



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:03 AM GMT

PDB ID : 2ZCI
Title : Structure of a GTP-dependent bacterial PEP-carboxykinase from *Corynebacterium glutamicum*
Authors : Aich, S.; Prasad, L.; Delbaere, L.T.J.
Deposited on : 2007-11-09
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

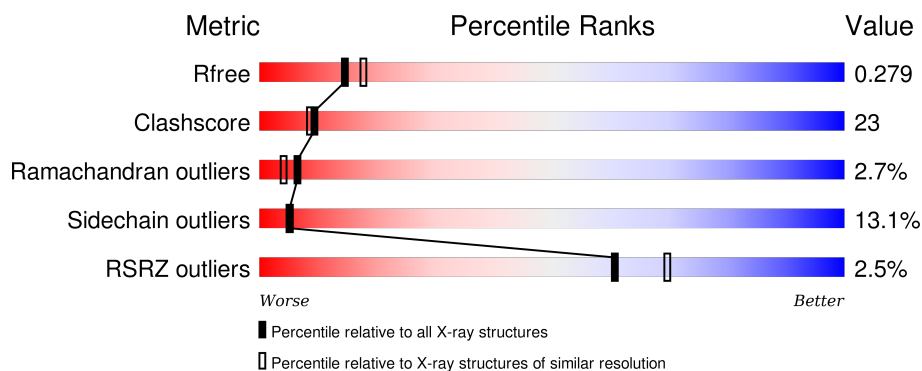
1 Overall quality at a glance

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	610	<div> <div>61%</div> <div>26%</div> <div>7%</div> <div>• •</div> </div>
1	B	610	<div> <div>52%</div> <div>34%</div> <div>8%</div> <div>• •</div> </div>
1	C	610	<div> <div>56%</div> <div>31%</div> <div>8%</div> <div>• •</div> </div>
1	D	610	<div> <div>50%</div> <div>33%</div> <div>10%</div> <div>• 5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18407 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 Phosphoenolpyruvate carboxykinase [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4539	2871	764	874	30			
1	B	584	Total	C	N	O	S	0	0	0
			4518	2858	761	869	30			
1	C	586	Total	C	N	O	S	0	0	0
			4535	2869	763	873	30			
1	D	578	Total	C	N	O	S	0	0	0
			4489	2840	755	864	30			

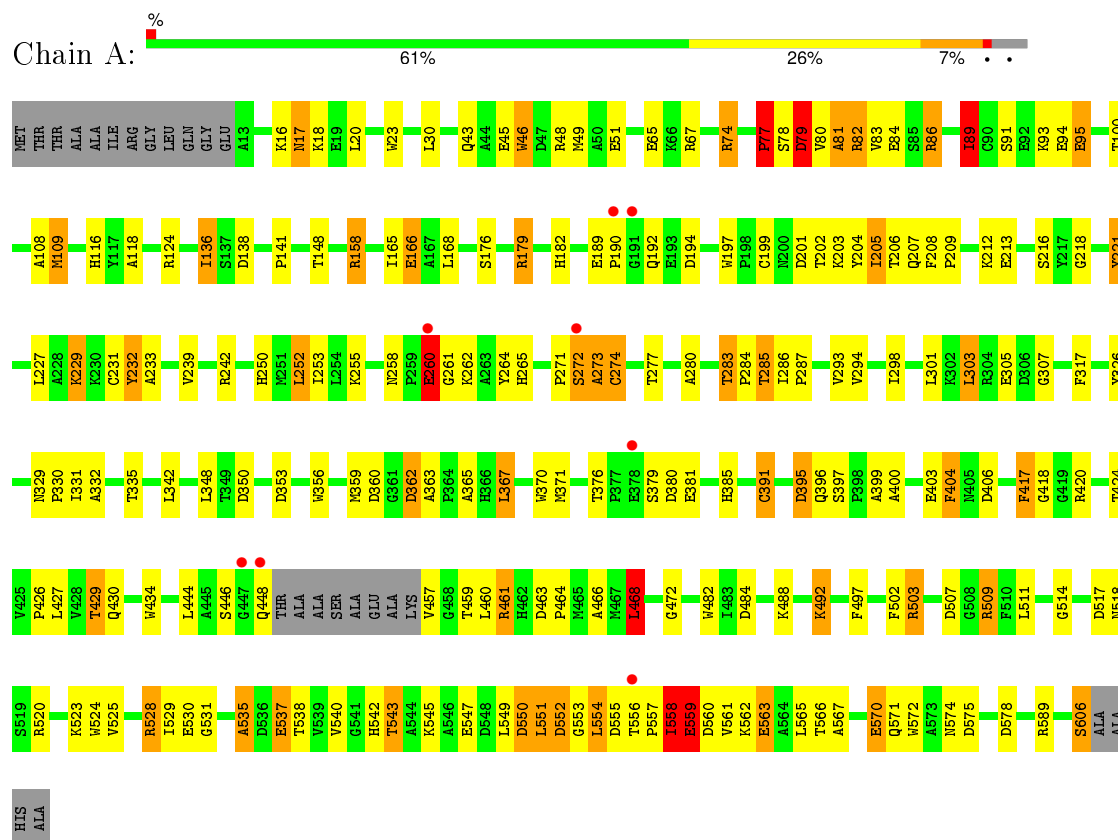
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total	O	0	0
			109	109		
2	B	69	Total	O	0	0
			69	69		
2	C	89	Total	O	0	0
			89	89		
2	D	59	Total	O	0	0
			59	59		

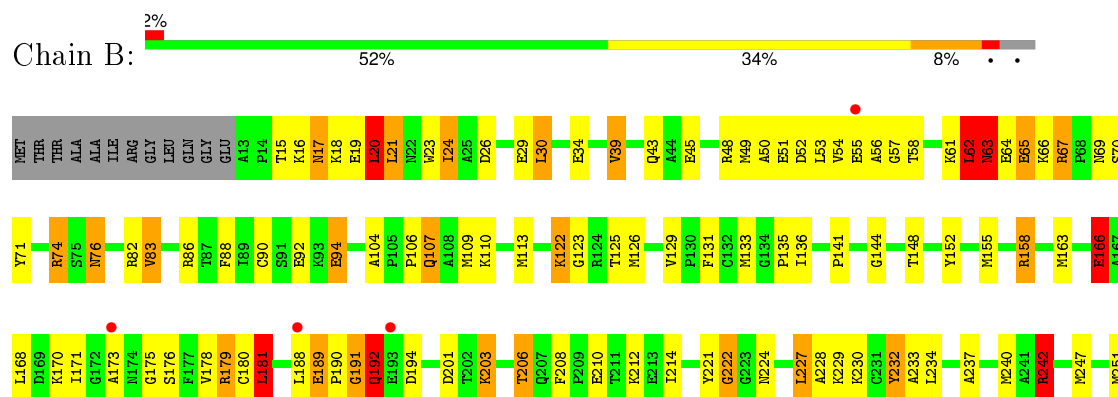
3 Residue-property plots

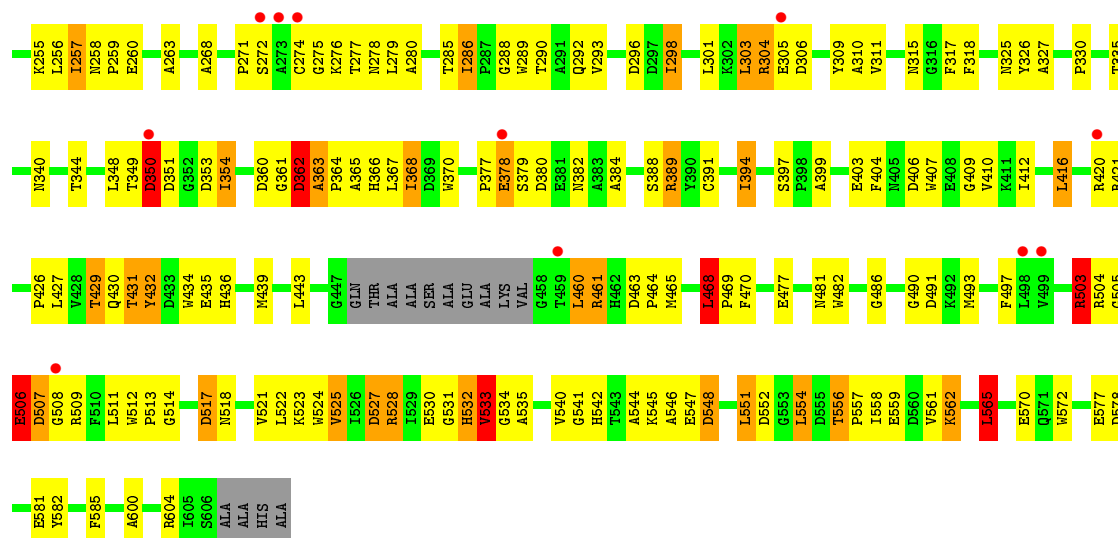
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Phosphoenolpyruvate carboxykinase [GTP]

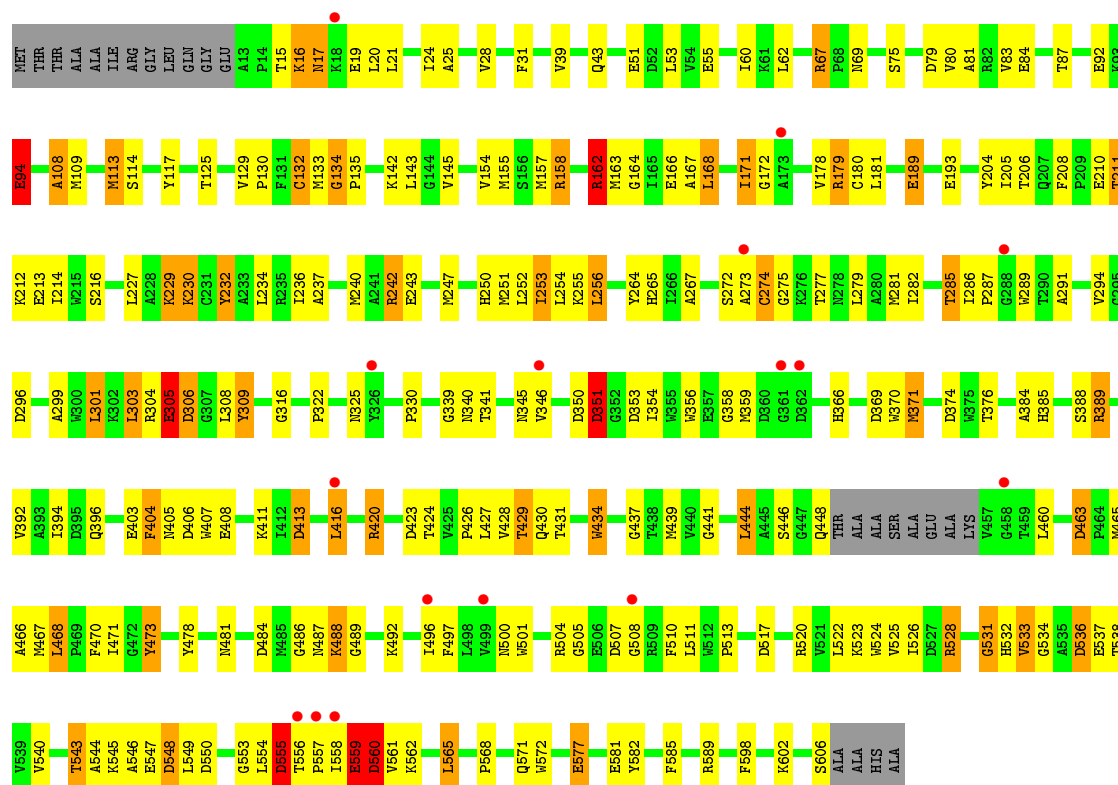


• Molecule 1: Phosphoenolpyruvate carboxykinase [GTP]





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E577	G508	T424	E336	I257	K170	E84
E581	F510	V425	E337	N258	A173	I89
P588	L511	P426	N340	E260	F177	E92
	G514	L427	T341	G261	V178	K93
P591	G514	V428	L342	K262	R179	E94
A600	N518	T429	L348	K263	G180	E95
	S519	Q430	T349	Y264	L181	P105
A603	R520	W434	D350	H265	E189	P106
	V521	W434	D351	I266	P190	Q107
R604	L522	L444	R351	A267	G191	A108
R605	K523	A445	I354	A268	Q192	M109
	S606	S446	K355	P271	E193	K110
ALA	V525	GLY	K356	S272	E193	S114
HIS	I526	GLN		A273	D194	
ALA	D527	THR	M359	C274	V195	Y117
HIS	R528	ALA	D360	G275	A196	A118
	I529	ALA	G361	K276		M121
ALA	E530	SER	D362	T277	W197	K122
	G531	ALA	A363	N278		G123
HIS	H532	GLU	R366	L279		R124
	V533	LYS	L367	A280		T125
V540		VAL	I368	N281	I205	M126
		GLY		T283	T206	Y127
T543	T459		G372	P284	Q207	V128
	A544	L460	N373		F208	V129
R545	R461		D374	G288	K212	P130
A546	H462		K375	N289	E213	F131
D463	D463		T376	T290		C132
D548	P464		P377		T214	M133
L549	M465		E378	V294	W215	P135
E550			S379		S216	I136
L551	L468		D380	D297		D140
D552	P469		E381	I298	L227	P141
G553	F470			A299	A228	K142
L554			R389	K300	K230	L143
D555	Y473		Y390	L301	C231	T148
THR			C391	K302		D149
PRO	Y478			L303		S150
I558	L479		I394	G319		E151
E559	Q480		D395			Y152
D560	N481		Q396	E305		V153
V561						V154
K562	M485		A401	N315		M155
E563	G486		P402	G316		R158
A564			E403	F317		S150
L565	D491		F404	G319		E151
T566			W405			R242
A567	S495		D406	N326		E243
P568	I496		W407	Y326		E244
A569	F497			A327		G245
E570	W501		V410	X276		W246
Q571				S328		
W572			I415	N329		H250
A573	B504		L416	P330		M251
M574	G505			I331		G164
D575	E506					I165
V576	D507		R420	K334		L254
			R421	T335		K255
						L256
						L168
						D169

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.34Å 118.06Å 152.93Å 90.00° 96.44° 90.00°	Depositor
Resolution (Å)	24.83 – 2.30 24.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.0 (24.83-2.30) 77.0 (24.83-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.188 , 0.279 0.189 , 0.279	Depositor DCC
R_{free} test set	4256 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 84798 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18407	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.39	16/4658 (0.3%)	1.27	33/6342 (0.5%)
1	B	1.31	8/4637 (0.2%)	1.21	35/6313 (0.6%)
1	C	1.40	24/4654 (0.5%)	1.23	21/6337 (0.3%)
1	D	1.25	12/4605 (0.3%)	1.17	14/6266 (0.2%)
All	All	1.34	60/18554 (0.3%)	1.22	103/25258 (0.4%)

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
1	A	0	3
1	B	0	1
1	C	0	3
1	D	0	2
All	All	0	9

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLU	CG-CD	9.11	1.65	1.51
1	C	577	GLU	CB-CG	7.57	1.66	1.52
1	C	274	CYS	CB-SG	7.41	1.94	1.82
1	C	305	GLU	CB-CG	7.28	1.66	1.52
1	C	108	ALA	CA-CB	7.20	1.67	1.52
1	C	84	GLU	CG-CD	7.09	1.62	1.51
1	A	65	GLU	CG-CD	6.92	1.62	1.51
1	A	51	GLU	CG-CD	6.61	1.61	1.51
1	C	478	TYR	CD2-CE2	-6.61	1.29	1.39
1	A	391	CYS	CB-SG	-6.42	1.71	1.82
1	C	309	TYR	CE2-CZ	6.39	1.46	1.38
1	A	197	TRP	CB-CG	6.33	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	351	ASP	CB-CG	6.22	1.64	1.51
1	A	570	GLU	CG-CD	6.21	1.61	1.51
1	D	92	GLU	CB-CG	6.18	1.63	1.52
1	B	260	GLU	CG-CD	6.15	1.61	1.51
1	A	166	GLU	CG-CD	6.12	1.61	1.51
1	C	94	GLU	CB-CG	6.07	1.63	1.52
1	C	145	VAL	CB-CG2	6.02	1.65	1.52
1	A	232	TYR	CD1-CE1	6.02	1.48	1.39
1	D	381	GLU	CG-CD	5.99	1.60	1.51
1	D	19	GLU	CD-OE1	5.96	1.32	1.25
1	C	55	GLU	CG-CD	5.86	1.60	1.51
1	C	525	VAL	CB-CG1	-5.86	1.40	1.52
1	D	38	PHE	CE1-CZ	5.83	1.48	1.37
1	A	365	ALA	CA-CB	5.81	1.64	1.52
1	D	300	TRP	CE3-CZ3	5.77	1.48	1.38
1	D	501	TRP	CB-CG	-5.73	1.40	1.50
1	C	55	GLU	CB-CG	5.72	1.63	1.52
1	A	570	GLU	CD-OE2	5.67	1.31	1.25
1	C	164	GLY	C-O	-5.63	1.14	1.23
1	D	51	GLU	CG-CD	5.61	1.60	1.51
1	B	90	CYS	CB-SG	-5.59	1.72	1.81
1	C	84	GLU	CB-CG	5.57	1.62	1.52
1	A	524	TRP	CE3-CZ3	5.54	1.47	1.38
1	A	189	GLU	CG-CD	5.53	1.60	1.51
1	C	189	GLU	CG-CD	5.50	1.60	1.51
1	A	65	GLU	CB-CG	5.47	1.62	1.52
1	A	260	GLU	CB-CG	5.39	1.62	1.52
1	C	242	ARG	CG-CD	5.37	1.65	1.51
1	A	417	PHE	CE2-CZ	5.36	1.47	1.37
1	C	189	GLU	CB-CG	5.32	1.62	1.52
1	D	152	TYR	CE1-CZ	5.30	1.45	1.38
1	D	315	ASN	CB-CG	5.30	1.63	1.51
1	A	221	TYR	CB-CG	-5.29	1.43	1.51
1	B	189	GLU	CG-CD	5.29	1.59	1.51
1	B	482	TRP	CB-CG	-5.26	1.40	1.50
1	D	215	TRP	CE3-CZ3	5.26	1.47	1.38
1	C	346	VAL	CB-CG2	5.26	1.63	1.52
1	C	384	ALA	CA-CB	5.25	1.63	1.52
1	C	434	TRP	CB-CG	-5.25	1.40	1.50
1	A	221	TYR	CE1-CZ	5.25	1.45	1.38
1	B	432	TYR	CD1-CE1	5.10	1.47	1.39
1	C	51	GLU	CG-CD	5.10	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GLU	CB-CG	5.09	1.61	1.52
1	D	19	GLU	CG-CD	5.07	1.59	1.51
1	C	446	SER	N-CA	5.07	1.56	1.46
1	B	525	VAL	CB-CG1	-5.07	1.42	1.52
1	D	461	ARG	CG-CD	5.07	1.64	1.51
1	C	473	TYR	CZ-OH	5.02	1.46	1.37

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ARG	NE-CZ-NH1	12.07	126.33	120.30
1	B	30	LEU	CA-CB-CG	11.09	140.81	115.30
1	C	158	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	A	303	LEU	CB-CG-CD2	-9.46	94.92	111.00
1	D	30	LEU	CA-CB-CG	9.45	137.04	115.30
1	D	235	ARG	NE-CZ-NH2	8.63	124.61	120.30
1	C	460	LEU	CB-CG-CD1	-8.49	96.56	111.00
1	A	503	ARG	CG-CD-NE	-8.19	94.61	111.80
1	A	606	SER	CA-C-O	8.09	137.09	120.10
1	C	406	ASP	CB-CG-OD1	8.01	125.51	118.30
1	D	181	LEU	CA-CB-CG	7.88	133.42	115.30
1	B	389	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	D	254	LEU	CB-CG-CD2	-7.53	98.20	111.00
1	C	406	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	D	395	ASP	CB-CA-C	-7.29	95.81	110.40
1	C	303	LEU	CB-CG-CD2	-7.13	98.87	111.00
1	B	74	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	463	ASP	CB-CG-OD2	7.04	124.64	118.30
1	B	179	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	C	133	MET	CG-SD-CE	6.96	111.34	100.20
1	D	254	LEU	CA-CB-CG	6.95	131.29	115.30
1	A	503	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	303	LEU	CA-CB-CG	6.78	130.90	115.30
1	B	256	LEU	CB-CG-CD1	-6.76	99.50	111.00
1	B	468	LEU	CB-CG-CD2	6.71	122.41	111.00
1	B	565	LEU	CA-CB-CG	6.58	130.43	115.30
1	A	406	ASP	CB-CG-OD1	6.57	124.21	118.30
1	D	460	LEU	CA-CB-CG	6.44	130.12	115.30
1	D	155	MET	CG-SD-CE	-6.43	89.91	100.20
1	A	158	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	395	ASP	CB-CA-C	-6.43	97.55	110.40
1	B	191	GLY	N-CA-C	-6.38	97.15	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	LEU	CA-CB-CG	6.36	129.93	115.30
1	A	79	ASP	CB-CG-OD2	6.35	124.02	118.30
1	D	282	ILE	CG1-CB-CG2	6.31	125.29	111.40
1	B	528	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	549	LEU	CA-CB-CG	6.31	129.81	115.30
1	B	406	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	367	LEU	CB-CG-CD2	-6.23	100.41	111.00
1	B	443	LEU	CB-CG-CD1	-6.22	100.43	111.00
1	D	468	LEU	C-N-CD	6.22	141.46	128.40
1	A	179	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	578	ASP	CB-CG-OD2	6.16	123.85	118.30
1	A	158	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	286	ILE	CB-CA-C	-6.16	99.29	111.60
1	A	303	LEU	CB-CG-CD1	6.15	121.46	111.00
1	A	201	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	86	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	575	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	549	LEU	CA-CB-CG	6.05	129.22	115.30
1	B	303	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	79	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	A	109	MET	CG-SD-CE	-6.04	90.54	100.20
1	B	39	VAL	CG1-CB-CG2	6.04	120.56	110.90
1	B	62	LEU	CB-CG-CD1	6.03	121.25	111.00
1	B	181	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	528	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	468	LEU	C-N-CD	5.80	140.59	128.40
1	A	192	GLN	N-CA-C	5.80	126.65	111.00
1	B	503	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	558	ILE	CB-CA-C	-5.79	100.03	111.60
1	B	460	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	242	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	421	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	B	517	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	74	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	533	VAL	CB-CA-C	5.61	122.05	111.40
1	A	48	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	484	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	26	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	89	ILE	CB-CA-C	5.52	122.65	111.60
1	B	179	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	536	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	B	242	ARG	NE-CZ-NH1	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	348	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	381	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	B	350	ASP	CB-CG-OD1	5.43	123.18	118.30
1	C	439	MET	CG-SD-CE	5.42	108.87	100.20
1	C	413	ASP	CB-CG-OD1	5.42	123.17	118.30
1	C	523	LYS	CD-CE-NZ	-5.34	99.41	111.70
1	C	501	TRP	CB-CA-C	-5.32	99.77	110.40
1	A	350	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	205	ILE	N-CA-C	-5.29	96.72	111.00
1	D	234	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	26	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	158	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	484	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	C	532	HIS	N-CA-C	-5.21	96.93	111.00
1	A	242	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	C	389	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	162	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	416	LEU	CB-CG-CD2	5.15	119.75	111.00
1	B	527	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	B	20	LEU	CA-CB-CG	5.14	127.13	115.30
1	C	296	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	D	540	VAL	CB-CA-C	-5.11	101.69	111.40
1	D	428	VAL	CB-CA-C	-5.10	101.70	111.40
1	C	134	GLY	N-CA-C	-5.08	100.41	113.10
1	A	528	ARG	CG-CD-NE	5.04	122.39	111.80
1	C	371	MET	CG-SD-CE	5.03	108.25	100.20
1	B	548	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	B	578	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	252	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide
1	A	559	GLU	Peptide
1	A	81	ALA	Peptide
1	B	350	ASP	Peptide
1	C	305	GLU	Peptide
1	C	560	ASP	Peptide
1	C	81	ALA	Peptide
1	D	15	THR	Peptide

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Mol	Chain	Res	Type	Group
1	D	361	GLY	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	4539	0	4342	151	0
1	B	4518	0	4320	225	0
1	C	4535	0	4336	209	0
1	D	4489	0	4292	228	0
2	A	109	0	0	9	0
2	B	69	0	0	6	0
2	C	89	0	0	8	0
2	D	59	0	0	9	0
All	All	18407	0	17290	802	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 23.

All (802) 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:D:355:TRP:HA	1:D:359:MET:CE	1.70	1.22
1:B:129:VAL:HG13	1:B:163:MET:CE	1.70	1.19
1:C:534:GLY:HA3	1:C:548:ASP:OD2	1.38	1.18
1:D:132:CYS:HB2	1:D:143:LEU:HD23	1.18	1.16
1:A:558:ILE:H	1:A:558:ILE:HD12	1.00	1.16
1:C:113:MET:HE1	1:C:206:THR:HB	1.30	1.11
1:B:129:VAL:CG1	1:B:163:MET:CE	2.29	1.10
1:B:129:VAL:CG1	1:B:163:MET:HE2	1.83	1.08
1:B:74:ARG:NH1	1:B:368:ILE:CD1	2.17	1.08
1:D:132:CYS:HB2	1:D:143:LEU:CD2	1.88	1.04
1:B:74:ARG:NH1	1:B:368:ILE:HD11	1.72	1.02
1:C:366:HIS:HE1	1:C:374:ASP:OD1	1.43	1.01
1:C:247:MET:HE1	1:C:308:LEU:HD21	1.43	1.01
1:A:558:ILE:CD1	1:A:558:ILE:H	1.70	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ARG:HH12	1:B:368:ILE:CD1	1.73	1.00
1:D:355:TRP:HA	1:D:359:MET:HE2	1.41	0.99
1:D:511:LEU:HD13	1:D:563:GLU:HG3	1.43	0.98
1:A:429:THR:HG22	2:A:627:HOH:O	1.62	0.98
1:A:550:ASP:O	1:A:551:LEU:HD13	1.63	0.97
1:B:180:CYS:HB3	1:B:227:LEU:HD23	1.47	0.97
1:B:129:VAL:HG13	1:B:163:MET:HE2	0.96	0.96
1:D:71:TYR:CE2	2:D:643:HOH:O	2.17	0.96
1:B:577:GLU:O	1:B:581:GLU:HG3	1.65	0.96
1:B:304:ARG:O	1:B:306:ASP:N	1.96	0.96
1:A:550:ASP:O	1:A:551:LEU:CD1	2.14	0.95
1:B:69:ASN:HD22	1:B:340:ASN:HD22	1.03	0.95
1:D:78:SER:O	1:D:79:ASP:HB2	1.63	0.95
1:A:558:ILE:HD12	1:A:558:ILE:N	1.82	0.94
1:D:63:ASN:HD22	1:D:66:LYS:HB2	1.34	0.93
1:D:17:ASN:HD22	1:D:18:LYS:H	1.12	0.93
1:C:16:LYS:N	1:C:16:LYS:HD3	1.84	0.92
1:C:273:ALA:O	1:C:274:CYS:SG	2.27	0.92
1:B:506:GLU:O	1:B:508:GLY:N	2.03	0.92
1:A:429:THR:CG2	2:A:627:HOH:O	2.16	0.91
1:D:49:MET:HG2	1:D:151:GLU:OE1	1.71	0.90
1:C:16:LYS:H	1:C:16:LYS:HD3	1.38	0.88
1:C:17:ASN:O	1:C:21:LEU:HD12	1.73	0.88
1:C:16:LYS:CD	1:C:16:LYS:H	1.87	0.88
1:C:341:THR:HG22	1:C:392:VAL:HB	1.53	0.88
1:D:376:THR:OG1	1:D:378:GLU:HG2	1.75	0.86
1:C:113:MET:HE1	1:C:206:THR:CB	2.05	0.85
1:D:278:ASN:O	1:D:282:ILE:HG23	1.76	0.85
1:B:43:GLN:HE22	1:B:158:ARG:HH12	1.22	0.85
1:A:507:ASP:OD1	1:A:509:ARG:HD2	1.77	0.85
1:D:278:ASN:O	1:D:282:ILE:CG2	2.25	0.85
1:C:179:ARG:HH11	1:C:179:ARG:HG2	1.40	0.85
1:C:285:THR:HG21	1:C:517:ASP:OD1	1.75	0.84
1:D:318:PHE:CE2	1:D:389:ARG:HD2	2.11	0.84
1:A:503:ARG:HH22	1:A:566:THR:CG2	1.91	0.84
1:A:457:VAL:HB	1:A:459:THR:HG23	1.60	0.83
1:B:109:MET:HE2	1:D:105:PRO:HD3	1.59	0.83
1:C:69:ASN:HD22	1:C:340:ASN:HD22	1.24	0.83
1:D:273:ALA:O	1:D:274:CYS:HB2	1.77	0.82
1:C:366:HIS:CE1	1:C:374:ASP:OD1	2.32	0.82
1:D:511:LEU:CD1	1:D:563:GLU:HG3	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:TRP:HA	1:D:359:MET:HE1	1.62	0.82
1:A:326:TYR:O	1:A:330:PRO:HG3	1.79	0.82
1:A:429:THR:HB	1:A:543:THR:HB	1.60	0.82
1:C:413:ASP:OD1	2:C:667:HOH:O	1.98	0.81
1:A:430:GLN:OE1	1:A:528:ARG:HD2	1.81	0.81
1:C:211:THR:OG1	1:C:213:GLU:HG3	1.81	0.80
1:D:325:ASN:OD1	1:D:328:SER:HB3	1.80	0.80
1:A:503:ARG:HH22	1:A:566:THR:HG23	1.46	0.80
1:C:113:MET:CE	1:C:206:THR:HB	2.11	0.80
1:A:558:ILE:O	1:A:560:ASP:N	2.15	0.79
1:B:544:ALA:O	1:B:565:LEU:HG	1.83	0.79
1:B:129:VAL:HG11	1:B:163:MET:CE	2.13	0.79
1:A:555:ASP:O	1:A:557:PRO:HD3	1.83	0.79
1:D:229:LYS:NZ	1:D:297:ASP:OD2	2.16	0.78
1:D:424:THR:HG22	1:D:571:GLN:HB3	1.64	0.78
1:B:561:VAL:O	1:B:565:LEU:HD22	1.84	0.78
1:B:255:LYS:HD3	1:B:292:GLN:HE21	1.49	0.77
1:B:74:ARG:CZ	1:B:368:ILE:HD11	2.14	0.77
1:A:86:ARG:HE	1:C:94:GLU:HG3	1.49	0.77
1:A:331:ILE:HD12	1:A:399:ALA:HB2	1.66	0.77
1:B:189:GLU:N	1:B:192:GLN:OE1	2.17	0.77
1:B:109:MET:CE	1:D:105:PRO:HD3	2.14	0.76
1:B:237:ALA:HA	1:B:240:MET:HE2	1.67	0.76
1:D:242:ARG:HH21	1:D:481:ASN:HD22	1.33	0.76
1:C:210:GLU:HG2	2:C:620:HOH:O	1.84	0.76
1:C:69:ASN:HD22	1:C:340:ASN:ND2	1.83	0.76
1:B:74:ARG:NH1	1:B:368:ILE:HD13	2.01	0.76
1:A:563:GLU:O	1:A:566:THR:HG22	1.86	0.76
1:D:17:ASN:ND2	1:D:18:LYS:H	1.84	0.75
1:C:242:ARG:HH11	1:C:481:ASN:HD22	1.34	0.75
1:A:79:ASP:HB2	2:A:694:HOH:O	1.86	0.75
1:C:179:ARG:NH1	2:C:670:HOH:O	2.17	0.75
1:C:407:TRP:HE3	1:C:407:TRP:H	1.34	0.75
1:D:509:ARG:NE	1:D:509:ARG:HA	2.02	0.75
1:D:274:CYS:SG	2:D:646:HOH:O	2.44	0.74
1:B:378:GLU:HG3	1:B:378:GLU:O	1.85	0.74
1:D:540:VAL:HG22	1:D:572:TRP:CZ2	2.23	0.74
1:A:136:ILE:HG22	2:A:651:HOH:O	1.88	0.74
1:B:364:PRO:HG2	1:B:367:LEU:HG	1.70	0.74
1:C:237:ALA:HA	1:C:240:MET:HE2	1.70	0.74
1:C:430:GLN:NE2	1:C:528:ARG:HE	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ARG:CG	1:C:179:ARG:HH11	1.99	0.73
1:D:600:ALA:O	1:D:604:ARG:HD3	1.89	0.73
1:B:62:LEU:HD21	1:B:354:ILE:HD13	1.71	0.73
1:D:240:MET:O	1:D:244:GLU:HB2	1.88	0.73
1:D:253:ILE:HD11	1:D:410:VAL:HG21	1.71	0.73
1:B:505:GLY:O	1:B:506:GLU:O	2.06	0.73
1:C:426:PRO:HG2	1:C:429:THR:CG2	2.19	0.73
1:B:429:THR:HG23	2:B:619:HOH:O	1.88	0.72
1:C:16:LYS:CD	1:C:16:LYS:N	2.51	0.72
1:D:327:ALA:O	1:D:328:SER:CB	2.37	0.72
1:C:20:LEU:CD2	1:C:24:ILE:HD11	2.19	0.72
1:B:506:GLU:C	1:B:508:GLY:H	1.93	0.72
1:B:503:ARG:HH11	1:B:503:ARG:HG2	1.54	0.71
1:B:275:GLY:H	1:B:278:ASN:HD22	1.38	0.71
1:C:286:ILE:HD11	1:C:520:ARG:CZ	2.20	0.71
1:D:255:LYS:NZ	1:D:257:ILE:HD11	2.05	0.71
1:B:271:PRO:HB3	1:B:463:ASP:OD2	1.91	0.71
1:B:17:ASN:HA	1:B:173:ALA:O	1.91	0.71
1:C:256:LEU:HD12	1:C:289:TRP:CZ3	2.25	0.71
1:B:129:VAL:CG1	1:B:163:MET:HE3	2.19	0.71
1:B:351:ASP:N	2:B:646:HOH:O	2.22	0.70
1:B:69:ASN:HD22	1:B:340:ASN:ND2	1.86	0.70
1:B:62:LEU:HB2	1:B:70:SER:O	1.91	0.70
1:C:53:LEU:HD12	1:C:155:MET:CE	2.21	0.70
1:B:427:LEU:HB3	1:B:565:LEU:HD13	1.73	0.70
1:B:34:GLU:HG2	1:B:123:GLY:H	1.57	0.70
1:A:430:GLN:HB2	1:A:497:PHE:CE2	2.27	0.70
1:B:201:ASP:OD2	1:D:588:PRO:HG3	1.92	0.70
1:B:69:ASN:ND2	1:B:340:ASN:HD22	1.86	0.70
1:A:82:ARG:HH12	1:A:84:GLU:HB2	1.55	0.70
1:A:206:THR:HG21	1:A:208:PHE:CZ	2.27	0.70
1:C:113:MET:CE	1:C:206:THR:CB	2.70	0.69
1:B:277:THR:HG22	1:B:296:ASP:OD2	1.91	0.69
1:C:511:LEU:HD22	1:C:561:VAL:HG11	1.74	0.69
1:C:206:THR:HG21	1:C:208:PHE:CZ	2.28	0.69
1:C:20:LEU:O	1:C:24:ILE:HG13	1.93	0.69
1:B:43:GLN:HE22	1:B:158:ARG:NH1	1.91	0.69
1:C:429:THR:HB	1:C:543:THR:HB	1.74	0.69
1:A:260:GLU:HA	1:A:260:GLU:OE2	1.90	0.69
1:D:50:ALA:HB1	1:D:71:TYR:CZ	2.27	0.69
1:C:431:THR:HB	1:C:496:ILE:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:GLU:HB2	1:D:192:GLN:HG3	1.75	0.68
1:A:514:GLY:HA2	1:A:518:ASN:OD1	1.94	0.68
1:D:376:THR:OG1	1:D:378:GLU:CG	2.41	0.68
1:C:256:LEU:CD1	1:C:289:TRP:CE3	2.76	0.68
1:D:205:ILE:HD11	1:D:231:CYS:SG	2.33	0.68
1:D:426:PRO:HG3	1:D:567:ALA:HB2	1.74	0.68
1:B:506:GLU:N	1:B:506:GLU:OE2	2.26	0.68
1:D:132:CYS:CB	1:D:143:LEU:HD23	2.11	0.68
1:D:349:THR:HG21	1:D:351:ASP:OD1	1.94	0.68
1:B:63:ASN:HD21	1:B:65:GLU:HB3	1.59	0.68
1:B:67:ARG:HD2	1:B:353:ASP:OD1	1.93	0.68
1:D:355:TRP:CA	1:D:359:MET:HE2	2.22	0.68
1:D:16:LYS:C	1:D:16:LYS:HD2	2.14	0.67
1:C:286:ILE:HD11	1:C:520:ARG:NH1	2.09	0.67
1:B:179:ARG:HD3	2:B:623:HOH:O	1.93	0.67
1:B:74:ARG:HH12	1:B:368:ILE:HD13	1.55	0.67
1:C:17:ASN:HD21	1:C:19:GLU:HB2	1.59	0.67
1:B:61:LYS:HG3	1:B:71:TYR:CE2	2.28	0.67
1:A:503:ARG:NH2	1:A:566:THR:CG2	2.57	0.67
1:D:509:ARG:CZ	1:D:509:ARG:HA	2.24	0.67
1:B:242:ARG:HH21	1:B:481:ASN:HD22	1.40	0.67
1:C:424:THR:HA	1:C:571:GLN:HE21	1.59	0.67
1:D:255:LYS:HZ2	1:D:257:ILE:HD11	1.59	0.67
1:D:17:ASN:HD22	1:D:18:LYS:N	1.90	0.67
1:A:380:ASP:OD2	2:A:697:HOH:O	2.13	0.67
1:C:582:TYR:O	1:C:585:PHE:HB3	1.94	0.67
1:A:255:LYS:HE3	1:A:403:GLU:OE2	1.95	0.67
1:C:179:ARG:CG	1:C:179:ARG:NH1	2.55	0.66
1:B:135:PRO:HG2	1:B:407:TRP:HA	1.78	0.66
1:C:553:GLY:O	1:C:554:LEU:HG	1.96	0.66
1:B:230:LYS:N	2:B:638:HOH:O	2.13	0.66
1:C:69:ASN:ND2	1:C:340:ASN:HD22	1.94	0.66
1:B:503:ARG:NH1	1:B:503:ARG:HG2	2.10	0.66
1:D:464:PRO:HD2	1:D:468:LEU:HD13	1.76	0.66
1:C:16:LYS:CE	1:C:16:LYS:H	2.08	0.65
1:A:17:ASN:ND2	1:A:20:LEU:H	1.95	0.65
1:D:305:GLU:OE2	1:D:305:GLU:N	2.26	0.65
1:B:524:TRP:NE1	1:B:533:VAL:CG1	2.59	0.65
1:B:362:ASP:O	1:B:363:ALA:CB	2.45	0.65
1:B:17:ASN:O	1:B:21:LEU:HD12	1.96	0.65
1:D:67:ARG:HH22	1:D:354:ILE:HD11	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:VAL:O	1:C:163:MET:HE3	1.97	0.65
1:B:394:ILE:HD13	1:B:404:PHE:CD1	2.32	0.65
1:D:511:LEU:HD22	1:D:560:ASP:HB3	1.77	0.65
1:C:304:ARG:HG3	1:C:309:TYR:CD1	2.33	0.64
1:D:16:LYS:HD2	1:D:17:ASN:N	2.11	0.64
1:A:427:LEU:HB3	1:A:565:LEU:HD23	1.78	0.64
1:A:89:ILE:HD13	1:A:472:GLY:O	1.97	0.64
1:B:107:GLN:NE2	1:B:107:GLN:H	1.97	0.63
1:C:487:ASN:C	1:C:489:GLY:N	2.51	0.63
1:B:171:ILE:O	1:B:175:GLY:HA3	1.98	0.63
1:B:311:VAL:HG12	1:B:409:GLY:CA	2.28	0.63
1:D:53:LEU:HD12	1:D:155:MET:CE	2.28	0.63
1:B:554:LEU:HD13	1:B:556:THR:HG22	1.81	0.63
1:D:507:ASP:HA	1:D:509:ARG:NH1	2.13	0.63
1:D:43:GLN:HE22	1:D:158:ARG:HH12	1.47	0.63
1:B:24:ILE:C	1:B:24:ILE:HD13	2.19	0.63
1:C:511:LEU:HB3	1:C:561:VAL:HG11	1.80	0.63
1:D:429:THR:HG23	2:D:634:HOH:O	1.98	0.62
1:B:86:ARG:HE	1:D:94:GLU:HG2	1.64	0.62
1:D:17:ASN:HB3	1:D:20:LEU:HB2	1.80	0.62
1:D:30:LEU:HD22	1:D:117:TYR:HB3	1.80	0.62
1:D:427:LEU:HB3	1:D:565:LEU:HD13	1.81	0.62
1:D:267:ALA:O	1:D:415:ILE:HA	1.98	0.62
1:A:553:GLY:O	1:A:555:ASP:N	2.32	0.62
1:B:430:GLN:NE2	1:B:528:ARG:HE	1.97	0.62
1:A:216:SER:HB2	1:A:227:LEU:HD21	1.82	0.62
1:B:304:ARG:HE	1:B:304:ARG:HA	1.64	0.62
1:C:426:PRO:HG2	1:C:429:THR:HG21	1.80	0.62
1:C:272:SER:HB2	1:C:275:GLY:HA3	1.82	0.62
1:D:507:ASP:OD1	1:D:509:ARG:NH1	2.32	0.62
1:B:430:GLN:HG2	1:B:431:THR:O	2.00	0.62
1:C:559:GLU:O	1:C:560:ASP:HB2	2.00	0.62
1:D:265:HIS:HE1	1:D:403:GLU:OE2	1.83	0.62
1:A:136:ILE:O	1:A:136:ILE:HG13	2.00	0.62
1:B:528:ARG:HH12	1:B:534:GLY:HA2	1.64	0.62
1:B:434:TRP:CD1	1:B:486:GLY:HA3	2.35	0.61
1:B:15:THR:HG21	1:B:20:LEU:HD13	1.82	0.61
1:C:540:VAL:HG22	1:C:572:TRP:CZ2	2.35	0.61
1:D:523:LYS:HG3	2:D:620:HOH:O	2.00	0.61
1:B:34:GLU:CG	1:B:123:GLY:H	2.13	0.61
1:D:277:THR:O	1:D:281:MET:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ARG:HD2	1:B:370:TRP:O	2.00	0.61
1:C:430:GLN:HE22	1:C:528:ARG:HE	1.46	0.61
1:A:17:ASN:HD22	1:A:20:LEU:H	1.46	0.61
1:B:524:TRP:NE1	1:B:533:VAL:HG11	2.16	0.61
1:D:208:PHE:HB2	1:D:213:GLU:HB2	1.82	0.61
1:D:234:LEU:HD11	1:D:250:HIS:CD2	2.36	0.61
1:A:503:ARG:NH2	1:A:566:THR:HG22	2.16	0.60
1:C:429:THR:HG23	2:C:635:HOH:O	2.02	0.60
1:C:53:LEU:HD12	1:C:155:MET:HE1	1.83	0.60
1:A:264:TYR:OH	1:A:530:GLU:OE2	2.13	0.60
1:C:109:MET:O	1:C:113:MET:HG3	2.01	0.60
1:C:256:LEU:HD13	1:C:289:TRP:HE3	1.65	0.60
1:A:67:ARG:HD2	1:A:353:ASP:OD2	2.02	0.60
1:A:550:ASP:O	1:A:551:LEU:HD12	2.00	0.60
1:B:530:GLU:HB3	1:B:532:HIS:CE1	2.36	0.60
1:A:511:LEU:HD23	1:A:563:GLU:HB3	1.83	0.60
1:C:256:LEU:HD12	1:C:289:TRP:CE3	2.37	0.60
1:B:379:SER:O	1:B:380:ASP:HB2	2.02	0.60
1:B:514:GLY:HA2	1:B:518:ASN:OD1	2.01	0.60
1:D:559:GLU:O	1:D:559:GLU:OE2	2.20	0.59
1:B:242:ARG:HD3	1:B:477:GLU:OE1	2.02	0.59
1:D:507:ASP:HA	1:D:509:ARG:HH12	1.67	0.59
1:B:129:VAL:HG11	1:B:163:MET:HE3	1.79	0.59
1:A:520:ARG:NE	1:A:554:LEU:HD23	2.18	0.59
1:A:551:LEU:O	1:A:552:ASP:HB2	2.02	0.59
1:B:432:TYR:CE2	1:B:541:GLY:HA2	2.37	0.59
1:A:86:ARG:HE	1:C:94:GLU:CG	2.15	0.59
1:D:195:VAL:HG12	1:D:196:ALA:H	1.66	0.59
1:B:349:THR:O	1:B:350:ASP:HB2	2.03	0.59
1:C:157:MET:HB3	1:C:163:MET:HE2	1.83	0.59
1:D:30:LEU:CD2	1:D:117:TYR:HB3	2.33	0.59
1:C:463:ASP:OD1	1:C:468:LEU:HB2	2.03	0.59
1:D:69:ASN:HB3	1:D:340:ASN:OD1	2.01	0.59
1:D:50:ALA:O	1:D:54:VAL:HG23	2.02	0.59
1:D:354:ILE:HD13	1:D:356:TRP:CZ3	2.38	0.59
1:B:535:ALA:CB	1:B:542:HIS:HB3	2.31	0.59
1:C:265:HIS:HE1	1:C:403:GLU:OE2	1.86	0.59
1:B:24:ILE:HD13	1:B:24:ILE:O	2.03	0.58
1:D:255:LYS:NZ	1:D:257:ILE:CD1	2.67	0.58
1:C:232:TYR:HA	1:C:236:ILE:CG1	2.34	0.58
1:C:306:ASP:O	1:C:411:LYS:NZ	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ILE:CD1	1:A:558:ILE:N	2.46	0.58
1:B:503:ARG:CG	1:B:503:ARG:HH11	2.17	0.58
1:B:528:ARG:NH1	1:B:534:GLY:HA2	2.18	0.58
1:B:325:ASN:ND2	1:B:327:ALA:HB3	2.18	0.58
1:B:344:THR:O	1:B:388:SER:HB2	2.03	0.58
1:D:416:LEU:HD11	1:D:522:LEU:HD11	1.85	0.58
1:D:514:GLY:HA2	1:D:518:ASN:OD1	2.04	0.58
1:B:43:GLN:NE2	1:B:158:ARG:HH12	1.95	0.58
1:B:63:ASN:HD22	1:B:63:ASN:C	2.06	0.58
1:B:63:ASN:HD22	1:B:65:GLU:H	1.50	0.58
1:A:464:PRO:HD2	1:A:468:LEU:HG	1.86	0.58
1:D:254:LEU:HD11	1:D:256:LEU:HD22	1.86	0.58
1:D:235:ARG:NH2	1:D:470:PHE:HD2	2.01	0.58
1:D:78:SER:O	1:D:79:ASP:CB	2.45	0.57
1:D:577:GLU:O	1:D:581:GLU:HG3	2.03	0.57
1:D:53:LEU:HD12	1:D:155:MET:HE1	1.86	0.57
1:B:521:VAL:O	1:B:525:VAL:HG23	2.04	0.57
1:A:77:PRO:HG3	1:A:371:MET:CE	2.34	0.57
1:A:43:GLN:OE1	1:A:158:ARG:NH1	2.37	0.57
1:A:80:VAL:CG1	1:A:80:VAL:O	2.53	0.57
1:D:114:SER:HA	1:D:117:TYR:HB2	1.85	0.57
1:A:80:VAL:HG11	1:A:385:HIS:NE2	2.20	0.57
1:C:350:ASP:OD2	1:C:366:HIS:HD2	1.88	0.57
1:D:136:ILE:O	1:D:170:LYS:NZ	2.33	0.57
1:C:330:PRO:HD2	2:C:627:HOH:O	2.04	0.56
1:C:255:LYS:HD2	1:C:265:HIS:CE1	2.41	0.56
1:C:166:GLU:HA	1:D:406:ASP:OD1	2.05	0.56
1:B:94:GLU:OE1	1:D:202:THR:HB	2.06	0.56
1:B:53:LEU:HD22	1:B:58:THR:OG1	2.05	0.56
1:B:82:ARG:HB2	1:B:82:ARG:CZ	2.36	0.56
1:D:49:MET:HB3	1:D:155:MET:HE2	1.88	0.56
1:D:67:ARG:HG3	1:D:67:ARG:NH2	2.21	0.56
1:B:325:ASN:HD21	1:B:327:ALA:HB3	1.71	0.56
1:D:465:MET:CE	1:D:479:LEU:HD23	2.35	0.56
1:B:122:LYS:HD2	1:B:188:LEU:O	2.05	0.56
1:D:189:GLU:H	1:D:192:GLN:NE2	2.03	0.56
1:C:487:ASN:O	1:C:489:GLY:N	2.38	0.56
1:C:214:ILE:HD11	1:C:236:ILE:HG12	1.88	0.56
1:D:465:MET:HG3	1:D:478:TYR:HE2	1.70	0.55
1:C:536:ASP:O	1:C:536:ASP:OD1	2.24	0.55
1:B:427:LEU:HB3	1:B:565:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:HB2	1:B:360:ASP:OD2	2.06	0.55
1:D:349:THR:CG2	1:D:351:ASP:OD1	2.53	0.55
1:B:524:TRP:NE1	1:B:533:VAL:HG13	2.21	0.55
1:D:279:LEU:HD11	1:D:522:LEU:HD21	1.89	0.55
1:D:17:ASN:HB3	1:D:20:LEU:CB	2.36	0.55
1:B:48:ARG:HH21	1:B:52:ASP:N	2.05	0.55
1:D:259:PRO:HA	1:D:288:GLY:O	2.07	0.55
1:D:244:GLU:HB3	1:D:246:TRP:CD1	2.42	0.54
1:B:214:ILE:HG21	1:B:227:LEU:HG	1.89	0.54
1:A:511:LEU:CD2	1:A:563:GLU:HB3	2.37	0.54
1:B:532:HIS:ND1	1:B:532:HIS:N	2.54	0.54
1:C:598:PHE:CE1	1:C:602:LYS:HD2	2.42	0.54
1:A:335:THR:O	1:A:396:GLN:NE2	2.36	0.54
1:C:17:ASN:C	1:C:17:ASN:HD22	2.11	0.54
1:C:487:ASN:O	1:C:488:LYS:C	2.46	0.54
1:B:255:LYS:CD	1:B:292:GLN:HE21	2.18	0.54
1:D:507:ASP:CG	1:D:509:ARG:HH12	2.11	0.54
1:B:63:ASN:ND2	1:B:65:GLU:H	2.06	0.54
1:B:82:ARG:HH11	1:B:82:ARG:HG3	1.72	0.54
1:C:264:TYR:CG	1:C:526:ILE:HD12	2.42	0.54
1:B:51:GLU:O	1:B:54:VAL:HG12	2.07	0.54
1:A:531:GLY:HA2	2:A:671:HOH:O	2.07	0.54
1:D:253:ILE:HG13	1:D:294:VAL:HB	1.90	0.54
1:B:259:PRO:HG3	1:B:288:GLY:HA3	1.90	0.54
1:D:421:ARG:HD2	1:D:446:SER:HB2	1.90	0.54
1:B:349:THR:HA	1:B:367:LEU:HD23	1.89	0.54
1:C:424:THR:HA	1:C:571:GLN:NE2	2.20	0.54
1:A:448:GLN:C	1:A:461:ARG:HH12	2.11	0.54
1:B:141:PRO:HG3	1:B:170:LYS:HG2	1.89	0.54
1:D:278:ASN:O	1:D:282:ILE:HG21	2.04	0.54
1:D:317:PHE:O	1:D:391:CYS:HA	2.07	0.54
1:D:571:GLN:O	1:D:574:ASN:HB3	2.08	0.54
1:B:17:ASN:O	1:B:21:LEU:CD1	2.56	0.53
1:B:524:TRP:CE2	1:B:533:VAL:HG11	2.43	0.53
1:D:465:MET:HG3	1:D:478:TYR:CE2	2.43	0.53
1:C:545:LYS:O	1:C:546:ALA:HB3	2.07	0.53
1:D:327:ALA:O	1:D:328:SER:HB3	2.06	0.53
1:B:311:VAL:HG12	1:B:409:GLY:HA2	1.90	0.53
1:B:528:ARG:NH1	1:B:534:GLY:CA	2.71	0.53
1:B:325:ASN:HD22	1:B:327:ALA:H	1.57	0.53
1:D:524:TRP:CZ2	1:D:544:ALA:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:ASP:HB2	1:C:559:GLU:OE2	2.08	0.53
1:D:368:ILE:HG23	1:D:372:GLY:O	2.08	0.53
1:C:256:LEU:CD1	1:C:289:TRP:HE3	2.20	0.53
1:C:254:LEU:HD11	1:C:291:ALA:HB1	1.90	0.53
1:A:540:VAL:HG22	1:A:572:TRP:CZ2	2.42	0.53
1:D:501:TRP:HA	1:D:501:TRP:HE3	1.73	0.53
1:A:550:ASP:C	1:A:551:LEU:HD12	2.28	0.53
1:D:335:THR:O	1:D:396:GLN:HG2	2.09	0.53
1:C:507:ASP:OD1	1:C:507:ASP:C	2.46	0.53
1:D:67:ARG:CG	1:D:67:ARG:HH21	2.22	0.53
1:A:555:ASP:O	2:A:706:HOH:O	2.18	0.53
1:C:487:ASN:C	1:C:489:GLY:H	2.11	0.53
1:D:368:ILE:HD12	2:D:619:HOH:O	2.08	0.53
1:A:221:TYR:C	1:A:221:TYR:CD2	2.82	0.52
1:D:255:LYS:HZ3	1:D:257:ILE:CD1	2.22	0.52
1:C:129:VAL:CG1	1:C:163:MET:HG3	2.39	0.52
1:A:461:ARG:HG2	1:A:461:ARG:O	2.09	0.52
1:D:121:MET:HG2	1:D:149:ASP:HB3	1.92	0.52
1:D:15:THR:OG1	1:D:15:THR:O	2.28	0.52
1:D:34:GLU:CD	1:D:123:GLY:H	2.13	0.52
1:C:83:VAL:HG23	1:C:205:ILE:HD13	1.92	0.52
1:B:255:LYS:HZ2	1:B:263:ALA:HB1	1.74	0.52
1:A:80:VAL:HG13	1:A:80:VAL:O	2.10	0.52
1:D:480:GLN:HA	1:D:591:PRO:HG3	1.91	0.52
1:D:165:ILE:HD12	1:D:165:ILE:N	2.24	0.52
1:B:426:PRO:HB2	1:B:429:THR:HG22	1.91	0.52
1:D:283:THR:OG1	1:D:331:ILE:CD1	2.58	0.52
1:B:62:LEU:HD21	1:B:354:ILE:CD1	2.38	0.52
1:B:71:TYR:CD1	1:B:71:TYR:N	2.77	0.52
1:B:464:PRO:HD2	1:B:468:LEU:HG	1.92	0.52
1:B:289:TRP:CZ2	1:B:523:LYS:HG3	2.45	0.52
1:C:538:THR:OG1	1:C:543:THR:CG2	2.58	0.52
1:C:511:LEU:HD22	1:C:561:VAL:CG1	2.38	0.52
1:D:501:TRP:HA	1:D:501:TRP:CE3	2.45	0.52
1:B:228:ALA:HA	1:B:232:TYR:HB3	1.91	0.52
1:C:252:LEU:O	1:C:267:ALA:HA	2.10	0.52
1:D:46:TRP:CD1	1:D:46:TRP:C	2.83	0.52
1:C:17:ASN:ND2	1:C:20:LEU:H	2.07	0.52
1:C:75:SER:OG	1:C:80:VAL:HG12	2.10	0.52
1:B:191:GLY:O	1:B:192:GLN:HB3	2.10	0.51
1:B:18:LYS:HA	1:B:21:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ALA:HA	1:D:276:LYS:HE3	1.91	0.51
1:D:235:ARG:NH2	1:D:470:PHE:CD2	2.78	0.51
1:B:388:SER:C	1:B:389:ARG:HG2	2.31	0.51
1:D:268:ALA:HA	1:D:416:LEU:O	2.11	0.51
1:C:429:THR:CG2	1:C:543:THR:HB	2.41	0.51
1:B:503:ARG:O	1:B:504:ARG:HG3	2.11	0.51
1:C:467:MET:O	1:C:468:LEU:C	2.47	0.51
1:D:121:MET:SD	1:D:126:MET:HB2	2.50	0.51
1:D:318:PHE:CD2	1:D:389:ARG:HD2	2.44	0.51
1:C:157:MET:HB2	1:C:163:MET:CE	2.41	0.51
1:C:230:LYS:HE2	1:C:470:PHE:CZ	2.46	0.51
1:A:554:LEU:HD22	1:A:554:LEU:O	2.11	0.51
1:B:533:VAL:O	1:B:548:ASP:OD2	2.29	0.51
1:A:537:GLU:OE2	1:A:542:HIS:ND1	2.42	0.51
1:C:25:ALA:O	1:C:28:VAL:HG12	2.10	0.51
1:D:229:LYS:O	1:D:233:ALA:HB3	2.11	0.51
1:B:503:ARG:C	1:B:504:ARG:HG3	2.31	0.51
1:D:254:LEU:O	1:D:265:HIS:HA	2.11	0.51
1:A:204:TYR:C	1:A:205:ILE:HD12	2.31	0.51
1:A:95:GLU:OE2	1:A:589:ARG:NH2	2.39	0.51
1:B:315:ASN:O	1:B:394:ILE:HG22	2.10	0.51
1:B:530:GLU:OE1	1:B:530:GLU:HA	2.11	0.51
1:A:77:PRO:HG3	1:A:371:MET:HE3	1.91	0.51
1:B:122:LYS:C	1:B:122:LYS:HD3	2.31	0.51
1:A:23:TRP:CZ2	1:A:179:ARG:HB3	2.46	0.50
1:A:108:ALA:HB2	1:C:108:ALA:CB	2.41	0.50
1:D:266:ILE:HD13	1:D:522:LEU:HD12	1.92	0.50
1:C:211:THR:O	1:C:211:THR:OG1	2.29	0.50
1:A:525:VAL:O	1:A:529:ILE:HG12	2.10	0.50
1:A:258:ASN:OD1	1:A:258:ASN:C	2.49	0.50
1:D:604:ARG:HD2	2:D:658:HOH:O	2.11	0.50
1:A:100:THR:HB	1:A:468:LEU:CD2	2.42	0.50
1:D:570:GLU:O	1:D:574:ASN:HB2	2.11	0.50
1:B:106:PRO:O	1:B:110:LYS:HG3	2.12	0.50
1:A:429:THR:HB	1:A:543:THR:CB	2.35	0.50
1:A:221:TYR:HB3	2:A:694:HOH:O	2.11	0.50
1:B:468:LEU:N	1:B:469:PRO:CD	2.74	0.50
1:A:272:SER:OG	1:A:420:ARG:NH2	2.43	0.50
1:A:285:THR:HG21	1:A:517:ASP:OD1	2.12	0.50
1:D:246:TRP:HB2	1:D:301:LEU:O	2.12	0.50
1:A:274:CYS:HA	1:A:277:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ASP:C	1:C:371:MET:H	2.16	0.50
1:B:275:GLY:H	1:B:278:ASN:ND2	2.07	0.50
1:A:523:LYS:HE3	1:A:551:LEU:HD11	1.94	0.49
1:A:280:ALA:HB1	1:A:293:VAL:HG23	1.93	0.49
1:D:67:ARG:HH22	1:D:354:ILE:CD1	2.24	0.49
1:B:507:ASP:OD2	1:B:509:ARG:HB3	2.11	0.49
1:B:382:ASN:HB3	1:B:384:ALA:O	2.12	0.49
1:B:64:GLU:HG3	1:B:64:GLU:O	2.12	0.49
1:B:136:ILE:HG21	1:B:166:GLU:HG3	1.92	0.49
1:C:167:ALA:O	1:C:171:ILE:HG23	2.11	0.49
1:D:278:ASN:ND2	1:D:328:SER:O	2.45	0.49
1:A:563:GLU:O	1:A:566:THR:CG2	2.58	0.49
1:C:407:TRP:CE3	1:C:407:TRP:N	2.70	0.49
1:D:430:GLN:HG3	1:D:497:PHE:CZ	2.46	0.49
1:D:17:ASN:ND2	1:D:18:LYS:N	2.56	0.49
1:D:189:GLU:H	1:D:192:GLN:HE21	1.61	0.49
1:B:82:ARG:HH11	1:B:82:ARG:CG	2.26	0.49
1:C:305:GLU:HB2	2:C:640:HOH:O	2.11	0.49
1:C:211:THR:OG1	1:C:213:GLU:CG	2.58	0.49
1:A:427:LEU:HB3	1:A:565:LEU:CD2	2.42	0.49
1:B:285:THR:HG23	1:B:285:THR:O	2.13	0.49
1:B:366:HIS:O	1:B:367:LEU:HG	2.12	0.49
1:C:424:THR:H	1:C:571:GLN:HE22	1.60	0.49
1:C:316:GLY:HA2	1:C:394:ILE:HG13	1.95	0.49
1:A:538:THR:OG1	1:A:543:THR:CG2	2.61	0.49
1:B:258:ASN:O	1:B:259:PRO:C	2.50	0.49
1:A:253:ILE:CG2	1:A:294:VAL:HB	2.43	0.49
1:A:307:GLY:HA2	1:A:492:LYS:HB2	1.94	0.49
1:C:53:LEU:HD12	1:C:155:MET:HE3	1.94	0.48
1:D:205:ILE:CD1	1:D:231:CYS:SG	3.01	0.48
1:B:432:TYR:CZ	1:B:541:GLY:HA2	2.48	0.48
1:A:271:PRO:HB3	1:A:463:ASP:OD2	2.12	0.48
1:A:550:ASP:HB3	1:A:552:ASP:H	1.78	0.48
1:C:142:LYS:HG2	1:C:240:MET:CE	2.43	0.48
1:D:428:VAL:O	1:D:543:THR:HG23	2.12	0.48
1:C:473:TYR:HB2	2:C:616:HOH:O	2.12	0.48
1:A:558:ILE:C	1:A:560:ASP:H	2.14	0.48
1:C:555:ASP:OD2	1:C:559:GLU:HG2	2.12	0.48
1:A:252:LEU:HB2	1:A:280:ALA:HB2	1.95	0.48
1:D:148:THR:HG21	1:D:153:VAL:HG22	1.96	0.48
1:C:429:THR:HB	1:C:543:THR:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:CG1	1:A:385:HIS:CE1	2.96	0.48
1:C:206:THR:CG2	1:C:208:PHE:CZ	2.96	0.48
1:D:403:GLU:O	1:D:404:PHE:C	2.52	0.48
1:C:232:TYR:CG	1:C:236:ILE:HD11	2.48	0.48
1:C:162:ARG:HD2	1:C:162:ARG:H	1.77	0.48
1:C:92:GLU:HG2	1:C:210:GLU:HG3	1.96	0.48
1:C:543:THR:O	1:C:544:ALA:C	2.50	0.48
1:C:546:ALA:HB2	1:C:565:LEU:HD23	1.95	0.48
1:D:434:TRP:CD1	1:D:486:GLY:HA3	2.49	0.48
1:B:43:GLN:NE2	1:B:158:ARG:NH1	2.57	0.48
1:D:572:TRP:O	1:D:576:VAL:HG23	2.14	0.48
1:B:524:TRP:CE2	1:B:533:VAL:CG1	2.96	0.48
1:C:129:VAL:HG13	1:C:163:MET:HG3	1.94	0.48
1:C:339:GLY:O	1:C:396:GLN:NE2	2.34	0.48
1:D:362:ASP:O	1:D:363:ALA:HB3	2.13	0.48
1:D:507:ASP:CG	1:D:509:ARG:NH1	2.67	0.48
1:D:241:ALA:HB1	1:D:246:TRP:O	2.14	0.48
1:A:253:ILE:HG22	1:A:294:VAL:HB	1.95	0.48
1:A:233:ALA:HB1	1:A:298:ILE:HG21	1.95	0.48
1:C:568:PRO:O	1:C:571:GLN:HB2	2.14	0.48
1:D:544:ALA:HB3	1:D:565:LEU:HD11	1.96	0.48
1:D:23:TRP:CZ2	1:D:179:ARG:HB3	2.49	0.48
1:B:362:ASP:O	1:B:363:ALA:HB3	2.14	0.47
1:C:232:TYR:CD2	1:C:236:ILE:HD11	2.48	0.47
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.65	0.47
1:D:68:PRO:O	1:D:69:ASN:C	2.52	0.47
1:B:577:GLU:O	1:B:581:GLU:CG	2.51	0.47
1:D:568:PRO:O	1:D:571:GLN:HB2	2.15	0.47
1:A:79:ASP:HB3	1:A:203:LYS:HE3	1.95	0.47
1:D:195:VAL:HG12	1:D:196:ALA:N	2.28	0.47
1:B:600:ALA:O	1:B:604:ARG:HG3	2.14	0.47
1:C:434:TRP:CD1	1:C:486:GLY:HA3	2.49	0.47
1:B:505:GLY:H	1:B:511:LEU:HD13	1.78	0.47
1:C:157:MET:CB	1:C:163:MET:CE	2.92	0.47
1:D:465:MET:HE2	1:D:479:LEU:HD23	1.95	0.47
1:A:199:CYS:HB2	1:A:218:GLY:O	2.15	0.47
1:A:286:ILE:HA	1:A:287:PRO:HD3	1.67	0.47
1:D:178:VAL:HG21	1:D:232:TYR:CZ	2.49	0.47
1:C:132:CYS:HB2	1:C:143:LEU:HD23	1.97	0.47
1:D:128:VAL:O	1:D:130:PRO:HD3	2.14	0.47
1:A:317:PHE:O	1:A:391:CYS:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:MET:CB	1:C:163:MET:HE2	2.45	0.47
1:D:135:PRO:HG2	1:D:407:TRP:HA	1.97	0.47
1:A:138:ASP:O	1:A:141:PRO:HG3	2.15	0.47
1:C:247:MET:CE	1:C:301:LEU:HB2	2.45	0.47
1:C:416:LEU:HD12	1:C:497:PHE:HB2	1.97	0.47
1:D:67:ARG:CG	1:D:67:ARG:NH2	2.75	0.47
1:B:436:HIS:HE1	1:B:540:VAL:O	1.98	0.47
1:B:514:GLY:O	1:B:517:ASP:HB2	2.14	0.47
1:A:271:PRO:HD2	1:A:418:GLY:O	2.15	0.47
1:A:262:LYS:NZ	2:A:709:HOH:O	2.48	0.47
1:A:426:PRO:HG3	1:A:567:ALA:HB2	1.95	0.47
1:B:317:PHE:O	1:B:391:CYS:HA	2.15	0.47
1:C:427:LEU:HA	1:C:500:ASN:O	2.14	0.47
1:B:365:ALA:HA	1:B:377:PRO:HD3	1.96	0.47
1:C:20:LEU:CD2	1:C:24:ILE:CD1	2.92	0.47
1:B:179:ARG:CD	2:B:623:HOH:O	2.57	0.47
1:B:62:LEU:HD11	1:B:354:ILE:HD13	1.96	0.47
1:B:34:GLU:HG2	1:B:123:GLY:N	2.26	0.47
1:D:194:ASP:OD2	1:D:195:VAL:N	2.42	0.47
1:C:471:ILE:HG22	1:C:473:TYR:H	1.80	0.47
1:A:148:THR:HA	1:A:182:HIS:O	2.14	0.47
1:B:562:LYS:HD2	1:B:562:LYS:HA	1.47	0.47
1:A:550:ASP:C	1:A:551:LEU:CD1	2.82	0.47
1:B:524:TRP:HE1	1:B:533:VAL:HG13	1.80	0.47
1:B:468:LEU:CB	1:B:469:PRO:HD3	2.45	0.47
1:B:251:MET:HA	1:B:268:ALA:O	2.15	0.47
1:B:16:LYS:HE2	1:B:16:LYS:HB2	1.40	0.47
1:C:253:ILE:HB	1:C:294:VAL:HB	1.97	0.46
1:B:505:GLY:N	1:B:511:LEU:HD13	2.30	0.46
1:C:513:PRO:HG3	1:C:554:LEU:HD22	1.97	0.46
1:D:34:GLU:HG2	1:D:124:ARG:N	2.31	0.46
1:C:31:PHE:HE2	1:C:117:TYR:CD2	2.32	0.46
1:B:122:LYS:HD3	1:B:123:GLY:N	2.30	0.46
1:B:110:LYS:HG2	1:B:208:PHE:CZ	2.51	0.46
1:C:251:MET:HB2	1:C:299:ALA:HB3	1.97	0.46
1:B:292:GLN:HA	1:B:399:ALA:O	2.15	0.46
1:B:122:LYS:CD	1:B:188:LEU:O	2.63	0.46
1:B:335:THR:HG23	1:B:397:SER:HA	1.97	0.46
1:D:122:LYS:HB2	1:D:122:LYS:HE2	1.70	0.46
1:B:113:MET:SD	1:B:206:THR:HG23	2.55	0.46
1:A:94:GLU:HG2	1:C:204:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ARG:HG2	1:A:502:PHE:CD1	2.51	0.46
1:C:279:LEU:HD11	1:C:522:LEU:HD11	1.98	0.46
1:B:461:ARG:HD2	1:B:461:ARG:HA	1.85	0.46
1:B:83:VAL:HG21	1:B:203:LYS:HD3	1.97	0.46
1:D:284:PRO:HB3	1:D:519:SER:CB	2.46	0.46
1:C:180:CYS:HB3	1:C:227:LEU:HD12	1.97	0.46
1:C:210:GLU:CG	2:C:620:HOH:O	2.52	0.46
1:D:43:GLN:NE2	1:D:158:ARG:HH12	2.11	0.46
1:A:116:HIS:CE1	1:A:202:THR:HG21	2.50	0.46
1:C:162:ARG:N	1:C:162:ARG:HD2	2.29	0.46
1:A:136:ILE:CD1	1:A:166:GLU:HB3	2.46	0.46
1:C:25:ALA:O	1:C:28:VAL:CG1	2.64	0.46
1:C:430:GLN:NE2	1:C:528:ARG:NE	2.61	0.46
1:C:53:LEU:CD1	1:C:155:MET:CE	2.93	0.46
1:C:132:CYS:HB2	1:C:143:LEU:CD2	2.46	0.46
1:D:71:TYR:HE2	2:D:643:HOH:O	1.72	0.46
1:C:429:THR:CB	1:C:543:THR:HB	2.44	0.46
1:C:255:LYS:HD2	1:C:265:HIS:HE1	1.80	0.46
1:C:83:VAL:CG2	1:C:205:ILE:CD1	2.94	0.46
1:D:134:GLY:O	1:D:135:PRO:C	2.53	0.46
1:D:89:ILE:HG22	1:D:89:ILE:O	2.15	0.46
1:D:49:MET:C	1:D:155:MET:HE2	2.35	0.45
1:A:272:SER:HB3	1:A:273:ALA:H	1.60	0.45
1:A:206:THR:CG2	1:A:208:PHE:CZ	2.99	0.45
1:B:86:ARG:HE	1:D:94:GLU:CG	2.28	0.45
1:C:274:CYS:HA	1:C:277:THR:HB	1.97	0.45
1:C:15:THR:HG21	1:C:20:LEU:HD13	1.97	0.45
1:C:341:THR:HG22	1:C:392:VAL:CB	2.38	0.45
1:D:326:TYR:O	1:D:330:PRO:HD3	2.15	0.45
1:D:230:LYS:HD3	1:D:230:LYS:HA	1.73	0.45
1:B:416:LEU:HD22	1:B:497:PHE:HB2	1.99	0.45
1:D:63:ASN:O	1:D:65:GLU:N	2.49	0.45
1:D:251:MET:HE1	1:D:415:ILE:HD13	1.99	0.45
1:A:417:PHE:HZ	1:A:482:TRP:CH2	2.34	0.45
1:C:322:PRO:HD3	1:C:388:SER:OG	2.17	0.45
1:C:531:GLY:C	1:C:533:VAL:H	2.10	0.45
1:C:255:LYS:HB2	1:C:265:HIS:CE1	2.51	0.45
1:D:416:LEU:HD11	1:D:522:LEU:CD1	2.46	0.45
1:D:362:ASP:O	1:D:363:ALA:CB	2.64	0.45
1:C:130:PRO:HG2	1:C:168:LEU:HG	1.99	0.45
1:D:327:ALA:O	1:D:328:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ILE:HB	1:B:290:THR:HG22	1.99	0.45
1:D:528:ARG:HD2	1:D:533:VAL:HG23	1.98	0.45
1:D:465:MET:HE1	1:D:479:LEU:HD23	1.98	0.45
1:A:540:VAL:CG2	1:A:572:TRP:CZ2	3.00	0.45
1:B:286:ILE:CG2	1:B:289:TRP:HD1	2.29	0.45
1:C:369:ASP:O	1:C:371:MET:N	2.50	0.45
1:B:88:PHE:HB2	1:B:206:THR:HB	1.98	0.45
1:A:124:ARG:NH2	1:A:194:ASP:OD2	2.49	0.45
1:C:404:PHE:C	1:C:404:PHE:CD1	2.89	0.45
1:C:212:LYS:HE2	1:C:240:MET:HG2	1.98	0.45
1:B:188:LEU:HD11	1:B:194:ASP:OD1	2.17	0.45
1:C:232:TYR:HA	1:C:236:ILE:HG13	1.99	0.45
1:D:31:PHE:HE1	1:D:181:LEU:HD12	1.80	0.45
1:A:424:THR:H	1:A:571:GLN:NE2	2.14	0.45
1:A:255:LYS:HD2	1:A:403:GLU:OE2	2.16	0.45
1:A:520:ARG:HE	1:A:554:LEU:HD23	1.81	0.45
1:C:39:VAL:HG22	1:C:129:VAL:HA	1.99	0.45
1:B:513:PRO:HG2	1:B:554:LEU:HD21	1.97	0.45
1:C:216:SER:HB2	1:C:227:LEU:HD21	1.99	0.45
1:B:257:ILE:HB	1:B:290:THR:CG2	2.47	0.45
1:C:67:ARG:HD3	1:C:353:ASP:OD2	2.17	0.45
1:D:298:ILE:O	2:D:637:HOH:O	2.21	0.45
1:A:554:LEU:HD13	1:A:557:PRO:HG2	1.99	0.44
1:A:509:ARG:HD3	1:A:509:ARG:O	2.17	0.44
1:B:431:THR:HB	1:B:436:HIS:ND1	2.32	0.44
1:B:34:GLU:HG3	1:B:123:GLY:CA	2.46	0.44
1:A:255:LYS:CE	1:A:403:GLU:OE2	2.63	0.44
1:D:524:TRP:CZ3	1:D:528:ARG:HG3	2.53	0.44
1:D:559:GLU:C	1:D:561:VAL:H	2.20	0.44
1:B:286:ILE:HG21	1:B:289:TRP:CD1	2.52	0.44
1:A:404:PHE:C	1:A:404:PHE:CD1	2.91	0.44
1:D:207:GLN:HE21	1:D:207:GLN:HB3	1.29	0.44
1:D:271:PRO:HB3	1:D:463:ASP:OD2	2.17	0.44
1:C:369:ASP:C	1:C:371:MET:N	2.70	0.44
1:D:93:LYS:HB2	1:D:93:LYS:HE2	1.81	0.44
1:C:504:ARG:NH2	1:C:510:PHE:CZ	2.85	0.44
1:C:555:ASP:OD2	1:C:559:GLU:CG	2.66	0.44
1:D:509:ARG:HG3	1:D:510:PHE:H	1.81	0.44
1:C:142:LYS:HG2	1:C:240:MET:HE1	2.00	0.44
1:C:424:THR:H	1:C:571:GLN:NE2	2.15	0.44
1:D:234:LEU:HD11	1:D:250:HIS:HD2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HA	1:C:168:LEU:HD23	1.77	0.44
1:A:424:THR:H	1:A:571:GLN:HE22	1.65	0.44
1:B:192:GLN:O	1:B:192:GLN:CG	2.65	0.44
1:C:264:TYR:CE1	1:C:526:ILE:HG21	2.53	0.44
1:B:546:ALA:H	1:B:562:LYS:HD3	1.83	0.44
1:B:222:GLY:HA2	1:B:318:PHE:CZ	2.52	0.44
1:D:603:ALA:O	1:D:604:ARG:C	2.56	0.43
1:D:522:LEU:O	1:D:526:ILE:HG23	2.17	0.43
1:C:242:ARG:NH1	1:C:481:ASN:HA	2.32	0.43
1:B:430:GLN:HE22	1:B:528:ARG:HE	1.63	0.43
1:B:286:ILE:CG2	1:B:289:TRP:CD1	3.02	0.43
1:A:124:ARG:NH1	1:A:194:ASP:OD1	2.50	0.43
1:A:424:THR:HA	1:A:571:GLN:HE21	1.83	0.43
1:D:334:LYS:O	1:D:337:GLU:HB2	2.18	0.43
1:D:257:ILE:HB	1:D:290:THR:HG22	1.99	0.43
1:B:107:GLN:CD	1:B:107:GLN:H	2.21	0.43
1:D:200:ASN:OD1	1:D:202:THR:N	2.43	0.43
1:D:109:MET:O	1:D:110:LYS:C	2.56	0.43
1:A:209:PRO:HB3	1:A:239:VAL:HG21	2.00	0.43
1:A:207:GLN:NE2	1:A:231:CYS:SG	2.91	0.43
1:B:104:ALA:HB3	1:B:109:MET:HG3	2.00	0.43
1:C:135:PRO:HB3	1:C:405:ASN:O	2.18	0.43
1:D:252:LEU:HB2	1:D:280:ALA:HB2	2.00	0.43
1:A:77:PRO:CG	1:A:371:MET:CE	2.96	0.43
1:D:501:TRP:CA	1:D:501:TRP:CE3	3.01	0.43
1:B:286:ILE:HD13	1:B:286:ILE:HG21	1.72	0.43
1:C:389:ARG:HH11	1:C:389:ARG:HD2	1.65	0.43
1:D:53:LEU:HD12	1:D:155:MET:HE3	1.97	0.43
1:D:426:PRO:HG2	1:D:429:THR:HG21	2.00	0.43
1:B:136:ILE:HG13	1:B:136:ILE:H	1.66	0.43
1:A:250:HIS:ND1	1:A:466:ALA:O	2.46	0.43
1:C:420:ARG:HG2	1:C:420:ARG:H	1.51	0.43
1:C:301:LEU:HA	1:C:309:TYR:O	2.19	0.43
1:C:31:PHE:CE2	1:C:117:TYR:CD2	3.06	0.43
1:C:250:HIS:HD2	1:C:466:ALA:O	2.01	0.43
1:B:125:THR:HG22	1:B:126:MET:N	2.34	0.43
1:D:416:LEU:HD23	1:D:497:PHE:HB2	2.00	0.43
1:A:80:VAL:HG11	1:A:385:HIS:CD2	2.54	0.43
1:B:403:GLU:HG3	1:B:410:VAL:CG1	2.49	0.43
1:D:141:PRO:O	1:D:142:LYS:HB2	2.18	0.43
1:B:272:SER:OG	1:B:274:CYS:O	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASN:HD22	1:B:76:ASN:HA	1.66	0.43
1:C:113:MET:HE2	1:C:206:THR:OG1	2.19	0.43
1:D:69:ASN:HA	2:D:643:HOH:O	2.18	0.43
1:B:506:GLU:H	1:B:506:GLU:CD	2.21	0.43
1:C:513:PRO:HG3	1:C:554:LEU:CD2	2.49	0.43
1:D:524:TRP:CH2	1:D:528:ARG:HG3	2.54	0.43
1:C:505:GLY:O	1:C:508:GLY:N	2.49	0.43
1:A:74:ARG:HD2	1:A:370:TRP:O	2.18	0.43
1:B:280:ALA:O	1:B:293:VAL:HG22	2.19	0.43
1:C:17:ASN:HB2	1:C:172:GLY:O	2.19	0.43
1:D:429:THR:HG22	1:D:543:THR:HG23	2.00	0.43
1:D:464:PRO:CD	1:D:468:LEU:HD13	2.47	0.43
1:D:528:ARG:HG2	1:D:533:VAL:HG23	2.00	0.43
1:B:326:TYR:O	1:B:330:PRO:HG3	2.19	0.43
1:D:17:ASN:CB	1:D:20:LEU:HB2	2.46	0.42
1:C:431:THR:HG21	1:C:437:GLY:CA	2.49	0.42
1:A:77:PRO:HG3	1:A:371:MET:HE2	2.01	0.42
1:A:280:ALA:O	1:A:293:VAL:HB	2.18	0.42
1:C:316:GLY:CA	1:C:394:ILE:HG13	2.49	0.42
1:A:356:TRP:CD1	1:A:359:MET:HG3	2.54	0.42
1:A:46:TRP:CD1	1:A:46:TRP:C	2.93	0.42
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.83	0.42
1:C:424:THR:N	1:C:571:GLN:NE2	2.67	0.42
1:B:234:LEU:HG	1:B:298:ILE:HD12	2.01	0.42
1:A:229:LYS:HB2	1:A:229:LYS:HE2	1.45	0.42
1:A:557:PRO:HA	1:A:558:ILE:HD12	2.00	0.42
1:B:512:TRP:HA	1:B:513:PRO:HD3	1.88	0.42
1:C:75:SER:N	1:C:345:ASN:OD1	2.44	0.42
1:D:177:PHE:CE1	1:D:179:ARG:HG2	2.54	0.42
1:D:316:GLY:HA2	1:D:394:ILE:HG13	2.02	0.42
1:B:230:LYS:HD2	1:B:470:PHE:CE2	2.54	0.42
1:D:234:LEU:HD13	1:D:470:PHE:HB2	2.00	0.42
1:C:178:VAL:HG21	1:C:236:ILE:CD1	2.50	0.42
1:B:82:ARG:NH1	1:B:82:ARG:CG	2.80	0.42
1:C:87:THR:HA	1:C:205:ILE:O	2.20	0.42
1:C:178:VAL:HG11	1:C:236:ILE:HD13	2.02	0.42
1:C:423:ASP:OD2	1:C:448:GLN:C	2.57	0.42
1:B:45:GLU:O	1:B:49:MET:HG3	2.20	0.42
1:D:421:ARG:NH2	1:D:424:THR:OG1	2.53	0.42
1:B:178:VAL:HG22	1:B:212:LYS:HB3	2.02	0.42
1:A:397:SER:HB3	1:A:400:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:THR:HG23	1:D:460:LEU:H	1.83	0.42
1:B:554:LEU:HD22	1:B:556:THR:HB	2.02	0.42
1:A:535:ALA:H	1:A:545:LYS:HE2	1.84	0.42
1:B:279:LEU:HD11	1:B:522:LEU:HD11	2.02	0.42
1:B:582:TYR:O	1:B:585:PHE:HB3	2.19	0.42
1:D:67:ARG:HA	1:D:67:ARG:HD2	1.60	0.42
1:D:473:TYR:OH	1:D:478:TYR:HA	2.19	0.42
1:A:202:THR:CG2	1:A:204:TYR:CE2	3.03	0.42
1:D:75:SER:HA	1:D:197:TRP:CD2	2.54	0.42
1:C:113:MET:CE	1:C:206:THR:OG1	2.67	0.42
1:D:189:GLU:O	1:D:191:GLY:N	2.53	0.42
1:D:401:ALA:O	1:D:404:PHE:HD1	2.03	0.42
1:B:301:LEU:HA	1:B:309:TYR:O	2.20	0.42
1:A:553:GLY:C	1:A:555:ASP:N	2.73	0.41
1:A:509:ARG:HD3	1:A:509:ARG:C	2.41	0.41
1:D:256:LEU:HD12	1:D:289:TRP:HE3	1.85	0.41
1:B:335:THR:HG23	1:B:397:SER:CA	2.50	0.41
1:A:45:GLU:O	1:A:49:MET:HG3	2.20	0.41
1:B:310:ALA:HB3	1:B:412:ILE:HD11	2.02	0.41
1:D:276:LYS:HE2	1:D:297:ASP:OD1	2.19	0.41
1:C:428:VAL:HG13	1:C:544:ALA:HB2	2.00	0.41
1:C:255:LYS:HD2	1:C:403:GLU:OE2	2.19	0.41
1:C:234:LEU:HB3	1:C:470:PHE:HB3	2.01	0.41
1:C:114:SER:HA	1:C:117:TYR:HB2	2.01	0.41
1:D:93:LYS:HB3	1:D:95:GLU:OE1	2.20	0.41
1:D:61:LYS:HE3	1:D:64:GLU:OE2	2.20	0.41
1:C:277:THR:HG23	1:C:281:MET:CE	2.50	0.41
1:B:506:GLU:C	1:B:508:GLY:N	2.57	0.41
1:B:82:ARG:CZ	1:B:82:ARG:CB	2.99	0.41
1:C:43:GLN:OE1	1:C:158:ARG:NH2	2.54	0.41
1:C:441:GLY:O	1:C:444:LEU:HB2	2.20	0.41
1:B:50:ALA:HB2	1:B:155:MET:HE1	2.02	0.41
1:C:492:LYS:HA	1:C:492:LYS:HD2	1.83	0.41
1:B:62:LEU:HD11	1:B:354:ILE:CD1	2.51	0.41
1:D:528:ARG:HD2	1:D:533:VAL:O	2.19	0.41
1:B:247:MET:HB2	1:B:301:LEU:HB2	2.03	0.41
1:C:524:TRP:CZ2	1:C:544:ALA:HA	2.54	0.41
1:A:82:ARG:HB3	1:A:83:VAL:H	1.44	0.41
1:A:255:LYS:HG3	1:A:265:HIS:CE1	2.55	0.41
1:B:551:LEU:O	1:B:552:ASP:C	2.59	0.41
1:D:554:LEU:HA	1:D:554:LEU:HD23	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.84	0.41
1:A:553:GLY:C	1:A:555:ASP:H	2.24	0.41
1:C:256:LEU:HD22	1:C:291:ALA:HB2	2.03	0.41
1:D:349:THR:CG2	1:D:351:ASP:CG	2.89	0.41
1:D:526:ILE:HG13	1:D:527:ASP:N	2.35	0.41
1:B:232:TYR:CD2	1:B:232:TYR:C	2.93	0.41
1:A:329:ASN:O	1:A:332:ALA:HB3	2.21	0.41
1:D:378:GLU:H	1:D:378:GLU:HG2	1.57	0.41
1:D:319:GLY:O	1:D:389:ARG:HA	2.21	0.41
1:C:212:LYS:NZ	1:C:243:GLU:OE1	2.49	0.41
1:C:528:ARG:HD2	1:C:533:VAL:HG12	2.03	0.41
1:C:286:ILE:HA	1:C:287:PRO:HD3	1.95	0.41
1:D:304:ARG:O	1:D:305:GLU:C	2.59	0.41
1:B:133:MET:HE1	1:B:233:ALA:HB2	2.03	0.41
1:B:131:PHE:CZ	1:B:144:GLY:HA3	2.55	0.41
1:D:549:LEU:HB3	1:D:551:LEU:HD21	2.02	0.41
1:B:557:PRO:O	1:B:559:GLU:N	2.54	0.41
1:B:23:TRP:CZ2	1:B:181:LEU:CD1	3.04	0.41
1:D:366:HIS:NE2	1:D:374:ASP:OD1	2.52	0.41
1:D:485:MET:HB3	1:D:485:MET:HE2	1.56	0.41
1:C:577:GLU:OE1	1:C:581:GLU:OE2	2.39	0.41
1:A:89:ILE:O	1:A:89:ILE:HG13	2.21	0.40
1:C:370:TRP:CZ2	1:C:385:HIS:HD2	2.39	0.40
1:D:63:ASN:C	1:D:65:GLU:H	2.25	0.40
1:B:429:THR:CG2	2:B:619:HOH:O	2.60	0.40
1:D:264:TYR:CE1	1:D:526:ILE:HD13	2.56	0.40
1:C:134:GLY:O	1:C:135:PRO:C	2.60	0.40
1:A:165:ILE:HD12	1:A:168:LEU:HD23	2.03	0.40
1:C:354:ILE:HD13	1:C:356:TRP:CZ3	2.56	0.40
1:C:325:ASN:ND2	1:C:358:GLY:O	2.53	0.40
1:B:304:ARG:HA	1:B:304:ARG:NE	2.31	0.40
1:A:503:ARG:HH22	1:A:566:THR:HG22	1.69	0.40
1:C:430:GLN:HB2	1:C:497:PHE:CE2	2.57	0.40
1:B:166:GLU:HA	1:B:166:GLU:OE2	2.21	0.40
1:A:305:GLU:O	1:A:492:LYS:HE3	2.22	0.40
1:A:283:THR:HA	1:A:284:PRO:HD3	1.92	0.40
1:D:562:LYS:O	1:D:566:THR:HG23	2.20	0.40
1:D:49:MET:HE3	1:D:155:MET:HG2	2.03	0.40
1:C:94:GLU:HG2	1:C:94:GLU:O	2.21	0.40
1:B:275:GLY:N	1:B:278:ASN:HD22	2.11	0.40
1:B:540:VAL:HG22	1:B:572:TRP:CZ2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:TYR:HA	1:C:236:ILE:HG12	2.02	0.40
1:A:448:GLN:C	1:A:461:ARG:NH1	2.73	0.40
1:B:66:LYS:HB3	1:B:66:LYS:HE2	1.82	0.40
1:B:221:TYR:O	1:B:224:ASN:HB2	2.21	0.40
1:D:242:ARG:NH2	1:D:481:ASN:HD22	2.10	0.40
1:B:527:ASP:HB3	1:B:533:VAL:CG2	2.51	0.40
1:D:34:GLU:HG2	1:D:124:ARG:H	1.86	0.40
1:A:434:TRP:NE1	1:A:482:TRP:O	2.43	0.40
1:A:424:THR:HA	1:A:571:GLN:NE2	2.36	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	582/610 (95%)	528 (91%)	39 (7%)	15 (3%)	7	4
1	B	580/610 (95%)	523 (90%)	38 (7%)	19 (3%)	5	3
1	C	582/610 (95%)	527 (90%)	42 (7%)	13 (2%)	8	6
1	D	572/610 (94%)	519 (91%)	37 (6%)	16 (3%)	6	4
All	All	2316/2440 (95%)	2097 (90%)	156 (7%)	63 (3%)	6	4

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLU
1	A	273	ALA
1	A	362	ASP
1	A	551	LEU
1	A	556	THR
1	A	559	GLU

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Mol	Chain	Res	Type
1	B	56	ALA
1	B	94	GLU
1	B	305	GLU
1	B	363	ALA
1	B	460	LEU
1	B	506	GLU
1	B	507	ASP
1	C	79	ASP
1	C	488	LYS
1	C	533	VAL
1	C	559	GLU
1	D	17	ASN
1	D	79	ASP
1	D	190	PRO
1	D	192	GLN
1	D	193	GLU
1	D	274	CYS
1	D	328	SER
1	D	362	ASP
1	D	424	THR
1	D	507	ASP
1	A	82	ARG
1	A	395	ASP
1	B	192	GLN
1	B	361	GLY
1	B	362	ASP
1	C	229	LYS
1	C	558	ILE
1	D	552	ASP
1	A	81	ALA
1	A	535	ALA
1	B	17	ASN
1	C	555	ASP
1	C	557	PRO
1	C	560	ASP
1	D	118	ALA
1	D	363	ALA
1	A	363	ALA
1	B	57	GLY
1	B	63	ASN
1	B	190	PRO
1	B	350	ASP

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Mol	Chain	Res	Type
1	B	490	GLY
1	B	531	GLY
1	C	351	ASP
1	D	64	GLU
1	D	546	ALA
1	A	118	ALA
1	A	552	ASP
1	B	558	ILE
1	C	162	ARG
1	C	531	GLY
1	C	550	ASP
1	D	18	LYS
1	A	561	VAL
1	B	222	GLY
1	A	77	PRO

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	474/487 (97%)	420 (89%)	54 (11%)	7	7
1	B	471/487 (97%)	408 (87%)	63 (13%)	5	5
1	C	473/487 (97%)	423 (89%)	50 (11%)	8	9
1	D	469/487 (96%)	389 (83%)	80 (17%)	2	2
All	All	1887/1948 (97%)	1640 (87%)	247 (13%)	5	5

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	17	ASN
1	A	18	LYS
1	A	30	LEU
1	A	46	TRP
1	A	74	ARG

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Mol	Chain	Res	Type
1	A	77	PRO
1	A	78	SER
1	A	79	ASP
1	A	89	ILE
1	A	91	SER
1	A	93	LYS
1	A	95	GLU
1	A	109	MET
1	A	136	ILE
1	A	176	SER
1	A	190	PRO
1	A	212	LYS
1	A	213	GLU
1	A	229	LYS
1	A	232	TYR
1	A	260	GLU
1	A	272	SER
1	A	274	CYS
1	A	283	THR
1	A	285	THR
1	A	301	LEU
1	A	303	LEU
1	A	348	LEU
1	A	360	ASP
1	A	362	ASP
1	A	376	THR
1	A	379	SER
1	A	404	PHE
1	A	429	THR
1	A	446	SER
1	A	460	LEU
1	A	461	ARG
1	A	468	LEU
1	A	488	LYS
1	A	492	LYS
1	A	509	ARG
1	A	537	GLU
1	A	543	THR
1	A	547	GLU
1	A	550	ASP
1	A	554	LEU
1	A	558	ILE

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Mol	Chain	Res	Type
1	A	559	GLU
1	A	562	LYS
1	A	563	GLU
1	A	570	GLU
1	A	574	ASN
1	A	606	SER
1	B	19	GLU
1	B	20	LEU
1	B	21	LEU
1	B	24	ILE
1	B	29	GLU
1	B	30	LEU
1	B	39	VAL
1	B	55	GLU
1	B	62	LEU
1	B	63	ASN
1	B	65	GLU
1	B	67	ARG
1	B	76	ASN
1	B	83	VAL
1	B	92	GLU
1	B	107	GLN
1	B	122	LYS
1	B	148	THR
1	B	152	TYR
1	B	166	GLU
1	B	168	LEU
1	B	176	SER
1	B	181	LEU
1	B	192	GLN
1	B	203	LYS
1	B	206	THR
1	B	227	LEU
1	B	229	LYS
1	B	232	TYR
1	B	242	ARG
1	B	257	ILE
1	B	276	LYS
1	B	298	ILE
1	B	303	LEU
1	B	304	ARG
1	B	348	LEU

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Mol	Chain	Res	Type
1	B	354	ILE
1	B	362	ASP
1	B	368	ILE
1	B	378	GLU
1	B	394	ILE
1	B	420	ARG
1	B	429	THR
1	B	431	THR
1	B	435	GLU
1	B	439	MET
1	B	461	ARG
1	B	465	MET
1	B	468	LEU
1	B	491	ASP
1	B	493	MET
1	B	503	ARG
1	B	506	GLU
1	B	532	HIS
1	B	533	VAL
1	B	545	LYS
1	B	547	GLU
1	B	551	LEU
1	B	554	LEU
1	B	556	THR
1	B	562	LYS
1	B	565	LEU
1	B	570	GLU
1	C	16	LYS
1	C	17	ASN
1	C	60	ILE
1	C	62	LEU
1	C	67	ARG
1	C	94	GLU
1	C	113	MET
1	C	125	THR
1	C	132	CYS
1	C	168	LEU
1	C	171	ILE
1	C	179	ARG
1	C	181	LEU
1	C	189	GLU
1	C	193	GLU

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Mol	Chain	Res	Type
1	C	211	THR
1	C	229	LYS
1	C	230	LYS
1	C	232	TYR
1	C	253	ILE
1	C	256	LEU
1	C	282	ILE
1	C	285	THR
1	C	301	LEU
1	C	303	LEU
1	C	305	GLU
1	C	306	ASP
1	C	351	ASP
1	C	359	MET
1	C	376	THR
1	C	404	PHE
1	C	408	GLU
1	C	416	LEU
1	C	420	ARG
1	C	429	THR
1	C	444	LEU
1	C	465	MET
1	C	468	LEU
1	C	528	ARG
1	C	537	GLU
1	C	543	THR
1	C	547	GLU
1	C	548	ASP
1	C	555	ASP
1	C	556	THR
1	C	559	GLU
1	C	562	LYS
1	C	565	LEU
1	C	589	ARG
1	C	606	SER
1	D	15	THR
1	D	16	LYS
1	D	20	LEU
1	D	29	GLU
1	D	34	GLU
1	D	51	GLU
1	D	64	GLU

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Mol	Chain	Res	Type
1	D	67	ARG
1	D	78	SER
1	D	83	VAL
1	D	84	GLU
1	D	107	GLN
1	D	114	SER
1	D	122	LYS
1	D	132	CYS
1	D	136	ILE
1	D	140	ASP
1	D	149	ASP
1	D	163	MET
1	D	165	ILE
1	D	168	LEU
1	D	170	LYS
1	D	190	PRO
1	D	202	THR
1	D	205	ILE
1	D	207	GLN
1	D	212	LYS
1	D	216	SER
1	D	227	LEU
1	D	229	LYS
1	D	232	TYR
1	D	244	GLU
1	D	253	ILE
1	D	254	LEU
1	D	256	LEU
1	D	262	LYS
1	D	272	SER
1	D	274	CYS
1	D	281	MET
1	D	282	ILE
1	D	290	THR
1	D	301	LEU
1	D	302	LYS
1	D	305	GLU
1	D	331	ILE
1	D	342	LEU
1	D	349	THR
1	D	351	ASP
1	D	360	ASP

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Mol	Chain	Res	Type
1	D	362	ASP
1	D	378	GLU
1	D	379	SER
1	D	403	GLU
1	D	420	ARG
1	D	428	VAL
1	D	429	THR
1	D	444	LEU
1	D	446	SER
1	D	461	ARG
1	D	465	MET
1	D	478	TYR
1	D	491	ASP
1	D	495	SER
1	D	504	ARG
1	D	506	GLU
1	D	507	ASP
1	D	509	ARG
1	D	522	LEU
1	D	526	ILE
1	D	529	ILE
1	D	530	GLU
1	D	533	VAL
1	D	547	GLU
1	D	551	LEU
1	D	552	ASP
1	D	555	ASP
1	D	559	GLU
1	D	562	LYS
1	D	565	LEU
1	D	570	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	101	ASN
1	A	102	ASN
1	A	207	GLN
1	A	265	HIS
1	A	480	GLN
1	A	571	GLN

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Mol	Chain	Res	Type
1	B	43	GLN
1	B	63	ASN
1	B	76	ASN
1	B	107	GLN
1	B	146	GLN
1	B	278	ASN
1	B	292	GLN
1	B	325	ASN
1	B	340	ASN
1	B	430	GLN
1	B	481	ASN
1	B	571	GLN
1	C	17	ASN
1	C	101	ASN
1	C	200	ASN
1	C	207	GLN
1	C	250	HIS
1	C	265	HIS
1	C	340	ASN
1	C	366	HIS
1	C	430	GLN
1	C	481	ASN
1	C	571	GLN
1	C	597	GLN
1	D	17	ASN
1	D	43	GLN
1	D	63	ASN
1	D	192	GLN
1	D	207	GLN
1	D	265	HIS
1	D	278	ASN
1	D	480	GLN
1	D	481	ASN
1	D	597	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	586/610 (96%)	-0.25	8 (1%) 78 83	14, 25, 44, 62	0
1	B	584/610 (95%)	-0.00	15 (2%) 59 68	15, 32, 51, 62	0
1	C	586/610 (96%)	-0.08	16 (2%) 58 67	17, 28, 46, 72	0
1	D	578/610 (94%)	0.08	19 (3%) 50 59	23, 35, 54, 74	0
All	All	2334/2440 (95%)	-0.06	58 (2%) 61 70	14, 30, 50, 74	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	557	PRO	7.3
1	D	508	GLY	6.7
1	C	556	THR	6.4
1	D	327	ALA	4.7
1	D	507	ASP	4.3
1	D	509	ARG	4.2
1	A	448	GLN	4.0
1	B	188	LEU	3.8
1	B	459	THR	3.6
1	D	193	GLU	3.6
1	A	191	GLY	3.5
1	D	531	GLY	3.5
1	A	447	GLY	3.3
1	D	555	ASP	3.3
1	B	508	GLY	3.3
1	D	190	PRO	3.1
1	D	173	ALA	3.1
1	C	173	ALA	3.1
1	D	261	GLY	3.0
1	B	498	LEU	3.0
1	C	362	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	499	VAL	2.9
1	C	416	LEU	2.9
1	D	362	ASP	2.9
1	D	305	GLU	2.8
1	C	558	ILE	2.8
1	B	193	GLU	2.8
1	C	361	GLY	2.8
1	A	556	THR	2.7
1	D	521	VAL	2.7
1	D	259	PRO	2.6
1	C	458	GLY	2.5
1	C	273	ALA	2.5
1	B	173	ALA	2.5
1	C	496	ILE	2.4
1	D	505	GLY	2.4
1	A	260	GLU	2.4
1	D	491	ASP	2.4
1	B	272	SER	2.3
1	C	508	GLY	2.3
1	A	190	PRO	2.3
1	C	346	VAL	2.3
1	D	282	ILE	2.3
1	B	378	GLU	2.3
1	A	378	GLU	2.3
1	B	350	ASP	2.2
1	B	55	GLU	2.2
1	B	305	GLU	2.2
1	B	273	ALA	2.2
1	C	18	LYS	2.1
1	C	326	TYR	2.1
1	B	420	ARG	2.1
1	D	510	PHE	2.1
1	C	288	GLY	2.0
1	A	272	SER	2.0
1	C	499	VAL	2.0
1	D	532	HIS	2.0
1	B	274	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.