD2	1:S:438:TRP:HZ3	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:ASP:HB2	1:G:172:ILE:HD12	1.95	0.47
1:A:76:LEU:HD22	1:A:96:TYR:CE1	2.49	0.47
2:T:331:GLU:HA	2:T:334:VAL:HG12	1.96	0.47
2:W:201:ARG:HD2	2:W:207:GLU:O	2.15	0.47
1:A:88:ILE:HA	1:A:324:TYR:HB3	1.96	0.47
1:G:344:PHE:O	1:G:349:LYS:HE2	2.15	0.47
2:H:119:VAL:CG1	2:H:156:THR:HG21	2.45	0.47
1:A:162:VAL:HG21	1:A:219:VAL:HG21	1.96	0.47
1:A:201:SER:HB2	2:B:276:PRO:HG2	1.96	0.47
1:G:438:TRP:CD1	1:G:438:TRP:N	2.83	0.47
1:A:157:VAL:HG23	1:A:159:SER:H	1.80	0.47
2:W:330:PHE:CE1	2:W:344:VAL:HG13	2.50	0.47
1:J:245:VAL:HG12	1:J:459:LEU:HB3	1.97	0.47
2:N:355:LEU:HD22	2:N:360:ILE:HG12	1.97	0.46
2:N:36:ASN:ND2	3:O:84:GLY:O	2.37	0.46
2:N:17:MET:CE	2:N:60:TYR:HB2	2.41	0.46
1:J:138:TRP:CE2	1:J:438:TRP:HH2	2.31	0.46
2:N:348:ILE:HA	2:N:352:LEU:HD22	1.97	0.46
1:D:100:VAL:HG12	1:D:223:ILE:HB	1.96	0.46
2:K:310:TYR:CE1	2:K:334:VAL:HG11	2.50	0.46
1:D:464:LEU:O	1:D:464:LEU:HD12	2.14	0.46
2:H:282:LYS:HD3	3:I:55:PHE:CE2	2.50	0.46
1:V:42:TYR:CE2	1:V:113:GLY:HA3	2.51	0.46
1:V:438:TRP:CH2	1:V:443:PRO:HG3	2.50	0.46
1:M:155:VAL:HG21	1:M:163:SER:HB2	1.96	0.46
1:A:189:GLY:H	1:A:205:GLN:NE2	2.13	0.46
1:V:316:ARG:O	1:V:321:ARG:NH2	2.48	0.46
1:A:77:VAL:HG21	1:A:114:LYS:HD3	1.97	0.46
2:H:17:MET:HE2	2:H:60:TYR:CB	2.37	0.46
1:A:174:GLN:HB3	1:A:175:PRO:HD3	1.97	0.46
1:P:83:THR:HG22	1:P:90:GLU:HA	1.97	0.46
2:K:331:GLU:HA	2:K:334:VAL:HG12	1.98	0.46
2:Q:41:PRO:HB3	2:Q:46:MET:HE2	1.97	0.46
1:S:174:GLN:HB3	1:S:175:PRO:HD3	1.97	0.46
3:I:46:GLU:O	3:I:47:ASN:HB2	2.15	0.46
2:Q:54:ASN:HB2	3:R:61:ARG:NH2	2.31	0.46
1:J:292:LEU:O	1:J:295:VAL:HG22	2.16	0.46
1:S:218:LEU:O	1:S:222:VAL:HG23	2.16	0.46
1:S:27:SER:O	1:S:30:ASP:HB2	2.16	0.46
1:S:6:SER:HB3	1:S:212:ARG:CZ	2.45	0.46
1:A:199:PHE:CD1	1:A:199:PHE:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:438:TRP:CZ3	1:S:443:PRO:HG3	2.51	0.46
1:G:68:PRO:HB3	1:G:112:VAL:HG11	1.98	0.46
1:G:86:SER:HB2	1:G:119:GLU:HG3	1.98	0.46
1:A:47:TYR:CE2	1:A:112:VAL:HG12	2.47	0.46
1:J:376:ARG:CG	1:J:376:ARG:HH11	2.13	0.46
1:S:81:LYS:CE	1:S:91:ASN:HA	2.40	0.46
1:D:44:THR:HB	1:D:114:LYS:HB2	1.98	0.46
2:W:21:THR:HG21	3:X:61:ARG:NH1	2.24	0.46
1:D:182:ILE:HG12	1:D:434:ILE:CD1	2.42	0.46
1:G:83:THR:HG22	1:G:90:GLU:HA	1.98	0.46
2:N:217:VAL:HG11	2:N:223:VAL:HA	1.98	0.46
2:E:8:VAL:HG12	2:E:158:PRO:HB2	1.98	0.46
1:P:318:ASP:HB2	1:P:336:TYR:CE1	2.50	0.46
2:B:100:PRO:HB3	2:B:123:ARG:NH2	2.15	0.46
2:E:73:HIS:NE2	2:E:103:THR:HB	2.31	0.46
1:A:155:VAL:CG2	1:A:163:SER:HB3	2.46	0.46
1:G:172:ILE:HD13	1:G:207:GLY:HA3	1.97	0.46
1:J:316:ARG:O	1:J:321:ARG:NH2	2.46	0.46
1:V:265:LEU:HD23	1:V:398:PRO:HA	1.98	0.46
2:H:21:THR:HG21	3:I:61:ARG:NH1	2.10	0.46
1:G:297:TYR:CE2	3:I:43:LEU:HD21	2.51	0.46
2:B:331:GLU:O	2:B:334:VAL:HG12	2.16	0.46
2:T:132:LYS:HE2	2:T:146:ARG:HH21	1.81	0.46
1:J:338:ARG:CG	3:L:17:GLU:OE1	2.63	0.46
1:S:318:ASP:HB2	1:S:336:TYR:CE1	2.50	0.46
2:N:117:LYS:HG2	2:N:118:LYS:N	2.30	0.46
2:N:398:GLU:HA	2:N:398:GLU:OE1	2.15	0.46
1:G:199:PHE:C	1:G:199:PHE:CD1	2.88	0.46
2:H:21:THR:HG22	2:H:54:ASN:ND2	2.31	0.45
1:P:306:ALA:HB3	1:P:307:PRO:CD	2.42	0.45
1:J:138:TRP:CZ2	1:J:438:TRP:CH2	3.04	0.45
2:W:141:LEU:HD12	3:X:87:VAL:HG22	1.98	0.45
1:M:72:LYS:HA	1:M:115:THR:HG22	1.99	0.45
1:D:143:VAL:HG12	1:D:145:GLY:H	1.80	0.45
2:E:106:TRP:CE3	1:G:293:PRO:HG3	2.51	0.45
2:W:310:TYR:CE1	2:W:334:VAL:HG11	2.51	0.45
2:K:379:ILE:HD13	2:K:384:ILE:HG13	1.99	0.45
1:G:377:LEU:HD23	1:G:377:LEU:HA	1.81	0.45
1:P:95:PRO:HG2	2:Q:46:MET:HE1	1.97	0.45
2:H:119:VAL:CG1	2:H:156:THR:CG2	2.95	0.45
1:V:9:GLU:O	1:V:13:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:57:LEU:HD22	1:S:65:PHE:CE1	2.51	0.45
1:P:25:VAL:HG12	1:P:51:LEU:HD12	1.97	0.45
1:V:318:ASP:HB2	1:V:336:TYR:CE1	2.52	0.45
1:V:422:VAL:N	1:V:423:PRO:CD	2.80	0.45
2:K:162:THR:HG22	2:K:164:GLU:N	2.31	0.45
2:H:8:VAL:HG12	2:H:158:PRO:HB2	1.98	0.45
1:J:422:VAL:N	1:J:423:PRO:CD	2.80	0.45
1:V:241:TRP:O	1:V:245:VAL:HG22	2.17	0.45
2:H:103:THR:HG23	2:H:104:ASN:OD1	2.13	0.45
2:H:170:LEU:HB3	2:H:220:PHE:CE1	2.52	0.45
1:V:171:SER:O	1:V:175:PRO:HG2	2.17	0.45
2:Q:396:MET:HE1	2:Q:403:PRO:HB3	1.98	0.45
1:P:90:GLU:O	1:P:91:ASN:CB	2.65	0.45
2:N:8:VAL:CG1	2:N:158:PRO:HB2	2.47	0.45
2:W:340:PRO:O	2:W:344:VAL:HG22	2.17	0.45
2:B:96:GLN:HB2	2:B:125:HIS:HB2	1.99	0.45
1:A:94:ALA:HA	1:A:95:PRO:HD3	1.80	0.45
2:B:340:PRO:O	2:B:344:VAL:HG22	2.16	0.45
2:N:95:SER:HB3	2:N:127:GLU:CB	2.47	0.45
1:S:104:LEU:HD11	1:S:164:LEU:CD2	2.47	0.45
1:S:318:ASP:HB2	1:S:336:TYR:CD1	2.52	0.45
2:B:141:LEU:HD23	3:C:85:PHE:CD2	2.50	0.45
2:W:85:TYR:HD2	2:W:87:ASP:OD1	1.99	0.45
1:J:155:VAL:HG23	1:J:163:SER:HB2	1.98	0.45
1:P:16:ARG:CB	1:P:18:GLU:OE2	2.65	0.45
1:A:234:ALA:HB1	1:A:236:VAL:HG23	1.98	0.45
1:D:172:ILE:CD1	1:D:207:GLY:HA3	2.47	0.45
1:S:157:VAL:HG23	1:S:159:SER:H	1.81	0.45
1:D:337:ALA:HA	3:F:15:ARG:O	2.17	0.45
1:M:126:THR:HG22	1:M:126:THR:O	2.16	0.45
2:T:211:ARG:HD3	4:T:707:ADP:C5	2.52	0.45
1:S:162:VAL:HG21	1:S:219:VAL:HG21	1.98	0.45
1:D:39:VAL:HG21	1:D:157:VAL:HG11	1.98	0.45
1:A:69:ILE:HD11	1:A:164:LEU:HD13	1.99	0.45
2:B:336:HIS:CE1	2:B:370:GLU:HG3	2.52	0.45
2:H:184:LYS:HB2	2:H:191:GLN:OE1	2.17	0.45
1:P:174:GLN:HB2	1:P:174:GLN:HE21	1.56	0.44
1:G:94:ALA:HA	1:G:95:PRO:HD3	1.81	0.44
2:N:95:SER:HB3	2:N:127:GLU:HB3	1.99	0.44
1:G:138:TRP:CE2	1:G:438:TRP:HZ3	2.34	0.44
1:J:384:LYS:O	1:J:387:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:132:LYS:HB2	2:K:146:ARG:HH21	1.82	0.44
2:W:137:GLY:O	3:X:90:ARG:HD2	2.17	0.44
2:N:170:LEU:HD12	2:N:223:VAL:HG21	1.99	0.44
1:G:397:THR:CG2	1:G:399:THR:O	2.64	0.44
1:M:234:ALA:HB1	1:M:236:VAL:HG23	1.99	0.44
2:W:355:LEU:HD21	2:W:365:SER:HB2	2.00	0.44
1:G:134:THR:HG22	1:G:144:PRO:HG3	1.98	0.44
1:A:270:LYS:HE3	1:A:274:GLU:OE2	2.17	0.44
2:Q:123:ARG:NH1	2:Q:125:HIS:ND1	2.64	0.44
1:S:178:PHE:CE2	1:S:402:PHE:CE2	3.05	0.44
1:P:1:MET:O	1:P:1:MET:HG2	2.17	0.44
1:M:353:MET:O	1:M:356:THR:HG23	2.17	0.44
1:V:174:GLN:N	1:V:175:PRO:CD	2.81	0.44
1:A:99:THR:O	1:A:103:ARG:HG3	2.18	0.44
1:V:356:THR:HG21	3:X:14:ALA:HB2	2.00	0.44
1:A:422:VAL:N	1:A:423:PRO:CD	2.80	0.44
1:J:403:LYS:O	1:J:406:GLU:HB2	2.17	0.44
1:S:98:ALA:HA	1:S:195:GLY:HA3	2.00	0.44
1:S:126:THR:O	1:S:126:THR:HG22	2.18	0.44
2:H:275:ASP:OD1	2:H:276:PRO:HD2	2.17	0.44
2:N:184:LYS:HB2	2:N:191:GLN:OE1	2.17	0.44
1:P:422:VAL:N	1:P:423:PRO:CD	2.81	0.44
1:P:376:ARG:HG3	1:P:376:ARG:O	2.17	0.44
2:T:21:THR:HG22	2:T:54:ASN:HD22	1.82	0.44
1:S:297:TYR:C	1:S:300:PRO:HD2	2.38	0.44
1:V:203:LEU:CD2	1:V:375:ARG:NH2	2.80	0.44
2:Q:346:TRP:O	2:Q:350:ASP:HB2	2.16	0.44
1:S:120:PHE:HE1	1:S:197:VAL:HG11	1.82	0.44
2:H:394:LYS:HE3	2:H:394:LYS:HB2	1.82	0.44
2:T:193:ARG:HH11	2:T:193:ARG:HG3	1.83	0.44
1:V:29:TYR:O	1:V:29:TYR:HD1	2.00	0.44
1:D:438:TRP:CH2	1:D:443:PRO:HG3	2.52	0.44
1:M:190:ARG:HD2	1:M:455:GLU:OE2	2.18	0.44
1:S:356:THR:HG21	3:U:14:ALA:HB2	2.00	0.44
1:M:68:PRO:HB3	1:M:112:VAL:HG21	1.99	0.44
1:M:134:THR:HG22	1:M:144:PRO:HG3	2.00	0.44
1:J:352:ILE:O	1:J:356:THR:HG23	2.16	0.44
1:J:292:LEU:HB2	1:J:295:VAL:CG2	2.47	0.44
2:N:402:THR:HG22	2:N:403:PRO:HD2	2.00	0.44
1:G:201:SER:HB2	2:H:276:PRO:HG2	1.98	0.44
2:E:374:GLU:OE1	2:E:402:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:374:GLU:OE2	2:E:404:SER:HB3	2.17	0.44
1:G:395:PRO:O	1:G:420:LEU:HD13	2.18	0.44
1:S:168:THR:HG21	1:S:199:PHE:CE2	2.53	0.44
1:S:46:LEU:HD11	1:S:80:GLU:HG3	2.00	0.44
1:G:258:LYS:HE2	1:G:289:GLU:HB3	1.99	0.44
1:P:115:THR:HG21	1:P:151:SER:OG	2.18	0.44
1:V:69:ILE:HD11	1:V:164:LEU:HD13	2.00	0.44
2:Q:310:TYR:CE1	2:Q:334:VAL:HG11	2.53	0.44
3:U:58:THR:HA	3:U:59:PRO:HD2	1.88	0.44
2:H:17:MET:HE1	2:H:61:ALA:N	2.33	0.44
1:J:155:VAL:O	1:J:211:ARG:HD2	2.18	0.44
1:G:376:ARG:HG2	1:G:380:ASN:ND2	2.33	0.44
2:H:85:TYR:CG	2:H:86:PRO:HD2	2.53	0.44
1:A:245:VAL:HG12	1:A:459:LEU:HB3	1.99	0.44
1:S:14:LEU:HD11	1:S:24:VAL:HG21	1.99	0.44
1:P:370:LYS:HZ2	3:R:45:THR:CB	2.21	0.43
1:J:138:TRP:CD2	1:J:438:TRP:CZ3	3.06	0.43
2:T:95:SER:HB3	2:T:127:GLU:CB	2.48	0.43
2:T:8:VAL:HG13	2:T:161:ARG:NH1	2.33	0.43
2:K:330:PHE:CE1	2:K:344:VAL:HG13	2.52	0.43
1:P:351:ARG:NH1	7:P:906:ASN:O	2.31	0.43
2:B:179:TYR:CE1	2:B:324:LYS:HB2	2.53	0.43
1:P:234:ALA:HB1	1:P:236:VAL:HG23	1.99	0.43
1:J:330:LYS:HG2	1:J:334:GLU:CD	2.38	0.43
2:W:320:LEU:CD2	2:W:326:VAL:HG12	2.48	0.43
1:S:354:LEU:HD11	3:U:34:LEU:HD13	1.99	0.43
1:G:298:SER:HB3	1:G:422:VAL:HG23	2.00	0.43
2:H:75:GLU:HG3	2:H:282:LYS:HG3	2.00	0.43
2:E:106:TRP:CZ3	1:G:293:PRO:HG3	2.54	0.43
2:W:35:PRO:HG3	3:X:85:PHE:CE2	2.54	0.43
1:J:294:HIS:HB2	1:J:381:ASP:OD2	2.18	0.43
1:D:21:PRO:O	1:D:25:VAL:HG23	2.18	0.43
1:P:214:GLU:OE2	1:P:463:TYR:CE1	2.71	0.43
1:A:32:TYR:CE1	1:A:36:GLU:HG2	2.53	0.43
1:V:157:VAL:HG23	1:V:159:SER:H	1.83	0.43
2:W:8:VAL:HG13	2:W:161:ARG:NH1	2.34	0.43
1:V:337:ALA:HA	3:X:15:ARG:O	2.18	0.43
1:G:300:PRO:HG2	3:I:39:GLN:CG	2.48	0.43
2:K:103:THR:HG23	2:K:104:ASN:OD1	2.18	0.43
1:A:42:TYR:CE2	1:A:113:GLY:HA3	2.54	0.43
1:S:199:PHE:C	1:S:199:PHE:CD1	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:212:ARG:NH2	1:V:472:TYR:CE1	2.86	0.43
2:N:141:LEU:HD12	3:O:87:VAL:HG22	1.99	0.43
1:S:403:LYS:O	1:S:406:GLU:HB2	2.19	0.43
2:B:399:THR:OG1	2:B:400:GLY:N	2.51	0.43
1:J:374:VAL:HG11	3:L:40:LEU:HD22	2.01	0.43
1:S:178:PHE:HE2	1:S:402:PHE:CE2	2.36	0.43
2:T:320:LEU:HD22	2:T:326:VAL:HG12	2.01	0.43
2:N:340:PRO:O	2:N:344:VAL:HG22	2.17	0.43
1:G:337:ALA:HA	3:I:15:ARG:O	2.19	0.43
1:J:185:LYS:NZ	1:J:429:LEU:O	2.49	0.43
2:N:368:LYS:HB3	2:N:370:GLU:OE2	2.18	0.43
1:J:138:TRP:NE1	1:J:438:TRP:HH2	2.16	0.43
1:A:171:SER:N	7:A:901:ASN:OD1	2.52	0.43
2:Q:402:THR:HG22	2:Q:403:PRO:HD2	1.99	0.43
1:S:422:VAL:N	1:S:423:PRO:CD	2.81	0.43
1:M:57:LEU:HD22	1:M:65:PHE:CE1	2.54	0.43
1:G:57:LEU:HD22	1:G:65:PHE:CE1	2.54	0.43
1:A:317:TYR:O	1:A:340:ARG:NH1	2.49	0.43
1:P:190:ARG:HG3	1:P:190:ARG:HH11	1.83	0.43
1:P:138:TRP:CZ2	1:P:438:TRP:CH2	3.06	0.43
3:C:58:THR:HA	3:C:59:PRO:HD2	1.81	0.43
1:P:117:LEU:O	1:P:129:SER:HB2	2.19	0.43
2:E:201:ARG:HG3	2:E:205:SER:HB3	2.01	0.43
2:K:396:MET:HE1	2:K:403:PRO:HB3	2.01	0.43
1:P:245:VAL:HG12	1:P:459:LEU:HB3	2.01	0.43
1:P:199:PHE:CD1	1:P:199:PHE:C	2.92	0.43
2:Q:348:ILE:HA	2:Q:352:LEU:HD22	2.00	0.43
2:E:255:THR:HG23	2:E:257:LYS:H	1.83	0.43
1:P:62:LEU:HA	1:P:63:PRO:HD3	1.85	0.43
2:W:3:GLU:OE2	2:W:235:ILE:HD13	2.19	0.43
1:M:354:LEU:HD21	3:O:33:ILE:HG21	2.00	0.43
1:A:404:PHE:HB3	2:E:390:LYS:HE3	2.00	0.43
2:Q:83:TYR:CZ	2:Q:88:LEU:HD22	2.54	0.43
3:U:33:ILE:O	3:U:37:ILE:HG12	2.19	0.43
2:E:262:ARG:HG2	2:E:262:ARG:H	1.50	0.43
2:B:302:ARG:NH2	2:B:328:ASP:OD1	2.52	0.43
2:K:252:ASP:CG	2:K:255:THR:HG22	2.39	0.43
2:N:90:LYS:NZ	2:N:128:GLU:OE2	2.42	0.43
1:V:49:LYS:NZ	1:V:80:GLU:HG2	2.34	0.43
1:G:279:GLU:HG3	1:G:468:LYS:NZ	2.34	0.43
1:S:337:ALA:HA	3:U:15:ARG:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:169:GLY:HA2	1:V:425:ASN:OD1	2.18	0.43
1:A:337:ALA:HA	3:C:15:ARG:O	2.18	0.43
2:B:146:ARG:HG2	2:B:146:ARG:NH1	2.32	0.43
2:T:360:ILE:CD1	2:T:366:PRO:HD3	2.49	0.43
2:H:156:THR:HG22	2:H:157:GLU:O	2.19	0.43
2:E:162:THR:HG22	2:E:164:GLU:N	2.32	0.43
1:P:292:LEU:HB2	1:P:295:VAL:HG22	2.01	0.43
1:P:292:LEU:O	1:P:295:VAL:HG22	2.19	0.43
2:H:396:MET:HE1	2:H:403:PRO:HB3	2.01	0.43
2:H:396:MET:HG3	2:H:406:ILE:HD11	2.00	0.43
1:V:126:THR:OG1	1:V:149:GLY:HA3	2.19	0.43
2:E:306:LEU:HB3	2:E:312:LEU:HD12	2.01	0.43
1:M:88:ILE:HG23	1:M:343:GLY:CA	2.30	0.42
2:Q:21:THR:HG22	2:Q:54:ASN:ND2	2.34	0.42
1:V:434:ILE:HA	1:V:434:ILE:HD12	1.82	0.42
2:W:297:GLU:OE2	2:W:302:ARG:HA	2.18	0.42
1:A:279:GLU:HG3	1:A:468:LYS:HZ1	1.78	0.42
1:G:90:GLU:O	1:G:91:ASN:CB	2.62	0.42
1:P:172:ILE:O	1:P:175:PRO:HD2	2.19	0.42
1:A:265:LEU:HD22	1:A:398:PRO:HA	2.00	0.42
2:E:80:ARG:HE	2:E:275:ASP:CG	2.23	0.42
3:F:58:THR:HA	3:F:59:PRO:HD2	1.83	0.42
2:T:41:PRO:HB3	2:T:46:MET:HE2	2.01	0.42
2:N:146:ARG:HH11	2:N:146:ARG:HG2	1.84	0.42
1:D:30:ASP:O	1:D:34:GLN:HG3	2.19	0.42
2:Q:355:LEU:CD2	2:Q:365:SER:HB2	2.50	0.42
1:P:370:LYS:NZ	3:R:45:THR:HB	2.22	0.42
2:T:11:LEU:H	2:T:156:THR:HB	1.85	0.42
1:S:172:ILE:HG22	1:S:173:ARG:N	2.33	0.42
2:H:282:LYS:HD3	3:I:55:PHE:CZ	2.54	0.42
1:A:72:LYS:HE2	1:A:117:LEU:HD13	2.01	0.42
1:S:94:ALA:HA	1:S:95:PRO:HD3	1.82	0.42
1:V:71:VAL:HB	1:V:114:LYS:NZ	2.25	0.42
1:P:94:ALA:HA	1:P:95:PRO:HD3	1.86	0.42
2:Q:85:TYR:HA	2:Q:86:PRO:HD3	1.93	0.42
2:B:360:ILE:HD11	2:B:364:GLU:O	2.20	0.42
1:A:32:TYR:CE1	1:A:36:GLU:CG	3.02	0.42
1:A:325:ARG:HA	1:A:339:THR:HG23	2.00	0.42
2:W:101:LEU:HD22	2:W:126:ILE:HD11	2.01	0.42
1:M:277:ILE:HD13	1:M:280:LEU:HD12	2.00	0.42
2:E:255:THR:HG21	2:E:259:TYR:OH	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ARG:NH2	3:F:14:ALA:O	2.49	0.42
2:W:95:SER:HB2	2:W:96:GLN:H	1.69	0.42
1:M:299:ILE:N	1:M:300:PRO:CD	2.81	0.42
2:W:170:LEU:HB3	2:W:220:PHE:CE1	2.55	0.42
1:S:138:TRP:CE2	1:S:438:TRP:HH2	2.37	0.42
2:T:95:SER:HB3	2:T:127:GLU:HB3	2.01	0.42
2:H:89:PRO:HG3	2:H:144:LEU:HD22	2.01	0.42
1:G:95:PRO:HG2	2:H:46:MET:HE1	1.99	0.42
1:V:178:PHE:CE1	1:V:397:THR:HG21	2.54	0.42
1:A:168:THR:HG22	1:A:302:TYR:OH	2.20	0.42
1:S:265:LEU:HD23	1:S:398:PRO:HA	2.02	0.42
1:G:226:TRP:CE2	1:G:235:LYS:HE2	2.54	0.42
1:M:83:THR:HG22	1:M:90:GLU:HA	2.02	0.42
1:V:438:TRP:CD1	1:V:438:TRP:N	2.86	0.42
2:T:355:LEU:CD2	2:T:365:SER:HB2	2.50	0.42
1:A:178:PHE:CE1	1:A:397:THR:HG21	2.55	0.42
1:P:337:ALA:HA	3:R:15:ARG:O	2.20	0.42
1:G:137:PRO:HB3	1:G:157:VAL:HG13	2.02	0.42
2:Q:64:ALA:O	2:Q:68:LEU:HG	2.19	0.42
2:N:360:ILE:HD11	2:N:364:GLU:O	2.20	0.42
2:Q:162:THR:HG22	2:Q:164:GLU:N	2.35	0.42
1:S:173:ARG:HH11	1:S:447:GLN:NE2	2.17	0.42
1:D:101:ILE:HA	1:D:104:LEU:HD12	2.01	0.42
1:G:297:TYR:O	1:G:300:PRO:HD2	2.19	0.42
1:V:94:ALA:HA	1:V:95:PRO:HD3	1.76	0.42
1:A:90:GLU:O	1:A:91:ASN:HB2	2.19	0.42
1:M:318:ASP:HB2	1:M:336:TYR:CE1	2.54	0.42
1:D:76:LEU:HD22	1:D:96:TYR:CE1	2.55	0.42
2:K:355:LEU:HD21	2:K:365:SER:HB2	2.02	0.42
1:J:348:VAL:O	1:J:352:ILE:HG13	2.19	0.42
1:A:265:LEU:HD11	1:A:395:PRO:HG2	2.01	0.42
1:P:213:THR:HG21	1:P:459:LEU:O	2.20	0.42
1:S:341:ASP:OD1	3:U:22:GLU:OE1	2.38	0.42
1:M:320:VAL:HG13	3:O:88:VAL:CG1	2.50	0.42
1:D:94:ALA:HA	1:D:95:PRO:HD3	1.77	0.42
2:T:80:ARG:HD2	2:T:273:PHE:CE2	2.55	0.42
1:M:312:SER:OG	2:N:82:HIS:NE2	2.35	0.42
1:M:136:ASN:HA	1:M:137:PRO:HD2	1.96	0.42
2:T:402:THR:OG1	2:T:405:GLN:CB	2.66	0.42
1:J:438:TRP:CD1	1:J:438:TRP:N	2.87	0.42
2:E:118:LYS:HZ1	1:G:291:SER:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:337:ALA:HA	3:L:15:ARG:O	2.20	0.42
1:M:162:VAL:HG21	1:M:219:VAL:HG21	2.01	0.42
1:G:25:VAL:CG1	1:G:51:LEU:HD13	2.50	0.42
1:D:6:SER:HB3	1:D:212:ARG:CZ	2.49	0.42
2:K:8:VAL:HG12	2:K:158:PRO:HB2	2.02	0.42
2:T:23:MET:CE	2:T:126:ILE:HG21	2.50	0.42
1:D:190:ARG:HD2	1:D:455:GLU:OE2	2.20	0.41
2:W:255:THR:HG23	2:W:257:LYS:H	1.85	0.41
2:E:252:ASP:OD2	2:E:255:THR:HG22	2.20	0.41
2:H:23:MET:HE2	2:H:126:ILE:HG21	2.01	0.41
1:G:437:ALA:C	1:G:438:TRP:CD1	2.93	0.41
1:V:57:LEU:HD12	1:V:110:LEU:HD21	2.02	0.41
1:S:325:ARG:HD2	1:S:335:MET:SD	2.59	0.41
2:W:374:GLU:OE2	2:W:404:SER:HB3	2.20	0.41
1:S:5:LYS:HB2	1:S:10:LEU:HD13	2.01	0.41
2:H:36:ASN:ND2	3:I:84:GLY:O	2.35	0.41
2:W:70:CYS:HB3	2:W:102:ALA:HB1	2.00	0.41
2:N:20:LYS:HE2	2:N:56:ARG:HH12	1.84	0.41
1:J:318:ASP:HB2	1:J:336:TYR:CE1	2.54	0.41
2:K:142:VAL:HB	3:L:86:PHE:HB2	2.01	0.41
1:J:145:GLY:CA	1:J:174:GLN:OE1	2.68	0.41
2:B:156:THR:HG23	2:B:157:GLU:O	2.20	0.41
1:G:13:LEU:HB3	1:G:19:VAL:CG1	2.46	0.41
1:P:172:ILE:CD1	1:P:207:GLY:HA3	2.50	0.41
1:D:98:ALA:HA	1:D:195:GLY:HA3	2.02	0.41
2:T:90:LYS:HD2	2:T:92:TYR:CE2	2.55	0.41
2:T:179:TYR:CE1	2:T:324:LYS:HB2	2.55	0.41
1:P:11:ARG:HG2	1:P:15:LYS:HE3	2.02	0.41
2:Q:365:SER:HA	2:Q:366:PRO:HD3	1.94	0.41
1:V:162:VAL:HG22	1:V:163:SER:N	2.35	0.41
1:J:329:TYR:HE2	3:L:89:PRO:HG3	1.85	0.41
1:M:137:PRO:HB3	1:M:157:VAL:HG13	2.02	0.41
1:J:25:VAL:CG1	1:J:51:LEU:HD12	2.51	0.41
2:W:40:CYS:HB2	2:W:41:PRO:HD2	2.01	0.41
1:V:344:PHE:O	1:V:349:LYS:HE2	2.20	0.41
2:N:202:PRO:O	2:N:205:SER:HB3	2.20	0.41
1:P:29:TYR:O	1:P:32:TYR:HB3	2.21	0.41
1:J:266:GLN:HA	1:J:267:PRO:HD3	1.91	0.41
1:A:21:PRO:O	1:A:25:VAL:HG23	2.20	0.41
2:T:17:MET:HE3	2:T:60:TYR:CB	2.50	0.41
2:Q:214:ILE:HD11	2:Q:230:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:VAL:HG21	1:G:163:SER:HB3	2.02	0.41
2:H:132:LYS:HG3	2:H:133:ASN:N	2.35	0.41
1:S:78:GLU:HB2	1:S:97:ASP:OD1	2.21	0.41
2:K:41:PRO:HB3	2:K:46:MET:HE2	2.02	0.41
2:W:365:SER:HA	2:W:366:PRO:HD3	1.94	0.41
1:A:136:ASN:HA	1:A:137:PRO:HD2	1.84	0.41
1:M:98:ALA:HA	1:M:195:GLY:HA3	2.02	0.41
3:I:58:THR:HA	3:I:59:PRO:HD2	1.87	0.41
2:H:20:LYS:HE2	2:H:56:ARG:NH1	2.28	0.41
3:R:46:GLU:O	3:R:47:ASN:CB	2.65	0.41
1:A:69:ILE:HD12	1:A:162:VAL:HG13	2.03	0.41
1:A:77:VAL:HG23	1:A:114:LYS:NZ	2.35	0.41
1:G:319:GLY:O	3:I:79:PRO:HG2	2.20	0.41
2:B:95:SER:CB	2:B:127:GLU:HB3	2.51	0.41
2:B:346:TRP:O	2:B:350:ASP:HB2	2.19	0.41
2:H:365:SER:HA	2:H:366:PRO:HD3	1.94	0.41
2:K:95:SER:CB	2:K:127:GLU:CB	2.97	0.41
1:V:21:PRO:HG3	1:V:65:PHE:CE2	2.55	0.41
1:D:279:GLU:OE2	1:D:282:LYS:HD2	2.21	0.41
1:M:65:PHE:O	1:M:108:GLY:O	2.38	0.41
1:V:99:THR:O	1:V:103:ARG:HG3	2.19	0.41
3:L:58:THR:HA	3:L:59:PRO:HD3	1.93	0.41
1:S:279:GLU:HG3	1:S:468:LYS:NZ	2.35	0.41
2:W:83:TYR:CZ	2:W:88:LEU:HD22	2.56	0.41
2:E:88:LEU:HA	2:E:89:PRO:HD2	1.85	0.41
1:G:49:LYS:HE2	1:G:53:GLN:NE2	2.35	0.41
1:J:111:ILE:HD12	1:J:111:ILE:N	2.35	0.41
2:K:156:THR:HG22	2:K:157:GLU:N	2.35	0.41
1:M:94:ALA:HA	1:M:95:PRO:HD3	1.85	0.41
2:B:213:GLU:OE1	2:B:215:LYS:CE	2.63	0.41
1:P:25:VAL:CG1	1:P:51:LEU:HD12	2.51	0.41
2:H:402:THR:HG22	2:H:403:PRO:HD2	2.03	0.41
1:V:178:PHE:HE1	1:V:397:THR:HG21	1.86	0.41
2:T:80:ARG:HE	2:T:275:ASP:CG	2.24	0.41
2:T:141:LEU:HD23	3:U:85:PHE:CD2	2.56	0.41
1:D:118:ASP:HB2	1:D:147:SER:HB3	2.03	0.41
1:J:303:TYR:CE2	1:J:415:TYR:HB3	2.56	0.41
1:M:463:TYR:O	1:M:467:GLN:HG2	2.21	0.41
1:J:94:ALA:HA	1:J:95:PRO:HD3	1.86	0.41
2:Q:129:ASP:CG	2:Q:146:ARG:HH11	2.24	0.41
1:D:138:TRP:CD2	1:D:438:TRP:HZ3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:252:ASP:CB	2:H:255:THR:HG22	2.38	0.41
1:M:138:TRP:NE1	1:M:438:TRP:HH2	2.19	0.41
2:B:252:ASP:CB	2:B:255:THR:HG22	2.46	0.41
1:A:174:GLN:CG	1:A:175:PRO:HD3	2.51	0.41
1:G:226:TRP:CD1	1:G:235:LYS:HG3	2.56	0.41
2:W:40:CYS:HB2	2:W:41:PRO:CD	2.51	0.41
1:S:412:ILE:HA	1:S:415:TYR:CD2	2.55	0.41
1:A:111:ILE:N	1:A:111:ILE:HD12	2.35	0.41
1:G:403:LYS:O	1:G:406:GLU:HB2	2.20	0.41
2:B:348:ILE:HA	2:B:352:LEU:HD22	2.03	0.41
1:J:182:ILE:HG12	1:J:434:ILE:HG12	2.03	0.41
1:J:434:ILE:HA	1:J:435:PRO:HD3	1.91	0.41
1:J:126:THR:O	1:J:126:THR:HG22	2.20	0.41
1:A:47:TYR:CZ	1:A:112:VAL:HG12	2.56	0.41
1:P:3:TRP:CZ2	1:P:31:ARG:HG3	2.56	0.41
1:V:339:THR:CG2	1:V:340:ARG:N	2.83	0.41
2:W:170:LEU:CD1	2:W:223:VAL:HG21	2.50	0.41
2:N:95:SER:HB2	2:N:96:GLN:H	1.71	0.41
2:B:107:VAL:HG23	2:B:121:ILE:HD11	2.03	0.41
1:S:88:ILE:HG13	1:S:343:GLY:HA3	2.03	0.41
1:A:434:ILE:HD12	1:A:465:TRP:CD1	2.55	0.41
1:M:76:LEU:HD22	1:M:96:TYR:CE1	2.56	0.41
1:D:67:ILE:HD13	1:D:67:ILE:N	2.36	0.41
2:B:39:VAL:CG1	2:B:40:CYS:N	2.81	0.40
1:M:138:TRP:CZ2	1:M:438:TRP:HH2	2.36	0.40
2:K:140:THR:OG1	3:L:91:VAL:N	2.46	0.40
2:N:396:MET:HG3	2:N:406:ILE:HD11	2.02	0.40
1:J:422:VAL:CG2	1:J:423:PRO:HD3	2.51	0.40
1:J:373:LYS:HE2	3:L:50:PRO:HD3	2.03	0.40
2:T:88:LEU:HA	2:T:89:PRO:HD2	1.98	0.40
1:G:212:ARG:O	1:G:215:ASP:HB2	2.21	0.40
3:F:33:ILE:O	3:F:37:ILE:HG12	2.20	0.40
1:P:203:LEU:HD21	1:P:426:LEU:HD23	2.03	0.40
1:G:314:LEU:HD23	1:G:352:ILE:HD11	2.02	0.40
1:J:155:VAL:CG2	1:J:163:SER:HB2	2.51	0.40
2:H:41:PRO:HB3	2:H:46:MET:HE2	2.03	0.40
2:H:119:VAL:HG12	2:H:156:THR:HG23	2.01	0.40
1:D:155:VAL:HG23	1:D:163:SER:HB2	2.03	0.40
1:J:418:ASP:HB3	1:J:422:VAL:HG13	2.02	0.40
1:P:426:LEU:HA	1:P:426:LEU:HD23	1.81	0.40
1:G:98:ALA:HA	1:G:195:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:LEU:HA	1:J:63:PRO:HD3	1.90	0.40
1:G:259:GLU:CD	1:G:292:LEU:H	2.25	0.40
1:V:234:ALA:HB1	1:V:236:VAL:HG23	2.04	0.40
1:J:270:LYS:HE3	1:J:274:GLU:OE2	2.22	0.40
1:D:1:MET:HG2	1:D:1:MET:O	2.21	0.40
2:E:225:LYS:HD3	2:E:225:LYS:HA	1.95	0.40
2:H:107:VAL:HG23	2:H:121:ILE:HD11	2.03	0.40
2:E:119:VAL:CG1	2:E:156:THR:CG2	2.98	0.40
1:S:143:VAL:HG12	1:S:145:GLY:N	2.30	0.40
1:A:171:SER:O	1:A:175:PRO:HG2	2.21	0.40
1:G:167:ASP:HA	1:G:171:SER:HB2	2.03	0.40
1:V:13:LEU:HB3	1:V:19:VAL:HG12	2.02	0.40
2:T:193:ARG:NH1	2:T:193:ARG:HG3	2.36	0.40
2:E:361:SER:HB2	2:E:363:GLU:OE1	2.21	0.40
1:V:67:ILE:HA	1:V:68:PRO:HD3	1.97	0.40
1:V:297:TYR:CE2	3:X:43:LEU:HD21	2.57	0.40
1:M:172:ILE:HD13	1:M:207:GLY:HA3	2.02	0.40
2:Q:305:ARG:HH11	2:Q:305:ARG:HG2	1.87	0.40
2:K:355:LEU:CD2	2:K:365:SER:HB2	2.51	0.40
2:T:162:THR:HG22	2:T:164:GLU:N	2.35	0.40
2:W:85:TYR:HA	2:W:86:PRO:HD3	1.93	0.40
1:V:62:LEU:HA	1:V:63:PRO:HD3	1.94	0.40
1:P:77:VAL:HG22	1:P:101:ILE:HG13	2.02	0.40
1:G:245:VAL:HG12	1:G:459:LEU:HB3	2.02	0.40
2:B:99:LYS:N	2:B:100:PRO:CD	2.83	0.40
2:T:252:ASP:CB	2:T:255:THR:HG22	2.49	0.40
1:G:57:LEU:HD12	1:G:110:LEU:HD11	2.04	0.40
2:Q:25:CYS:SG	2:Q:43:CYS:HB3	2.62	0.40
1:S:68:PRO:HB3	1:S:112:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

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	476/478 (100%)	455 (96%)	19 (4%)	2 (0%)	39	48
1	D	476/478 (100%)	456 (96%)	18 (4%)	2 (0%)	39	48
1	G	476/478 (100%)	453 (95%)	21 (4%)	2 (0%)	39	48
1	J	476/478 (100%)	457 (96%)	17 (4%)	2 (0%)	39	48
1	M	476/478 (100%)	456 (96%)	18 (4%)	2 (0%)	39	48
1	P	476/478 (100%)	454 (95%)	20 (4%)	2 (0%)	39	48
1	S	476/478 (100%)	454 (95%)	20 (4%)	2 (0%)	39	48
1	V	476/478 (100%)	454 (95%)	20 (4%)	2 (0%)	39	48
2	B	408/478 (85%)	393 (96%)	15 (4%)	0	100	100
2	E	408/478 (85%)	394 (97%)	14 (3%)	0	100	100
2	H	408/478 (85%)	394 (97%)	14 (3%)	0	100	100
2	K	408/478 (85%)	393 (96%)	14 (3%)	1 (0%)	52	64
2	N	408/478 (85%)	394 (97%)	14 (3%)	0	100	100
2	Q	408/478 (85%)	395 (97%)	13 (3%)	0	100	100
2	T	408/478 (85%)	396 (97%)	12 (3%)	0	100	100
2	W	408/478 (85%)	395 (97%)	13 (3%)	0	100	100
3	C	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
3	F	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
3	I	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
3	L	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
3	O	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
3	R	89/94 (95%)	89 (100%)	0	0	100	100
3	U	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
3	X	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
All	All	7784/8400 (93%)	7490 (96%)	277 (4%)	17 (0%)	52	64

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	LEU
1	S	2	LEU
1	S	409	GLU
1	G	2	LEU
1	G	65	PHE
1	J	2	LEU

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Mol	Chain	Res	Type
1	M	2	LEU
1	M	65	PHE
1	V	2	LEU
1	A	2	LEU
1	A	65	PHE
1	J	65	PHE
1	P	2	LEU
1	D	65	PHE
2	K	113	ASN
1	P	65	PHE
1	V	65	PHE

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	406/406 (100%)	388 (96%)	18 (4%)	35	46
1	D	406/406 (100%)	383 (94%)	23 (6%)	25	34
1	G	406/406 (100%)	391 (96%)	15 (4%)	41	55
1	J	406/406 (100%)	379 (93%)	27 (7%)	20	26
1	M	406/406 (100%)	385 (95%)	21 (5%)	29	38
1	P	406/406 (100%)	380 (94%)	26 (6%)	22	28
1	S	406/406 (100%)	382 (94%)	24 (6%)	24	32
1	V	406/406 (100%)	388 (96%)	18 (4%)	35	46
2	B	364/427 (85%)	346 (95%)	18 (5%)	31	41
2	E	364/427 (85%)	346 (95%)	18 (5%)	31	41
2	H	364/427 (85%)	346 (95%)	18 (5%)	31	41
2	K	364/427 (85%)	346 (95%)	18 (5%)	31	41
2	N	364/427 (85%)	344 (94%)	20 (6%)	27	36
2	Q	364/427 (85%)	343 (94%)	21 (6%)	25	33
2	T	364/427 (85%)	347 (95%)	17 (5%)	32	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	364/427 (85%)	348 (96%)	16 (4%)	35	46
3	C	86/89 (97%)	80 (93%)	6 (7%)	19	23
3	F	86/89 (97%)	83 (96%)	3 (4%)	43	58
3	I	86/89 (97%)	81 (94%)	5 (6%)	25	33
3	L	86/89 (97%)	82 (95%)	4 (5%)	32	43
3	O	86/89 (97%)	82 (95%)	4 (5%)	32	43
3	R	86/89 (97%)	82 (95%)	4 (5%)	32	43
3	U	86/89 (97%)	81 (94%)	5 (6%)	25	33
3	X	86/89 (97%)	81 (94%)	5 (6%)	25	33
All	All	6848/7376 (93%)	6494 (95%)	354 (5%)	29	38

All (354) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	29	TYR
1	A	57	LEU
1	A	62	LEU
1	A	69	ILE
1	A	115	THR
1	A	159	SER
1	A	164	LEU
1	A	174	GLN
1	A	190	ARG
1	A	199	PHE
1	A	228	GLU
1	A	245	VAL
1	A	279	GLU
1	A	295	VAL
1	A	356	THR
1	A	417	SER
1	A	478	THR
2	B	21	THR
2	B	39	VAL
2	B	74	GLU
2	B	98	GLU
2	B	103	THR
2	B	156	THR
2	B	162	THR

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Mol	Chain	Res	Type
2	B	189	LYS
2	B	213	GLU
2	B	244	VAL
2	B	250	THR
2	B	323	HIS
2	B	344	VAL
2	B	360	ILE
2	B	402	THR
2	B	405	GLN
2	B	406	ILE
2	B	412	LEU
3	C	34	LEU
3	C	38	ASP
3	C	46	GLU
3	C	52	ILE
3	C	70	ASP
3	C	92	VAL
1	D	10	LEU
1	D	11	ARG
1	D	29	TYR
1	D	51	LEU
1	D	57	LEU
1	D	62	LEU
1	D	88	ILE
1	D	89	LEU
1	D	115	THR
1	D	117	LEU
1	D	164	LEU
1	D	174	GLN
1	D	181	VAL
1	D	199	PHE
1	D	245	VAL
1	D	270	LYS
1	D	295	VAL
1	D	356	THR
1	D	376	ARG
1	D	384	LYS
1	D	388	GLU
1	D	397	THR
1	D	434	ILE
2	E	34	GLU
2	E	39	VAL

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Mol	Chain	Res	Type
2	E	98	GLU
2	E	103	THR
2	E	113	ASN
2	E	139	LYS
2	E	232	GLU
2	E	244	VAL
2	E	262	ARG
2	E	278	LEU
2	E	323	HIS
2	E	341	LYS
2	E	344	VAL
2	E	352	LEU
2	E	364	GLU
2	E	387	LYS
2	E	402	THR
2	E	412	LEU
3	F	34	LEU
3	F	39	GLN
3	F	46	GLU
1	G	10	LEU
1	G	51	LEU
1	G	57	LEU
1	G	59	GLU
1	G	62	LEU
1	G	78	GLU
1	G	89	LEU
1	G	115	THR
1	G	117	LEU
1	G	164	LEU
1	G	199	PHE
1	G	245	VAL
1	G	327	LYS
1	G	356	THR
1	G	397	THR
2	H	21	THR
2	H	39	VAL
2	H	98	GLU
2	H	103	THR
2	H	109	LEU
2	H	113	ASN
2	H	123	ARG
2	H	132	LYS

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Mol	Chain	Res	Type
2	H	162	THR
2	H	203	LYS
2	H	225	LYS
2	H	266	GLU
2	H	323	HIS
2	H	344	VAL
2	H	395	GLU
2	H	402	THR
2	H	403	PRO
2	H	412	LEU
3	I	39	GLN
3	I	52	ILE
3	I	70	ASP
3	I	81	ARG
3	I	92	VAL
1	J	10	LEU
1	J	29	TYR
1	J	56	SER
1	J	57	LEU
1	J	59	GLU
1	J	62	LEU
1	J	78	GLU
1	J	89	LEU
1	J	112	VAL
1	J	115	THR
1	J	162	VAL
1	J	164	LEU
1	J	174	GLN
1	J	181	VAL
1	J	185	LYS
1	J	199	PHE
1	J	201	SER
1	J	205	GLN
1	J	240	GLU
1	J	245	VAL
1	J	279	GLU
1	J	295	VAL
1	J	356	THR
1	J	376	ARG
1	J	434	ILE
1	J	458	LEU
1	J	478	THR

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Mol	Chain	Res	Type
2	K	21	THR
2	K	39	VAL
2	K	74	GLU
2	K	103	THR
2	K	109	LEU
2	K	113	ASN
2	K	115	GLU
2	K	132	LYS
2	K	134	ILE
2	K	189	LYS
2	K	201	ARG
2	K	245	VAL
2	K	266	GLU
2	K	344	VAL
2	K	352	LEU
2	K	360	ILE
2	K	365	SER
2	K	412	LEU
3	L	34	LEU
3	L	52	ILE
3	L	91	VAL
3	L	92	VAL
1	M	8	SER
1	M	10	LEU
1	M	40	LYS
1	M	51	LEU
1	M	57	LEU
1	M	62	LEU
1	M	88	ILE
1	M	89	LEU
1	M	112	VAL
1	M	115	THR
1	M	117	LEU
1	M	174	GLN
1	M	199	PHE
1	M	211	ARG
1	M	245	VAL
1	M	250	LYS
1	M	299	ILE
1	M	325	ARG
1	M	356	THR
1	M	434	ILE

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Mol	Chain	Res	Type
1	M	478	THR
2	N	21	THR
2	N	39	VAL
2	N	95	SER
2	N	98	GLU
2	N	103	THR
2	N	134	ILE
2	N	141	LEU
2	N	162	THR
2	N	203	LYS
2	N	250	THR
2	N	323	HIS
2	N	344	VAL
2	N	358	LYS
2	N	360	ILE
2	N	387	LYS
2	N	390	LYS
2	N	391	GLU
2	N	395	GLU
2	N	402	THR
2	N	412	LEU
3	O	34	LEU
3	O	38	ASP
3	O	52	ILE
3	O	81	ARG
1	P	10	LEU
1	P	29	TYR
1	P	31	ARG
1	P	40	LYS
1	P	51	LEU
1	P	57	LEU
1	P	59	GLU
1	P	62	LEU
1	P	78	GLU
1	P	89	LEU
1	P	115	THR
1	P	162	VAL
1	P	164	LEU
1	P	174	GLN
1	P	185	LYS
1	P	199	PHE
1	P	240	GLU

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Mol	Chain	Res	Type
1	P	245	VAL
1	P	279	GLU
1	P	291	SER
1	P	295	VAL
1	P	325	ARG
1	P	356	THR
1	P	458	LEU
1	P	464	LEU
1	P	478	THR
2	Q	21	THR
2	Q	39	VAL
2	Q	74	GLU
2	Q	103	THR
2	Q	106	TRP
2	Q	109	LEU
2	Q	123	ARG
2	Q	132	LYS
2	Q	201	ARG
2	Q	210	THR
2	Q	245	VAL
2	Q	255	THR
2	Q	302	ARG
2	Q	323	HIS
2	Q	344	VAL
2	Q	352	LEU
2	Q	360	ILE
2	Q	365	SER
2	Q	402	THR
2	Q	405	GLN
2	Q	412	LEU
3	R	34	LEU
3	R	45	THR
3	R	52	ILE
3	R	56	GLU
1	S	10	LEU
1	S	11	ARG
1	S	29	TYR
1	S	51	LEU
1	S	57	LEU
1	S	59	GLU
1	S	62	LEU
1	S	69	ILE

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Mol	Chain	Res	Type
1	S	89	LEU
1	S	117	LEU
1	S	164	LEU
1	S	181	VAL
1	S	192	SER
1	S	199	PHE
1	S	242	SER
1	S	245	VAL
1	S	295	VAL
1	S	356	THR
1	S	376	ARG
1	S	384	LYS
1	S	389	VAL
1	S	392	ILE
1	S	458	LEU
1	S	464	LEU
2	T	21	THR
2	T	39	VAL
2	T	74	GLU
2	T	98	GLU
2	T	103	THR
2	T	123	ARG
2	T	189	LYS
2	T	214	ILE
2	T	232	GLU
2	T	244	VAL
2	T	245	VAL
2	T	262	ARG
2	T	341	LYS
2	T	344	VAL
2	T	406	ILE
2	T	407	VAL
2	T	412	LEU
3	U	34	LEU
3	U	52	ILE
3	U	54	GLU
3	U	68	SER
3	U	70	ASP
1	V	10	LEU
1	V	29	TYR
1	V	57	LEU
1	V	62	LEU

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Mol	Chain	Res	Type
1	V	89	LEU
1	V	115	THR
1	V	117	LEU
1	V	124	SER
1	V	143	VAL
1	V	190	ARG
1	V	199	PHE
1	V	245	VAL
1	V	279	GLU
1	V	295	VAL
1	V	325	ARG
1	V	356	THR
1	V	434	ILE
1	V	478	THR
2	W	21	THR
2	W	39	VAL
2	W	46	MET
2	W	74	GLU
2	W	109	LEU
2	W	123	ARG
2	W	203	LYS
2	W	210	THR
2	W	233	ARG
2	W	244	VAL
2	W	250	THR
2	W	344	VAL
2	W	364	GLU
2	W	402	THR
2	W	406	ILE
2	W	412	LEU
3	X	34	LEU
3	X	38	ASP
3	X	39	GLN
3	X	46	GLU
3	X	52	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	S	447	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ASN	A	901	1	4,7,8	0.93	0	1,8,10	1.45	0
4	ADP	B	701	-	22,29,29	1.08	2 (9%)	27,45,45	1.73	2 (7%)
7	ASN	D	902	1	4,7,8	0.54	0	1,8,10	1.22	0
4	ADP	E	702	-	22,29,29	0.95	1 (4%)	27,45,45	1.84	5 (18%)
7	ASN	G	903	1	4,7,8	0.89	0	1,8,10	1.45	0
4	ADP	H	703	-	22,29,29	1.04	1 (4%)	27,45,45	1.67	2 (7%)
7	ASN	J	904	1	4,7,8	0.95	0	1,8,10	1.79	0
4	ADP	K	704	-	22,29,29	1.04	2 (9%)	27,45,45	1.85	3 (11%)
7	ASN	M	905	1	4,7,8	0.74	0	1,8,10	1.41	0
4	ADP	N	705	-	22,29,29	1.09	2 (9%)	27,45,45	1.69	4 (14%)
7	ASN	P	906	1	4,7,8	0.76	0	1,8,10	1.55	0
4	ADP	Q	706	-	22,29,29	1.06	2 (9%)	27,45,45	1.73	5 (18%)
7	ASN	S	907	1	4,7,8	1.24	1 (25%)	1,8,10	1.29	0
4	ADP	T	707	-	22,29,29	1.01	1 (4%)	27,45,45	1.69	4 (14%)
7	ASN	V	908	1	4,7,8	1.21	0	1,8,10	1.90	0
4	ADP	W	708	-	22,29,29	1.01	1 (4%)	27,45,45	1.65	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ASN	A	901	1	-	0/3/7/8	0/0/0/0
4	ADP	B	701	-	-	0/12/32/32	0/3/3/3
7	ASN	D	902	1	-	0/3/7/8	0/0/0/0
4	ADP	E	702	-	-	0/12/32/32	0/3/3/3
7	ASN	G	903	1	-	0/3/7/8	0/0/0/0
4	ADP	H	703	-	-	0/12/32/32	0/3/3/3
7	ASN	J	904	1	-	0/3/7/8	0/0/0/0
4	ADP	K	704	-	-	0/12/32/32	0/3/3/3
7	ASN	M	905	1	-	0/3/7/8	0/0/0/0
4	ADP	N	705	-	-	0/12/32/32	0/3/3/3
7	ASN	P	906	1	-	0/3/7/8	0/0/0/0
4	ADP	Q	706	-	-	0/12/32/32	0/3/3/3
7	ASN	S	907	1	-	0/3/7/8	0/0/0/0
4	ADP	T	707	-	-	0/12/32/32	0/3/3/3
7	ASN	V	908	1	-	0/3/7/8	0/0/0/0
4	ADP	W	708	-	-	0/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ADP	O4'-C1'	2.01	1.43	1.41
7	S	907	ASN	CB-CG	2.07	1.56	1.49
4	K	704	ADP	O4'-C1'	2.15	1.43	1.41
4	Q	706	ADP	O4'-C1'	2.23	1.44	1.41
4	N	705	ADP	O4'-C1'	2.29	1.44	1.41
4	E	702	ADP	C5-C4	3.06	1.47	1.40
4	T	707	ADP	C5-C4	3.10	1.47	1.40
4	K	704	ADP	C5-C4	3.16	1.47	1.40
4	Q	706	ADP	C5-C4	3.20	1.47	1.40
4	W	708	ADP	C5-C4	3.23	1.47	1.40
4	H	703	ADP	C5-C4	3.25	1.47	1.40
4	N	705	ADP	C5-C4	3.32	1.48	1.40
4	B	701	ADP	C5-C4	3.51	1.48	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	704	ADP	N3-C2-N1	-7.46	123.19	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	702	ADP	N3-C2-N1	-7.11	123.45	128.89
4	H	703	ADP	N3-C2-N1	-6.86	123.64	128.89
4	N	705	ADP	N3-C2-N1	-6.55	123.88	128.89
4	B	701	ADP	N3-C2-N1	-6.52	123.90	128.89
4	T	707	ADP	N3-C2-N1	-6.46	123.95	128.89
4	Q	706	ADP	N3-C2-N1	-6.39	124.00	128.89
4	W	708	ADP	N3-C2-N1	-5.94	124.35	128.89
4	B	701	ADP	C4-C5-N7	-3.44	106.32	109.48
4	W	708	ADP	C4-C5-N7	-3.42	106.34	109.48
4	Q	706	ADP	C4-C5-N7	-3.29	106.45	109.48
4	T	707	ADP	C4-C5-N7	-2.96	106.76	109.48
4	E	702	ADP	PA-O3A-PB	-2.95	122.77	132.67
4	E	702	ADP	C4-C5-N7	-2.82	106.89	109.48
4	K	704	ADP	PA-O3A-PB	-2.65	123.78	132.67
4	Q	706	ADP	PA-O3A-PB	-2.63	123.84	132.67
4	T	707	ADP	PA-O3A-PB	-2.46	124.42	132.67
4	W	708	ADP	PA-O3A-PB	-2.45	124.45	132.67
4	N	705	ADP	C4-C5-N7	-2.39	107.28	109.48
4	E	702	ADP	C1'-N9-C4	-2.24	123.57	126.94
4	H	703	ADP	C4-C5-N7	-2.11	107.54	109.48
4	Q	706	ADP	C1'-N9-C4	-2.10	123.77	126.94
4	K	704	ADP	C4-C5-N7	-2.06	107.58	109.48
4	N	705	ADP	C2-N1-C6	2.01	122.36	118.77
4	N	705	ADP	O3B-PB-O2B	2.06	115.22	107.38
4	W	708	ADP	O3B-PB-O2B	2.06	115.24	107.38
4	E	702	ADP	O3B-PB-O2B	2.20	115.76	107.38
4	Q	706	ADP	O3B-PB-O2B	2.44	116.68	107.38
4	T	707	ADP	O3B-PB-O2B	2.50	116.89	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	901	ASN	1	0
4	B	701	ADP	1	0
7	D	902	ASN	1	0
7	P	906	ASN	1	0
7	S	907	ASN	1	0
4	T	707	ADP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	478/478 (100%)	0.01	8 (1%) 73 79	23, 44, 71, 79	0
1	D	478/478 (100%)	-0.07	8 (1%) 73 79	29, 44, 71, 80	0
1	G	478/478 (100%)	0.03	2 (0%) 93 95	29, 43, 71, 79	0
1	J	478/478 (100%)	0.02	4 (0%) 87 90	28, 43, 71, 79	0
1	M	478/478 (100%)	-0.03	1 (0%) 95 97	29, 43, 71, 79	0
1	P	478/478 (100%)	0.03	2 (0%) 93 95	28, 43, 71, 79	0
1	S	478/478 (100%)	-0.04	6 (1%) 79 84	29, 44, 71, 79	0
1	V	478/478 (100%)	-0.03	5 (1%) 84 88	29, 44, 71, 79	0
2	B	410/478 (85%)	0.17	8 (1%) 68 75	28, 54, 85, 103	0
2	E	410/478 (85%)	0.25	25 (6%) 25 33	29, 54, 85, 103	0
2	H	410/478 (85%)	0.22	19 (4%) 36 45	29, 54, 85, 103	0
2	K	410/478 (85%)	0.30	16 (3%) 43 52	29, 54, 85, 103	0
2	N	410/478 (85%)	0.21	13 (3%) 51 60	29, 54, 85, 103	0
2	Q	410/478 (85%)	0.27	10 (2%) 62 71	28, 54, 85, 103	0
2	T	410/478 (85%)	0.27	23 (5%) 28 36	28, 54, 85, 103	0
2	W	410/478 (85%)	0.21	9 (2%) 65 73	29, 54, 85, 103	0
3	C	91/94 (96%)	0.19	1 (1%) 82 86	39, 50, 64, 68	0
3	F	91/94 (96%)	0.13	1 (1%) 82 86	39, 50, 64, 67	0
3	I	91/94 (96%)	0.12	1 (1%) 82 86	39, 50, 64, 68	0
3	L	91/94 (96%)	0.21	2 (2%) 65 73	39, 50, 64, 67	0
3	O	91/94 (96%)	0.19	1 (1%) 82 86	39, 50, 64, 68	0
3	R	91/94 (96%)	0.23	1 (1%) 82 86	39, 50, 64, 67	0
3	U	91/94 (96%)	0.06	2 (2%) 65 73	39, 50, 64, 68	0
3	X	91/94 (96%)	0.14	2 (2%) 65 73	39, 50, 64, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7832/8400 (93%)	0.11	170 (2%) 65 73	23, 47, 79, 103	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	242	GLY	6.3
2	H	262	ARG	5.4
2	N	408	GLU	5.4
2	T	412	LEU	5.3
2	W	406	ILE	5.2
2	K	408	GLU	5.1
2	E	384	ILE	4.9
2	T	408	GLU	4.8
2	Q	406	ILE	4.5
2	N	262	ARG	4.5
2	E	262	ARG	4.5
2	E	242	GLY	4.5
2	E	408	GLU	4.4
2	H	267	ALA	4.3
2	T	406	ILE	4.2
2	B	384	ILE	4.2
2	H	241	GLY	4.1
2	N	267	ALA	4.1
2	T	264	LYS	4.1
1	A	57	LEU	4.1
2	E	403	PRO	4.0
2	E	407	VAL	3.9
2	T	265	GLU	3.9
2	N	241	GLY	3.8
3	O	92	VAL	3.7
2	B	360	ILE	3.6
2	K	406	ILE	3.6
2	N	384	ILE	3.6
2	T	407	VAL	3.6
2	T	262	ARG	3.6
2	K	265	GLU	3.6
1	V	10	LEU	3.5
2	T	111	LEU	3.5
2	Q	262	ARG	3.5
2	H	239	GLU	3.4
2	H	261	MET	3.4
2	T	263	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	N	405	GLN	3.4
3	F	8	LEU	3.3
1	D	54	ALA	3.3
2	K	262	ARG	3.2
1	D	19	VAL	3.2
2	H	408	GLU	3.2
1	S	10	LEU	3.2
2	H	266	GLU	3.1
2	E	267	ALA	3.1
1	P	19	VAL	3.1
2	E	245	VAL	3.1
2	Q	384	ILE	3.1
2	T	241	GLY	3.1
2	E	264	LYS	3.1
1	A	1	MET	3.0
2	H	265	GLU	3.0
1	A	22	LYS	3.0
1	D	57	LEU	3.0
3	L	89	PRO	2.9
2	E	263	THR	2.9
2	H	231	ILE	2.9
1	D	464	LEU	2.9
2	E	385	SER	2.9
2	T	259	TYR	2.9
2	Q	408	GLU	2.8
1	S	19	VAL	2.8
2	K	264	LYS	2.8
2	Q	266	GLU	2.8
1	A	19	VAL	2.7
2	B	264	LYS	2.7
2	T	403	PRO	2.7
2	N	407	VAL	2.7
2	B	383	VAL	2.7
1	G	478	THR	2.7
3	U	91	VAL	2.7
2	Q	379	ILE	2.7
2	Q	263	THR	2.7
3	U	92	VAL	2.7
2	T	192	LEU	2.6
1	S	58	LYS	2.6
2	W	265	GLU	2.6
2	H	238	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	406	ILE	2.6
2	H	4	LYS	2.6
2	B	265	GLU	2.6
1	J	7	LEU	2.6
2	E	200	ILE	2.6
2	H	354	LEU	2.6
2	E	359	GLY	2.5
2	E	265	GLU	2.5
2	W	407	VAL	2.5
1	A	54	ALA	2.5
2	N	232	GLU	2.5
2	T	239	GLU	2.5
2	T	399	THR	2.5
1	D	7	LEU	2.5
3	I	92	VAL	2.5
2	K	266	GLU	2.5
2	K	337	PHE	2.5
1	V	19	VAL	2.4
2	K	106	TRP	2.4
2	Q	265	GLU	2.4
1	A	10	LEU	2.4
1	D	10	LEU	2.4
2	K	267	ALA	2.4
2	W	375	LEU	2.4
2	T	405	GLN	2.4
2	E	261	MET	2.4
2	H	111	LEU	2.4
1	G	265	LEU	2.3
3	L	91	VAL	2.3
2	E	373	ALA	2.3
2	E	375	LEU	2.3
2	H	263	THR	2.3
1	S	66	GLY	2.3
2	B	375	LEU	2.3
2	K	335	ARG	2.3
3	X	5	GLU	2.3
2	K	404	SER	2.3
2	H	372	LEU	2.3
2	W	264	LYS	2.3
2	E	379	ILE	2.3
2	E	405	GLN	2.3
1	A	131	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	30	ASP	2.3
2	W	106	TRP	2.3
3	X	92	VAL	2.2
1	A	7	LEU	2.2
2	E	251	PHE	2.2
2	H	264	LYS	2.2
2	E	111	LEU	2.2
2	E	266	GLU	2.2
2	K	388	ILE	2.2
2	T	388	ILE	2.2
3	C	92	VAL	2.2
2	K	401	LYS	2.2
2	Q	106	TRP	2.2
2	K	383	VAL	2.2
2	W	258	THR	2.2
1	V	26	GLU	2.2
1	D	51	LEU	2.2
1	V	7	LEU	2.2
2	N	264	LYS	2.1
2	E	397	VAL	2.1
2	B	239	GLU	2.1
1	D	18	GLU	2.1
2	H	289	GLU	2.1
2	K	402	THR	2.1
1	J	10	LEU	2.1
1	M	7	LEU	2.1
2	N	406	ILE	2.1
2	W	200	ILE	2.1
2	N	244	VAL	2.1
2	Q	220	PHE	2.1
2	W	317	ALA	2.1
1	J	18	GLU	2.1
3	R	66	HIS	2.1
2	K	263	THR	2.1
2	T	188	GLU	2.1
1	S	198	ALA	2.1
2	E	388	ILE	2.1
2	H	74	GLU	2.0
2	N	265	GLU	2.0
1	J	478	THR	2.0
2	T	168	LEU	2.0
1	P	18	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	S	162	VAL	2.0
2	T	250	THR	2.0
2	N	412	LEU	2.0
2	T	310	TYR	2.0
2	E	31	PHE	2.0
2	H	109	LEU	2.0
2	T	375	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MG	B	801	1/1	0.98	0.19	7.28	10,10,10,10	0
5	MG	Q	806	1/1	0.95	0.18	4.56	21,21,21,21	0
5	MG	W	808	1/1	0.97	0.17	3.29	18,18,18,18	0
5	MG	T	807	1/1	1.00	0.18	2.99	15,15,15,15	0
5	MG	N	805	1/1	0.97	0.20	2.98	16,16,16,16	0
5	MG	H	803	1/1	0.98	0.19	2.03	10,10,10,10	0
6	ZN	B	901	1/1	1.00	0.16	1.99	37,37,37,37	0
7	ASN	M	905	8/9	0.90	0.16	1.98	32,33,34,36	0
5	MG	K	804	1/1	0.98	0.16	1.45	11,11,11,11	0
4	ADP	H	703	27/27	0.83	0.16	1.12	44,48,63,65	27
6	ZN	T	907	1/1	0.99	0.14	1.10	37,37,37,37	0
7	ASN	D	902	8/9	0.88	0.13	1.01	39,40,40,41	0
6	ZN	H	903	1/1	1.00	0.15	0.92	33,33,33,33	0
7	ASN	A	901	8/9	0.92	0.14	0.80	33,33,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	ZN	Q	906	1/1	0.99	0.15	0.60	30,30,30,30	0
5	MG	E	802	1/1	0.97	0.13	0.53	19,19,19,19	0
6	ZN	W	908	1/1	0.99	0.13	0.50	33,33,33,33	0
6	ZN	N	905	1/1	1.00	0.14	0.33	36,36,36,36	0
7	ASN	G	903	8/9	0.93	0.12	0.25	28,30,31,31	0
4	ADP	W	708	27/27	0.83	0.15	0.13	48,50,68,70	27
6	ZN	K	904	1/1	1.00	0.13	0.02	29,29,29,29	0
4	ADP	B	701	27/27	0.90	0.14	-0.01	46,49,65,66	27
4	ADP	N	705	27/27	0.88	0.16	-0.02	49,52,63,65	27
4	ADP	E	702	27/27	0.88	0.15	-0.05	59,60,72,73	27
4	ADP	T	707	27/27	0.88	0.14	-0.06	51,52,70,71	27
7	ASN	V	908	8/9	0.94	0.10	-0.15	29,30,31,32	0
7	ASN	P	906	8/9	0.90	0.12	-0.24	28,32,33,34	0
6	ZN	E	902	1/1	0.98	0.10	-0.39	40,40,40,40	0
4	ADP	Q	706	27/27	0.87	0.14	-0.52	44,46,65,66	27
7	ASN	S	907	8/9	0.96	0.09	-0.53	28,32,33,33	0
4	ADP	K	704	27/27	0.87	0.14	-0.83	40,41,64,66	27
7	ASN	J	904	8/9	0.96	0.10	-1.34	26,28,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.