



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 12:43 PM EDT

PDB ID : 3G05
Title : Crystal structure of N-terminal domain (2-550) of E.coli MnmG
Authors : Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : unknown
Resolution : 3.49 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

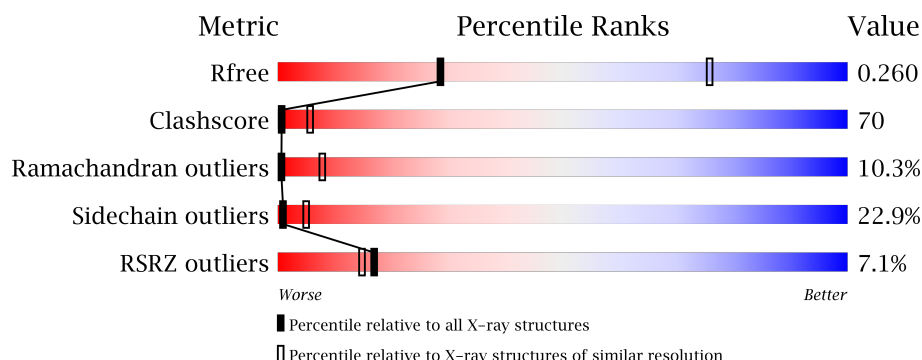
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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	576	<div> <div>5%</div> <div>25%</div> <div>48%</div> <div>16%</div> <div>9%</div> </div>
1	B	576	<div> <div>9%</div> <div>21%</div> <div>48%</div> <div>19%</div> <div>9%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8156 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4073	2551	728	776	18			
1	B	524	Total	C	N	O	S	0	0	0
			4063	2540	730	775	18			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	EXPRESSION TAG	UNP Q8XAY0
A	-26	GLY	-	EXPRESSION TAG	UNP Q8XAY0
A	-25	SER	-	EXPRESSION TAG	UNP Q8XAY0
A	-24	SER	-	EXPRESSION TAG	UNP Q8XAY0
A	-23	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-22	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-21	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-20	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-19	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-18	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-17	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-16	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-15	ASP	-	EXPRESSION TAG	UNP Q8XAY0
A	-14	TYR	-	EXPRESSION TAG	UNP Q8XAY0
A	-13	ASP	-	EXPRESSION TAG	UNP Q8XAY0
A	-12	ILE	-	EXPRESSION TAG	UNP Q8XAY0
A	-11	PRO	-	EXPRESSION TAG	UNP Q8XAY0
A	-10	THR	-	EXPRESSION TAG	UNP Q8XAY0
A	-9	THR	-	EXPRESSION TAG	UNP Q8XAY0
A	-8	GLU	-	EXPRESSION TAG	UNP Q8XAY0
A	-7	ASN	-	EXPRESSION TAG	UNP Q8XAY0
A	-6	LEU	-	EXPRESSION TAG	UNP Q8XAY0
A	-5	TYR	-	EXPRESSION TAG	UNP Q8XAY0
A	-4	PHE	-	EXPRESSION TAG	UNP Q8XAY0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLN	-	EXPRESSION TAG	UNP Q8XAY0
A	-2	GLY	-	EXPRESSION TAG	UNP Q8XAY0
A	-1	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-27	MET	-	EXPRESSION TAG	UNP Q8XAY0
B	-26	GLY	-	EXPRESSION TAG	UNP Q8XAY0
B	-25	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-24	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-23	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-22	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-21	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-20	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-19	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-18	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-17	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-16	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-15	ASP	-	EXPRESSION TAG	UNP Q8XAY0
B	-14	TYR	-	EXPRESSION TAG	UNP Q8XAY0
B	-13	ASP	-	EXPRESSION TAG	UNP Q8XAY0
B	-12	ILE	-	EXPRESSION TAG	UNP Q8XAY0
B	-11	PRO	-	EXPRESSION TAG	UNP Q8XAY0
B	-10	THR	-	EXPRESSION TAG	UNP Q8XAY0
B	-9	THR	-	EXPRESSION TAG	UNP Q8XAY0
B	-8	GLU	-	EXPRESSION TAG	UNP Q8XAY0
B	-7	ASN	-	EXPRESSION TAG	UNP Q8XAY0
B	-6	LEU	-	EXPRESSION TAG	UNP Q8XAY0
B	-5	TYR	-	EXPRESSION TAG	UNP Q8XAY0
B	-4	PHE	-	EXPRESSION TAG	UNP Q8XAY0
B	-3	GLN	-	EXPRESSION TAG	UNP Q8XAY0
B	-2	GLY	-	EXPRESSION TAG	UNP Q8XAY0
B	-1	SER	-	EXPRESSION TAG	UNP Q8XAY0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

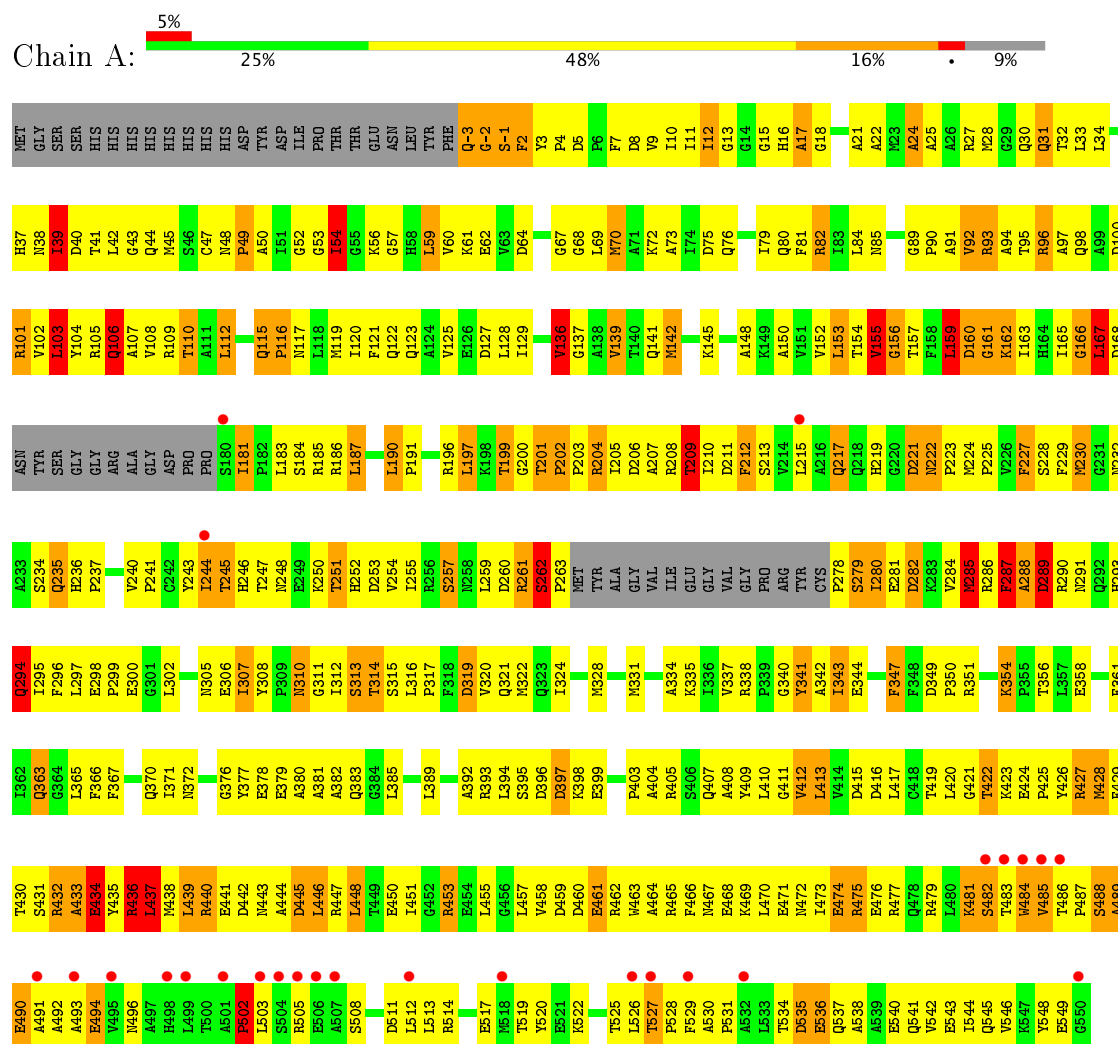


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

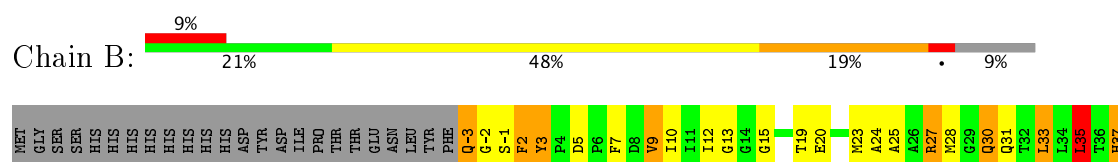
3 Residue-property plots

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

- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG



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T534	I472	L410	F347	F287	V226	H164	I103	I338
D535	I473	G411	F348	A288	F227	I165	Y104	I339
E536	E474	V412	D949	D289	S228	G166	Q106	D40
Q537	R475	L413	P350	R290	F229	LEU	Q105	
A538	E476	V414	R351	N291	N230	ASP	A107	Q44
A539		D415	P355	Q292	G231	ASN	V108	K45
E540	R479	D416	T356	H293	H232	TYR	R109	S46
Q541	L480	L417	T357	Q294	A233	SER	T110	C47
Y542	K481		S234	L295	S234	GLY	A111	N48
E543	S482	L420	S358	F296	Q235	GLY	L112	P49
T544	T483	G421	S359	L297	H236	ARG	E113	A50
Q545	W484	T422	K360	E298	P237	ALA	N114	I51
Y546	V485	K423	F361	P299	Q238	GLY	Q115	
K547	T486	E424	I362	E300	Q239	ASP	P116	
Y548	P487	P425	Q363	G301	V240	PRO	N117	
E549	A488	Y426	G364	L302	P241	PRO	L118	
G550	A489	R427	L365	T303	C242	S180	M119	
	E490	M428	F366	S304	Y243	I181	I120	
	A491	P429	F367	N305	T244	P182	I121	
	A492	T430	A366	E306	T245	L183	Q122	
	A493	S431	G369	I307	H246	S184	Q123	
	E494	R432	Q370	Y308	T247	R185	A124	
	V495	A433	I371	P309	N248	R186	E62	
	N496	E434	N372	N310	E249	L187	V125	
	A497	Y435	G373	G311	K250	R188	E126	
	H498	R436		I312	T251	E189	D127	
	E499	L437	G376	S313	H252	L190	L128	
	T500	M438	Y377	T314	D253	P191	I129	
	A501	L439	E378	S315	V254	L192	V130	
	P502	R440	E379	L316	T255	R193	E131	
	L503	P441	A380	P317	R256	V194	N132	
	S504	D442	A381	F318		G195	D133	
	R505	M443	A382	D319	L259	R196	R134	
	E506	A444	Q383	V320	D260	L197	V135	
	A507	D445	G384	Q321	R261	K198	V136	
	S508	L446	L385	M322	S262	T199	D75	
	G509	R447	L386	Q323	PRO	G200	A138	
	E510	L448	A387	I324	MET	G200	V139	
	D511	T449	G388	V325	TYR	T201	A77	
	L512	E450	L389	R326	ALA	R204	G78	
	L513	I451	N390	S327	GLY	I205	L144	
	R514	G452	A391	M328	VAL	D206	K145	
	R515	R453	A392	Q329	ILE	A207	F146	
	P516	E454	R393	G330	GLU	R208	R147	
	E517	L455	L394	M331	GLY	T209	A148	
	M518	G456	S395	E332	VAL	I210	K149	
	T519	L457	D396	N333	GLY	D211	A150	
	Y520	V458	D397	A334	PRO	F212	V151	
	E521	D459	K398	K335	ARG	S213	V152	
	K522	D460	E399	I336	TYR	V214	V92	
	L523	E461	G400	V337	CYS	L215	L153	
	T524	R462	W401	R338	P278	A216	A93	
	T525	W463	A402	P339	S279	G156	A94	
	L526	P403	P403	G340	I280	Q217	T95	
	T527	F466	A404	Y341	E281	Q218	T157	
	P528	M467	R405	A342	D282	E219	F158	
	F529	E468	S406	I343	K283		A97	
		R469	Q407	E344	V284	N222	I159	
		L470	A408	Y345	M285	P223	D160	
		A532	L533		R286	K224	G161	
						P225	K162	
							I101	
							V102	

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.59Å 144.59Å 271.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.49 49.74 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.49) 99.7 (49.74-3.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.265 0.224 , 0.260	Depositor DCC
R_{free} test set	2137 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	91.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8156	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.84	1/4146 (0.0%)	1.15	20/5615 (0.4%)
1	B	0.75	0/4134	1.11	15/5596 (0.3%)
All	All	0.80	1/8280 (0.0%)	1.13	35/11211 (0.3%)

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	1	7
1	B	0	4
All	All	1	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	ARG	CZ-NH2	24.30	1.64	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	B	290	ARG	N-CA-C	-10.74	82.01	111.00
1	A	505	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	B	100	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	505	ARG	NH1-CZ-NH2	-7.68	110.95	119.40
1	B	101	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	B	112	LEU	CB-CG-CD2	-6.81	99.43	111.00
1	B	385	LEU	CA-CB-CG	-6.75	99.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	THR	CB-CA-C	-6.61	93.74	111.60
1	A	112	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	A	202	PRO	C-N-CD	6.54	142.14	128.40
1	B	402	ALA	C-N-CD	6.41	141.85	128.40
1	A	434	GLU	CB-CA-C	6.38	123.16	110.40
1	B	35	LEU	CA-CB-CG	6.33	129.86	115.30
1	A	103	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	A	314	THR	CB-CA-C	-6.18	94.91	111.60
1	A	197	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	204	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	416	ASP	CB-CG-OD1	-5.94	112.96	118.30
1	A	47	CYS	CA-CB-SG	-5.88	103.42	114.00
1	B	152	VAL	CB-CA-C	-5.78	100.42	111.40
1	A	427	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	75	ASP	CB-CG-OD1	-5.66	113.20	118.30
1	B	376	GLY	N-CA-C	5.54	126.95	113.10
1	A	446	LEU	CA-CB-CG	-5.44	102.78	115.30
1	A	59	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	B	159	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	103	LEU	CA-CB-CG	-5.29	103.13	115.30
1	B	112	LEU	CA-CB-CG	-5.19	103.36	115.30
1	A	197	LEU	N-CA-C	-5.16	97.06	111.00
1	A	101	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	197	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	505	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	436	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	B	155	VAL	CB-CA-C	-5.00	101.90	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	291	ASN	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	SER	Mainchain,Peptide
1	A	159	LEU	Peptide
1	A	261	ARG	Peptide
1	A	287	PHE	Peptide
1	A	288	ALA	Peptide
1	A	289	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	159	LEU	Peptide
1	B	241	PRO	Peptide
1	B	436	ARG	Peptide
1	B	89	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	4073	0	4026	563	0
1	B	4063	0	4029	581	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
All	All	8156	0	8055	1141	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 70.

All (1141) 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:289:ASP:CA	1:A:291:ASN:HA	1.56	1.32
1:B:180:SER:O	1:B:181:ILE:HG22	1.24	1.31
1:B:154:THR:O	1:B:155:VAL:CG1	1.79	1.29
1:A:285:MET:CE	1:A:285:MET:HA	1.59	1.26
1:A:289:ASP:C	1:A:291:ASN:HA	1.56	1.26
1:A:432:ARG:HB2	1:A:436:ARG:NH1	1.52	1.25
1:A:285:MET:CA	1:A:285:MET:HE2	1.67	1.23
1:A:404:ALA:HB3	1:A:407:GLN:CG	1.68	1.23
1:B:12:ILE:O	1:B:154:THR:CG2	1.86	1.22
1:A:204:ARG:NH1	1:A:300:GLU:OE1	1.76	1.18
1:B:139:VAL:HG13	1:B:145:LYS:HG2	1.27	1.17
1:A:156:GLY:O	1:A:157:THR:HG22	1.43	1.16
1:B:154:THR:CG2	1:B:155:VAL:H	1.59	1.15
1:A:13:GLY:O	1:A:154:THR:HG21	1.47	1.15
1:A:262:SER:CB	1:A:263:PRO:HD2	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG21	1:A:328:MET:HE1	1.29	1.14
1:A:314:THR:HG22	1:A:316:LEU:H	1.05	1.14
1:B:12:ILE:O	1:B:154:THR:HG22	0.97	1.14
1:A:404:ALA:HB3	1:A:407:GLN:HG3	1.15	1.13
1:A:209:THR:CG2	1:A:335:LYS:HG3	1.79	1.13
1:A:209:THR:HG21	1:A:335:LYS:CG	1.79	1.12
1:A:314:THR:HG21	1:A:316:LEU:HB2	1.21	1.12
1:B:191:PRO:HB2	1:B:361:PHE:HE1	1.15	1.11
1:B:90:PRO:HB2	1:B:440:ARG:HD2	1.32	1.11
1:A:439:LEU:HD23	1:A:439:LEU:N	1.56	1.11
1:A:448:LEU:HD23	1:A:451:ILE:HD11	1.29	1.10
1:A:163:ILE:HG23	1:A:341:TYR:HD2	1.10	1.10
1:B:154:THR:HG23	1:B:155:VAL:H	0.94	1.09
1:A:285:MET:CA	1:A:285:MET:CE	2.25	1.08
1:A:284:VAL:O	1:A:286:ARG:N	1.85	1.08
1:A:-3:GLN:HG3	1:A:-3:GLN:O	1.46	1.08
1:A:290:ARG:N	1:A:291:ASN:HA	1.62	1.08
1:B:191:PRO:HB2	1:B:361:PHE:CE1	1.89	1.07
1:B:209:THR:OG1	1:B:334:ALA:HA	1.55	1.07
1:A:209:THR:HB	1:A:334:ALA:HA	1.36	1.07
1:B:401:TRP:CZ2	1:B:403:PRO:HB3	1.89	1.07
1:A:262:SER:CB	1:A:263:PRO:CD	2.32	1.06
1:B:461:GLU:HG2	1:B:461:GLU:O	1.54	1.06
1:A:404:ALA:CB	1:A:407:GLN:HG3	1.84	1.06
1:B:230:MET:HE3	1:B:230:MET:HA	1.31	1.06
1:A:289:ASP:CA	1:A:291:ASN:CA	2.33	1.06
1:B:347:PHE:HB2	1:B:371:ILE:O	1.55	1.06
1:B:154:THR:O	1:B:155:VAL:HG12	0.89	1.05
1:B:81:PHE:CE2	1:B:236:HIS:CD2	2.43	1.05
1:A:250:LYS:O	1:A:254:VAL:HG23	1.57	1.05
1:A:440:ARG:HH21	1:A:544:ILE:HG21	1.17	1.04
1:B:154:THR:C	1:B:155:VAL:HG12	1.75	1.04
1:B:154:THR:HG23	1:B:155:VAL:N	1.64	1.04
1:A:314:THR:HG22	1:A:315:SER:N	1.74	1.03
1:A:351:ARG:HD2	1:A:421:GLY:CA	1.88	1.03
1:A:314:THR:HG22	1:A:315:SER:H	1.23	1.03
1:A:45:MET:CE	1:A:49:PRO:HA	1.89	1.03
1:B:45:MET:HG2	1:B:377:TYR:CE2	1.94	1.02
1:B:156:GLY:O	1:B:157:THR:HG23	1.57	1.02
1:B:180:SER:O	1:B:181:ILE:CG2	2.07	1.02
1:A:166:GLY:N	1:A:315:SER:O	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:MET:CE	1:B:230:MET:HA	1.89	1.01
1:A:205:ILE:HG21	1:A:210:ILE:HD11	1.42	1.01
1:B:252:HIS:HD2	1:B:284:VAL:HG11	1.26	1.01
1:A:262:SER:OG	1:A:263:PRO:HD2	1.57	1.01
1:B:155:VAL:HG22	1:B:155:VAL:O	1.56	1.01
1:A:159:LEU:HB3	1:A:160:ASP:HA	1.42	1.00
1:B:210:ILE:HG22	1:B:212:PHE:CD2	1.97	1.00
1:B:209:THR:HG1	1:B:334:ALA:HA	1.19	0.99
1:B:205:ILE:CD1	1:B:336:ILE:HA	1.92	0.99
1:A:81:PHE:HB3	1:A:225:PRO:HG2	1.43	0.99
1:A:163:ILE:CG2	1:A:341:TYR:HD2	1.75	0.98
1:A:108:VAL:O	1:A:112:LEU:HD12	1.63	0.98
1:A:448:LEU:CD2	1:A:451:ILE:HD11	1.92	0.98
1:B:33:LEU:HD21	1:B:35:LEU:HD23	1.43	0.98
1:A:154:THR:O	1:A:155:VAL:HG12	1.62	0.97
1:A:45:MET:HE2	1:A:49:PRO:HA	1.44	0.97
1:A:448:LEU:O	1:A:451:ILE:HG12	1.63	0.97
1:A:163:ILE:HG23	1:A:341:TYR:CD2	1.98	0.96
1:B:394:LEU:HD23	1:B:394:LEU:C	1.83	0.96
1:A:289:ASP:N	1:A:291:ASN:CB	2.28	0.96
1:A:424:GLU:CD	1:A:436:ARG:HH22	1.67	0.96
1:A:166:GLY:HA3	1:A:317:PRO:HG3	1.48	0.96
1:B:191:PRO:CB	1:B:361:PHE:HE1	1.78	0.96
1:B:33:LEU:HD21	1:B:35:LEU:CD2	1.94	0.96
1:B:48:ASN:HB3	1:B:308:TYR:CE2	1.99	0.96
1:B:13:GLY:HA3	1:B:154:THR:CG2	1.96	0.96
1:A:338:ARG:HH21	1:B:39:ILE:HB	1.30	0.95
1:A:443:ASN:OD1	1:A:447:ARG:HD3	1.66	0.95
1:A:314:THR:HG22	1:A:316:LEU:N	1.80	0.95
1:A:285:MET:CE	1:A:285:MET:N	2.29	0.94
1:B:78:GLY:HA2	1:B:98:GLN:O	1.67	0.94
1:B:90:PRO:O	1:B:92:VAL:N	2.00	0.94
1:B:250:LYS:O	1:B:254:VAL:HG23	1.67	0.94
1:A:247:THR:HG22	1:A:293:HIS:H	1.29	0.94
1:A:424:GLU:OE2	1:A:436:ARG:NH2	2.01	0.94
1:A:289:ASP:N	1:A:291:ASN:HA	1.83	0.93
1:B:13:GLY:HA3	1:B:154:THR:HG21	1.47	0.93
1:B:314:THR:HG23	1:B:316:LEU:HB2	1.49	0.92
1:B:431:SER:O	1:B:433:ALA:N	2.00	0.92
1:B:31:GLN:HA	1:B:31:GLN:NE2	1.81	0.92
1:A:155:VAL:CG1	1:A:156:GLY:N	2.29	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:O	1:A:213:SER:N	2.03	0.92
1:B:139:VAL:HG13	1:B:145:LYS:CG	1.99	0.92
1:B:314:THR:CG2	1:B:316:LEU:HB2	1.99	0.92
1:B:210:ILE:CG2	1:B:212:PHE:CE2	2.51	0.92
1:A:439:LEU:N	1:A:439:LEU:CD2	2.33	0.92
1:A:314:THR:CG2	1:A:316:LEU:HB2	2.01	0.91
1:A:203:PRO:HB3	1:A:340:GLY:H	1.34	0.91
1:A:285:MET:HA	1:A:285:MET:HE2	0.93	0.91
1:A:437:LEU:HD12	1:A:437:LEU:O	1.70	0.91
1:A:155:VAL:HG13	1:A:156:GLY:N	1.86	0.90
1:A:320:VAL:O	1:A:324:ILE:HG13	1.71	0.90
1:A:101:ARG:NH1	1:A:300:GLU:OE2	2.04	0.90
1:A:285:MET:HE3	1:A:285:MET:N	1.86	0.90
1:B:217:GLN:NE2	1:B:219:HIS:NE2	2.20	0.90
1:B:79:ILE:HA	1:B:239:GLN:NE2	1.86	0.90
1:B:210:ILE:CG2	1:B:212:PHE:HE2	1.84	0.89
1:A:347:PHE:CG	1:A:347:PHE:O	2.25	0.89
1:B:160:ASP:CG	1:B:161:GLY:H	1.73	0.89
1:A:314:THR:CG2	1:A:316:LEU:H	1.86	0.89
1:B:101:ARG:HH12	1:B:300:GLU:CD	1.75	0.89
1:B:321:GLN:O	1:B:325:VAL:HG23	1.72	0.89
1:A:530:ALA:HB1	1:A:531:PRO:HA	1.54	0.89
1:B:427:ARG:HH21	1:B:428:MET:HE1	1.37	0.89
1:B:252:HIS:HD2	1:B:284:VAL:CG1	1.86	0.89
1:B:386:LEU:HD12	1:B:389:LEU:HD23	1.54	0.88
1:A:289:ASP:HA	1:A:291:ASN:CA	2.02	0.88
1:B:2:PHE:O	1:B:3:TYR:C	2.11	0.88
1:A:432:ARG:CB	1:A:436:ARG:NH1	2.34	0.88
1:A:351:ARG:HD2	1:A:421:GLY:N	1.89	0.86
1:A:289:ASP:C	1:A:291:ASN:CA	2.44	0.86
1:A:8:ASP:OD2	1:A:31:GLN:N	2.08	0.86
1:A:156:GLY:HA3	2:A:551:SO4:O4	1.74	0.86
1:B:201:THR:HG22	1:B:341:TYR:O	1.75	0.86
1:B:79:ILE:O	1:B:80:GLN:HB3	1.71	0.86
1:B:45:MET:HE3	1:B:104:TYR:CD1	2.10	0.86
1:B:469:LYS:O	1:B:473:ILE:HG13	1.76	0.86
1:B:518:MET:SD	1:B:523:LEU:HB2	2.15	0.86
1:B:127:ASP:HA	1:B:183:LEU:HB2	1.56	0.86
1:B:417:LEU:O	1:B:421:GLY:HA2	1.74	0.86
1:B:3:TYR:HD2	1:B:5:ASP:H	1.22	0.86
1:B:158:PHE:O	1:B:159:LEU:C	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PHE:N	1:B:361:PHE:CD2	2.40	0.85
1:A:288:ALA:O	1:A:291:ASN:CB	2.25	0.85
1:B:81:PHE:HB3	1:B:225:PRO:HG2	1.58	0.84
1:B:222:ASN:HD22	1:B:223:PRO:HA	1.40	0.84
1:A:284:VAL:C	1:A:286:ARG:H	1.79	0.84
1:B:476:GLU:HG3	1:B:476:GLU:O	1.75	0.84
1:A:139:VAL:HG13	1:A:145:LYS:HG2	1.58	0.84
1:A:122:GLN:HG2	1:A:122:GLN:O	1.75	0.84
1:A:163:ILE:CG2	1:A:341:TYR:CD2	2.59	0.84
1:B:361:PHE:N	1:B:361:PHE:HD2	1.71	0.84
1:A:440:ARG:HH21	1:A:544:ILE:CG2	1.90	0.84
1:B:181:ILE:HG23	1:B:184:SER:HB2	1.58	0.84
1:A:351:ARG:HD2	1:A:421:GLY:HA3	1.60	0.84
1:A:253:ASP:O	1:A:257:SER:OG	1.95	0.84
1:A:262:SER:HB2	1:A:263:PRO:HD2	1.57	0.84
1:B:314:THR:HG23	1:B:316:LEU:H	1.42	0.83
1:B:282:ASP:O	1:B:284:VAL:N	2.11	0.83
1:B:256:ARG:HA	1:B:259:LEU:HD12	1.59	0.83
1:B:38:ASN:O	1:B:40:ASP:N	2.12	0.83
1:A:436:ARG:O	1:A:437:LEU:HB2	1.79	0.83
1:B:314:THR:HG23	1:B:316:LEU:N	1.94	0.83
1:A:290:ARG:N	1:A:291:ASN:CA	2.36	0.83
1:A:81:PHE:CB	1:A:225:PRO:HG2	2.07	0.83
1:A:262:SER:OG	1:A:263:PRO:CD	2.25	0.83
1:B:205:ILE:HD11	1:B:336:ILE:HA	1.60	0.83
1:A:289:ASP:HA	1:A:291:ASN:CB	2.10	0.82
1:A:201:THR:HG22	1:A:202:PRO:HD2	1.61	0.82
1:B:13:GLY:CA	1:B:154:THR:HG21	2.10	0.82
1:B:210:ILE:HG22	1:B:212:PHE:CE2	2.13	0.82
1:B:226:VAL:HG21	1:B:232:ASN:HA	1.62	0.82
1:A:159:LEU:HB3	1:A:160:ASP:CA	2.09	0.81
1:A:440:ARG:NH2	1:A:544:ILE:HG21	1.94	0.81
1:A:289:ASP:CA	1:A:291:ASN:CB	2.58	0.81
1:B:541:GLN:HG3	1:B:545:GLN:HE21	1.45	0.81
1:B:427:ARG:HH21	1:B:428:MET:CE	1.93	0.81
1:B:81:PHE:CE2	1:B:236:HIS:HD2	1.93	0.81
1:B:96:ARG:HG2	1:B:96:ARG:O	1.78	0.81
1:B:366:PHE:CE1	1:B:391:ALA:HB2	2.15	0.81
1:B:453:ARG:NH2	1:B:460:ASP:OD1	2.13	0.81
1:B:540:GLU:O	1:B:544:ILE:HG12	1.80	0.81
1:A:234:SER:O	1:A:236:HIS:N	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ARG:HB2	1:A:436:ARG:HH11	1.46	0.81
1:B:210:ILE:HG22	1:B:212:PHE:HD2	1.44	0.80
1:A:527:THR:N	1:A:528:PRO:HD2	1.96	0.80
1:A:453:ARG:HG2	1:A:463:TRP:CE2	2.16	0.80
1:B:100:ASP:HB3	1:B:103:LEU:HB2	1.63	0.80
1:A:154:THR:O	1:A:155:VAL:CG1	2.29	0.80
1:B:37:HIS:C	1:B:37:HIS:ND1	2.36	0.80
1:B:94:ALA:HA	1:B:441:GLU:OE2	1.82	0.79
1:A:289:ASP:N	1:A:291:ASN:CA	2.44	0.79
1:B:156:GLY:O	1:B:157:THR:CG2	2.29	0.79
1:A:372:ASN:HD22	1:A:383:GLN:HE21	1.31	0.78
1:A:382:ALA:HB1	1:A:410:LEU:HD23	1.64	0.78
1:B:541:GLN:HG3	1:B:545:GLN:NE2	1.97	0.78
1:B:210:ILE:HG21	1:B:212:PHE:HE2	1.49	0.78
1:B:79:ILE:O	1:B:80:GLN:CB	2.33	0.77
1:B:158:PHE:O	1:B:158:PHE:CG	2.37	0.77
1:B:209:THR:HG21	1:B:335:LYS:HB2	1.66	0.77
1:B:191:PRO:CG	1:B:361:PHE:CE1	2.67	0.77
1:A:49:PRO:HB3	1:A:101:ARG:NH1	1.99	0.77
1:B:73:ALA:HB1	1:B:104:TYR:CE2	2.18	0.77
1:B:33:LEU:CD2	1:B:35:LEU:HD23	2.15	0.77
1:A:199:THR:O	1:A:343:ILE:HD12	1.85	0.77
1:A:205:ILE:CG2	1:A:210:ILE:HD11	2.14	0.77
1:B:191:PRO:CB	1:B:361:PHE:CE1	2.60	0.77
1:B:7:PHE:O	1:B:148:ALA:HA	1.85	0.77
1:B:287:PHE:O	1:B:288:ALA:CB	2.33	0.77
1:A:139:VAL:CG1	1:A:145:LYS:HG2	2.15	0.76
1:A:156:GLY:O	1:A:157:THR:CG2	2.29	0.76
1:A:473:ILE:HG23	1:A:542:VAL:HG23	1.67	0.76
1:B:247:THR:HG23	1:B:248:ASN:N	2.00	0.76
1:A:439:LEU:HD23	1:A:439:LEU:H	1.46	0.76
1:B:155:VAL:O	1:B:155:VAL:CG2	2.29	0.76
1:B:54:ILE:HD11	1:B:85:ASN:ND2	2.01	0.76
1:A:30:GLN:HA	1:A:30:GLN:NE2	2.01	0.76
1:B:165:ILE:HG22	1:B:341:TYR:HA	1.68	0.76
1:B:45:MET:HG2	1:B:377:TYR:HE2	1.51	0.76
1:A:288:ALA:C	1:A:291:ASN:CB	2.54	0.76
1:B:483:THR:HG22	1:B:529:PHE:HE1	1.51	0.75
1:B:247:THR:HG23	1:B:248:ASN:H	1.50	0.75
1:A:122:GLN:CG	1:A:122:GLN:O	2.33	0.75
1:B:131:GLU:O	1:B:132:ASN:HB2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:THR:O	1:B:357:LEU:HB2	1.87	0.75
1:B:252:HIS:CD2	1:B:284:VAL:HG11	2.16	0.75
1:B:459:ASP:O	1:B:461:GLU:N	2.20	0.75
1:B:476:GLU:O	1:B:476:GLU:CG	2.35	0.75
1:A:347:PHE:O	1:A:347:PHE:CD1	2.39	0.75
1:A:424:GLU:CD	1:A:436:ARG:NH2	2.40	0.75
1:B:197:LEU:HD12	1:B:345:TYR:HB2	1.68	0.74
1:B:511:ASP:OD1	1:B:514:ARG:NH2	2.20	0.74
1:A:96:ARG:HH11	1:A:96:ARG:CG	2.01	0.74
1:A:389:LEU:HD22	1:A:457:LEU:HD11	1.69	0.74
1:B:90:PRO:CB	1:B:440:ARG:HD2	2.14	0.74
1:A:27:ARG:NH2	1:A:67:GLY:C	2.40	0.74
1:A:424:GLU:OE1	1:A:436:ARG:NH2	2.20	0.74
1:A:465:ARG:NH1	1:A:535:ASP:OD2	2.17	0.74
1:B:72:LYS:O	1:B:73:ALA:C	2.25	0.74
1:B:241:PRO:HB2	1:B:243:TYR:HE2	1.52	0.74
1:B:210:ILE:HD13	1:B:331:MET:HE1	1.69	0.74
1:B:461:GLU:CG	1:B:461:GLU:O	2.35	0.74
1:A:262:SER:HB2	1:A:263:PRO:CD	2.15	0.74
1:A:210:ILE:HG22	1:A:212:PHE:CD2	2.23	0.73
1:B:320:VAL:O	1:B:324:ILE:HG13	1.88	0.73
1:B:58:HIS:CE1	1:B:429:PHE:CZ	2.75	0.73
1:A:103:LEU:O	1:A:106:GLN:HB3	1.87	0.73
1:A:389:LEU:HD13	1:A:457:LEU:HD21	1.69	0.73
1:B:416:ASP:O	1:B:420:LEU:HD12	1.88	0.73
1:B:156:GLY:C	1:B:157:THR:CG2	2.57	0.73
1:A:200:GLY:HA2	1:A:342:ALA:HA	1.70	0.73
1:A:13:GLY:HA3	1:A:154:THR:CG2	2.18	0.73
1:A:204:ARG:HB2	1:A:338:ARG:HB2	1.71	0.72
1:A:129:ILE:HG22	1:A:136:VAL:HG13	1.71	0.72
1:A:404:ALA:CB	1:A:407:GLN:CG	2.55	0.72
1:B:20:GLU:HG3	1:B:381:ALA:HB1	1.71	0.72
1:B:389:LEU:HD11	1:B:455:LEU:HD13	1.72	0.72
1:A:289:ASP:C	1:A:291:ASN:O	2.28	0.72
1:A:385:LEU:C	1:A:385:LEU:HD23	2.09	0.72
1:B:27:ARG:HH11	1:B:27:ARG:HG2	1.55	0.72
1:A:28:MET:HE2	1:A:392:ALA:HB1	1.71	0.72
1:B:190:LEU:HD11	1:B:362:ILE:HD11	1.70	0.72
1:B:155:VAL:HG13	1:B:155:VAL:O	1.87	0.72
1:A:440:ARG:NH2	1:A:544:ILE:CG2	2.51	0.72
1:B:431:SER:O	1:B:432:ARG:C	2.27	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:THR:HG22	1:B:529:PHE:CE1	2.25	0.71
1:A:382:ALA:HB1	1:A:410:LEU:CD2	2.20	0.71
1:B:101:ARG:NH1	1:B:300:GLU:CD	2.42	0.71
1:B:24:ALA:HA	1:B:27:ARG:NH1	2.06	0.71
1:A:62:GLU:OE1	1:A:408:ALA:HB1	1.91	0.71
1:B:210:ILE:HG21	1:B:212:PHE:CE2	2.22	0.71
1:B:239:GLN:C	1:B:240:VAL:HG12	2.11	0.71
1:A:413:LEU:HD11	1:A:417:LEU:HD11	1.72	0.71
1:A:432:ARG:HB2	1:A:436:ARG:HH12	1.50	0.71
1:B:292:GLN:HA	1:B:292:GLN:HE21	1.56	0.71
1:B:401:TRP:CH2	1:B:403:PRO:HB3	2.25	0.71
1:A:2:PHE:CD1	1:A:145:LYS:HB2	2.25	0.71
1:B:389:LEU:HD13	1:B:457:LEU:HD11	1.71	0.71
1:B:405:ARG:HG2	1:B:405:ARG:O	1.90	0.71
1:B:191:PRO:HG2	1:B:361:PHE:CE1	2.26	0.70
1:B:155:VAL:HG11	1:B:371:ILE:HB	1.73	0.70
1:A:209:THR:HB	1:A:334:ALA:CA	2.19	0.70
1:B:126:GLU:O	1:B:182:PRO:HG2	1.90	0.70
1:B:127:ASP:HB2	1:B:182:PRO:HG2	1.74	0.70
1:B:159:LEU:HB3	1:B:160:ASP:HA	1.73	0.70
1:B:160:ASP:CG	1:B:161:GLY:N	2.44	0.70
1:B:252:HIS:CD2	1:B:284:VAL:CG1	2.71	0.70
1:B:45:MET:CG	1:B:377:TYR:CE2	2.72	0.70
1:A:203:PRO:HD2	1:A:203:PRO:O	1.90	0.70
1:B:100:ASP:OD2	1:B:103:LEU:HD12	1.92	0.70
1:A:39:ILE:HD12	1:A:122:GLN:HB2	1.73	0.70
1:A:10:ILE:HG12	1:A:33:LEU:HB3	1.74	0.69
1:A:-3:GLN:O	1:A:-2:GLY:C	2.30	0.69
1:A:511:ASP:HA	1:A:514:ARG:HH21	1.57	0.69
1:B:9:VAL:HG21	1:B:25:ALA:HB1	1.72	0.69
1:B:309:PRO:HB2	1:B:312:ILE:HD11	1.74	0.69
1:A:28:MET:HE1	1:A:392:ALA:HB3	1.74	0.69
1:B:78:GLY:CA	1:B:98:GLN:O	2.41	0.69
1:A:468:GLU:O	1:A:472:ASN:HB2	1.92	0.69
1:A:222:ASN:HD22	1:A:223:PRO:HA	1.58	0.69
1:B:470:LEU:O	1:B:473:ILE:N	2.19	0.69
1:A:284:VAL:C	1:A:286:ARG:N	2.41	0.69
1:B:45:MET:CE	1:B:104:TYR:CD1	2.77	0.69
1:B:2:PHE:O	1:B:3:TYR:O	2.10	0.68
1:B:347:PHE:CD1	1:B:373:GLY:HA3	2.29	0.68
1:A:393:ARG:HH21	1:A:399:GLU:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASN:HD22	1:A:383:GLN:NE2	1.91	0.68
1:A:453:ARG:HG2	1:A:463:TRP:CD2	2.29	0.68
1:A:13:GLY:HA3	1:A:154:THR:HG23	1.74	0.68
1:B:394:LEU:CD2	1:B:394:LEU:C	2.61	0.68
1:B:61:LYS:HG3	1:B:441:GLU:HG2	1.75	0.68
1:A:28:MET:CE	1:A:392:ALA:HB3	2.24	0.68
1:A:404:ALA:HB3	1:A:407:GLN:CD	2.13	0.68
1:A:473:ILE:HG23	1:A:542:VAL:CG2	2.24	0.68
1:B:467:ASN:O	1:B:470:LEU:N	2.22	0.68
1:A:102:VAL:HG12	1:A:103:LEU:N	2.09	0.68
1:A:45:MET:HE1	1:A:49:PRO:HA	1.74	0.68
1:B:-3:GLN:C	1:B:-1:SER:H	1.96	0.68
1:A:435:TYR:C	1:A:436:ARG:O	2.30	0.68
1:B:393:ARG:O	1:B:396:ASP:N	2.26	0.68
1:A:154:THR:O	1:A:155:VAL:CB	2.40	0.67
1:B:10:ILE:HB	1:B:151:VAL:HG22	1.77	0.67
1:B:55:GLY:O	1:B:58:HIS:HB2	1.94	0.67
1:A:365:LEU:HG	1:A:367:PHE:HE1	1.59	0.67
1:A:351:ARG:CD	1:A:421:GLY:HA3	2.24	0.67
1:A:13:GLY:C	1:A:154:THR:HG21	2.13	0.67
1:B:205:ILE:HG23	1:B:206:ASP:N	2.09	0.67
1:B:409:TYR:CE2	1:B:429:PHE:HE1	2.13	0.67
1:B:542:VAL:HG12	1:B:543:GLU:N	2.07	0.67
1:A:206:ASP:OD1	1:A:208:ARG:HD3	1.95	0.67
1:A:33:LEU:HD12	1:A:34:LEU:N	2.10	0.67
1:A:408:ALA:HA	1:A:447:ARG:HH21	1.60	0.66
1:B:190:LEU:HB3	1:B:191:PRO:HD2	1.76	0.66
1:A:115:GLN:O	1:A:115:GLN:HG3	1.95	0.66
1:A:48:ASN:HB2	1:A:49:PRO:HD2	1.76	0.66
1:B:451:ILE:O	1:B:455:LEU:HB2	1.96	0.66
1:A:293:HIS:O	1:A:294:GLN:C	2.34	0.66
1:B:109:ARG:O	1:B:111:ALA:N	2.28	0.66
1:B:230:MET:CE	1:B:230:MET:CA	2.71	0.66
1:A:458:VAL:HG13	1:A:462:ARG:HD2	1.78	0.66
1:B:310:ASN:HD22	1:B:311:GLY:N	1.94	0.66
1:A:234:SER:OG	1:A:235:GLN:N	2.29	0.66
1:A:28:MET:HE2	1:A:392:ALA:CB	2.26	0.66
1:B:295:ILE:HD11	1:B:311:GLY:O	1.96	0.66
1:A:165:ILE:C	1:A:166:GLY:O	2.31	0.66
1:B:347:PHE:CE1	1:B:373:GLY:HA3	2.31	0.66
1:B:80:GLN:OE1	1:B:242:CYS:SG	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLN:NE2	1:A:219:HIS:NE2	2.44	0.65
1:B:347:PHE:CD1	1:B:373:GLY:CA	2.79	0.65
1:B:372:ASN:HD22	1:B:383:GLN:HE22	1.42	0.65
1:B:80:GLN:H	1:B:239:GLN:NE2	1.93	0.65
1:A:314:THR:HG21	1:A:316:LEU:CB	2.13	0.65
1:A:-3:GLN:O	1:A:-3:GLN:CG	2.30	0.65
1:A:95:THR:CG2	1:A:227:PHE:CE2	2.80	0.65
1:B:206:ASP:HB3	1:B:209:THR:HG23	1.78	0.65
1:B:314:THR:HG23	1:B:316:LEU:CB	2.26	0.65
1:B:409:TYR:CZ	1:B:429:PHE:HE1	2.14	0.65
1:A:347:PHE:C	1:A:347:PHE:CD1	2.67	0.65
1:A:481:LYS:O	1:A:483:THR:N	2.29	0.65
1:B:292:GLN:CA	1:B:292:GLN:HE21	2.09	0.65
1:B:70:MET:CG	1:B:70:MET:O	2.44	0.65
1:A:2:PHE:O	1:A:3:TYR:C	2.32	0.65
1:B:180:SER:C	1:B:181:ILE:HG22	2.14	0.65
1:B:81:PHE:CZ	1:B:236:HIS:CD2	2.85	0.65
1:A:481:LYS:C	1:A:483:THR:H	2.00	0.65
1:A:52:GLY:HA2	1:A:56:LYS:HB3	1.78	0.65
1:B:243:TYR:N	1:B:243:TYR:CD2	2.64	0.65
1:B:356:THR:HG22	1:B:390:ASN:OD1	1.96	0.65
1:A:155:VAL:HG12	1:A:156:GLY:H	1.61	0.64
1:A:244:ILE:HD13	1:A:296:PHE:CE1	2.32	0.64
1:A:285:MET:N	1:A:285:MET:HE2	1.99	0.64
1:A:417:LEU:N	1:A:417:LEU:HD23	2.11	0.64
1:B:226:VAL:CG2	1:B:232:ASN:HA	2.26	0.64
1:A:219:HIS:CE1	1:A:241:PRO:HB3	2.32	0.64
1:A:203:PRO:CB	1:A:340:GLY:H	2.06	0.64
1:B:154:THR:CG2	1:B:155:VAL:N	2.31	0.64
1:B:241:PRO:HB2	1:B:243:TYR:CE2	2.32	0.64
1:B:241:PRO:CB	1:B:243:TYR:CE2	2.80	0.64
1:B:251:THR:O	1:B:255:ILE:HG13	1.97	0.64
1:B:38:ASN:HD22	1:B:40:ASP:H	1.45	0.64
1:A:82:ARG:HA	1:A:221:ASP:OD1	1.97	0.64
1:A:203:PRO:CD	1:A:203:PRO:O	2.44	0.64
1:A:155:VAL:HG12	1:A:156:GLY:N	2.12	0.64
1:A:405:ARG:HD2	1:A:415:ASP:OD2	1.97	0.64
1:B:247:THR:CG2	1:B:248:ASN:N	2.60	0.64
1:A:282:ASP:OD1	1:A:286:ARG:NH1	2.30	0.64
1:B:-3:GLN:O	1:B:-1:SER:N	2.27	0.64
1:A:289:ASP:C	1:A:291:ASN:C	2.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:CA	1:A:154:THR:CG2	2.76	0.63
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.12	0.63
1:A:314:THR:CG2	1:A:316:LEU:N	2.53	0.63
1:A:432:ARG:O	1:A:434:GLU:N	2.32	0.63
1:B:314:THR:HG21	1:B:316:LEU:HB2	1.79	0.63
1:A:201:THR:CG2	1:A:202:PRO:HD2	2.29	0.63
1:B:191:PRO:CG	1:B:361:PHE:HE1	2.10	0.63
1:B:399:GLU:OE1	1:B:400:GLY:N	2.29	0.63
1:B:197:LEU:CD1	1:B:345:TYR:HB2	2.28	0.63
1:B:58:HIS:CE1	1:B:429:PHE:HZ	2.14	0.63
1:B:205:ILE:CG2	1:B:206:ASP:N	2.60	0.63
1:B:446:LEU:HD23	1:B:466:PHE:CZ	2.33	0.63
1:B:210:ILE:HD13	1:B:331:MET:CE	2.29	0.63
1:A:166:GLY:CA	1:A:315:SER:O	2.47	0.63
1:A:392:ALA:O	1:A:395:SER:N	2.31	0.63
1:B:195:GLY:HA3	1:B:347:PHE:CE2	2.34	0.63
1:B:38:ASN:C	1:B:40:ASP:H	2.01	0.63
1:A:28:MET:CE	1:A:392:ALA:CB	2.77	0.62
1:A:430:THR:O	1:A:433:ALA:HB3	1.98	0.62
1:A:206:ASP:HB2	1:A:337:VAL:CG2	2.29	0.62
1:A:343:ILE:N	1:A:343:ILE:HD12	2.15	0.62
1:A:408:ALA:HB2	1:A:448:LEU:HD11	1.81	0.62
1:A:48:ASN:HB2	1:A:49:PRO:CD	2.29	0.62
1:B:15:GLY:O	1:B:19:THR:OG1	2.13	0.62
1:A:343:ILE:HD12	1:A:343:ILE:H	1.64	0.62
1:B:453:ARG:NH1	1:B:463:TRP:HB2	2.14	0.62
1:B:379:GLU:O	1:B:383:GLN:HG3	2.00	0.62
1:B:222:ASN:HA	1:B:223:PRO:C	2.20	0.62
1:A:95:THR:HG22	1:A:227:PHE:HE2	1.63	0.62
1:B:54:ILE:HD11	1:B:85:ASN:HD21	1.64	0.62
1:A:209:THR:CB	1:A:334:ALA:HA	2.23	0.62
1:B:126:GLU:HB3	1:B:139:VAL:O	2.00	0.62
1:B:318:PHE:CE1	1:B:336:ILE:HG21	2.35	0.62
1:B:377:TYR:N	1:B:377:TYR:CD1	2.68	0.62
1:B:394:LEU:HD23	1:B:394:LEU:O	1.99	0.62
1:B:248:ASN:OD1	1:B:250:LYS:HB2	2.00	0.61
1:B:401:TRP:CE2	1:B:403:PRO:HB3	2.34	0.61
1:A:108:VAL:O	1:A:112:LEU:CD1	2.46	0.61
1:B:122:GLN:O	1:B:123:GLN:HG2	2.00	0.61
1:A:11:ILE:HG13	1:A:22:ALA:HB2	1.82	0.61
1:B:158:PHE:O	1:B:159:LEU:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:CG2	1:B:341:TYR:CB	2.78	0.61
1:B:-3:GLN:C	1:B:-1:SER:N	2.53	0.61
1:B:194:VAL:CG2	1:B:348:PHE:CE1	2.83	0.61
1:B:522:LYS:O	1:B:525:THR:HB	2.00	0.61
1:B:287:PHE:O	1:B:288:ALA:HB2	1.99	0.61
1:B:366:PHE:CD1	1:B:391:ALA:HB2	2.35	0.61
1:B:38:ASN:C	1:B:40:ASP:N	2.52	0.61
1:A:191:PRO:HG2	1:A:361:PHE:CE2	2.35	0.61
1:A:201:THR:HG22	1:A:202:PRO:CD	2.29	0.61
1:B:7:PHE:N	1:B:147:ARG:O	2.28	0.61
1:B:544:ILE:O	1:B:548:TYR:HD1	1.84	0.61
1:A:210:ILE:HG22	1:A:212:PHE:CE2	2.36	0.61
1:A:247:THR:HG22	1:A:293:HIS:N	2.10	0.61
1:A:312:ILE:HG21	1:A:328:MET:CE	2.19	0.61
1:A:341:TYR:N	1:A:341:TYR:HD1	1.99	0.61
1:A:37:HIS:NE2	1:A:157:THR:HG23	2.15	0.61
1:B:62:GLU:HG2	1:B:448:LEU:HD12	1.82	0.61
1:A:202:PRO:HA	1:A:313:SER:HA	1.81	0.60
1:B:127:ASP:O	1:B:138:ALA:HB1	2.01	0.60
1:B:290:ARG:HD2	1:B:291:ASN:HD22	1.65	0.60
1:A:300:GLU:HB2	1:A:306:GLU:O	2.02	0.60
1:A:491:ALA:C	1:A:493:ALA:H	2.02	0.60
1:A:530:ALA:HB1	1:A:531:PRO:CA	2.30	0.60
1:B:201:THR:HG21	1:B:341:TYR:CE1	2.36	0.60
1:B:79:ILE:O	1:B:79:ILE:CG1	2.49	0.60
1:A:96:ARG:NH1	1:A:96:ARG:CG	2.63	0.60
1:B:163:ILE:HD12	1:B:163:ILE:H	1.66	0.60
1:B:318:PHE:HE1	1:B:336:ILE:HG21	1.65	0.60
1:A:465:ARG:HD2	1:A:465:ARG:O	2.01	0.60
1:B:282:ASP:C	1:B:284:VAL:H	2.04	0.60
1:A:53:GLY:N	1:A:96:ARG:HB3	2.17	0.60
1:A:215:LEU:HD13	1:A:245:THR:HG22	1.81	0.60
1:A:351:ARG:CD	1:A:421:GLY:CA	2.71	0.60
1:A:75:ASP:OD1	1:A:236:HIS:HE1	1.85	0.60
1:B:492:ALA:O	1:B:496:ASN:ND2	2.35	0.60
1:A:425:PRO:HB2	1:A:428:MET:CG	2.32	0.60
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.66	0.60
1:B:38:ASN:HA	1:B:122:GLN:OE1	2.01	0.60
1:B:247:THR:HB	1:B:293:HIS:O	2.00	0.60
1:A:153:LEU:HD22	1:A:154:THR:N	2.17	0.60
1:A:445:ASP:OD2	1:A:469:LYS:NZ	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:SER:O	1:B:512:LEU:HD23	2.02	0.59
1:A:393:ARG:HH11	1:A:455:LEU:CD2	2.15	0.59
1:A:139:VAL:HG13	1:A:145:LYS:CG	2.32	0.59
1:A:203:PRO:HB3	1:A:321:GLN:OE1	2.02	0.59
1:A:72:LYS:O	1:A:75:ASP:HB2	2.03	0.59
1:B:109:ARG:O	1:B:110:THR:C	2.41	0.59
1:A:425:PRO:HB2	1:A:428:MET:HG2	1.83	0.59
1:A:448:LEU:O	1:A:451:ILE:CG1	2.47	0.59
1:B:37:HIS:ND1	1:B:38:ASN:HB2	2.17	0.59
1:A:240:VAL:HG23	1:A:241:PRO:N	2.18	0.59
1:A:341:TYR:CD1	1:A:341:TYR:N	2.71	0.59
1:A:408:ALA:O	1:A:411:GLY:N	2.35	0.59
1:B:79:ILE:HA	1:B:239:GLN:HE21	1.65	0.59
1:A:228:SER:OG	1:A:229:PHE:N	2.34	0.59
1:A:247:THR:CG2	1:A:293:HIS:H	2.09	0.59
1:B:154:THR:O	1:B:155:VAL:CB	2.50	0.59
1:B:72:LYS:O	1:B:75:ASP:N	2.36	0.59
1:A:477:ARG:NH1	1:A:545:GLN:OE1	2.36	0.59
1:B:165:ILE:CG2	1:B:341:TYR:HB3	2.33	0.59
1:A:211:ASP:O	1:A:211:ASP:OD1	2.21	0.58
1:A:446:LEU:HD13	1:A:541:GLN:NE2	2.18	0.58
1:B:426:TYR:O	1:B:427:ARG:C	2.40	0.58
1:A:199:THR:HG22	1:A:343:ILE:HD13	1.85	0.58
1:A:349:ASP:OD1	1:A:350:PRO:HD2	2.03	0.58
1:A:152:VAL:HG22	1:A:366:PHE:HB2	1.84	0.58
1:A:527:THR:N	1:A:528:PRO:CD	2.67	0.58
1:A:230:MET:CE	1:A:230:MET:HA	2.33	0.58
1:B:360:LYS:C	1:B:361:PHE:HD2	2.05	0.58
1:A:106:GLN:O	1:A:110:THR:HG23	2.03	0.58
1:A:61:LYS:HG3	1:A:441:GLU:HG2	1.85	0.58
1:B:191:PRO:HB2	1:B:361:PHE:CZ	2.37	0.58
1:B:37:HIS:CE1	1:B:38:ASN:HB2	2.37	0.58
1:B:48:ASN:HB3	1:B:308:TYR:HE2	1.63	0.58
1:A:210:ILE:CG2	1:A:212:PHE:CE2	2.86	0.58
1:A:278:PRO:CG	1:A:279:SER:H	2.16	0.58
1:B:188:ARG:HH11	1:B:188:ARG:HB2	1.66	0.58
1:A:42:LEU:O	1:A:105:ARG:HG2	2.04	0.58
1:A:17:ALA:HB2	1:A:380:ALA:HB1	1.85	0.58
1:B:443:ASN:OD1	1:B:447:ARG:NH1	2.37	0.58
1:A:491:ALA:C	1:A:493:ALA:N	2.57	0.58
1:B:110:THR:O	1:B:114:ASN:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PHE:C	1:B:159:LEU:O	2.40	0.58
1:B:404:ALA:O	1:B:406:SER:N	2.28	0.58
1:B:30:GLN:N	1:B:30:GLN:HE21	2.01	0.57
1:B:48:ASN:ND2	1:B:50:ALA:HB3	2.18	0.57
1:B:537:GLN:O	1:B:540:GLU:HB3	2.04	0.57
1:A:465:ARG:HH12	1:A:535:ASP:CG	2.08	0.57
1:B:326:ARG:HH21	1:B:333:ASN:HA	1.69	0.57
1:B:452:GLY:O	1:B:453:ARG:C	2.43	0.57
1:B:232:ASN:N	1:B:232:ASN:HD22	2.02	0.57
1:B:70:MET:HG2	1:B:70:MET:O	2.03	0.57
1:B:95:THR:N	1:B:441:GLU:OE2	2.37	0.57
1:A:389:LEU:HD21	1:A:455:LEU:HD13	1.86	0.57
1:A:10:ILE:HG13	1:A:148:ALA:HB2	1.87	0.57
1:A:448:LEU:HD23	1:A:451:ILE:CD1	2.20	0.57
1:B:12:ILE:HG22	1:B:12:ILE:O	2.04	0.57
1:B:243:TYR:N	1:B:243:TYR:HD2	2.01	0.57
1:B:409:TYR:CZ	1:B:429:PHE:CE1	2.93	0.57
1:A:289:ASP:HA	1:A:291:ASN:C	2.25	0.57
1:A:453:ARG:HG2	1:A:463:TRP:CZ2	2.39	0.57
1:A:45:MET:HE1	1:A:50:ALA:N	2.20	0.57
1:A:53:GLY:CA	1:A:96:ARG:HB3	2.35	0.57
1:B:156:GLY:C	1:B:157:THR:HG22	2.25	0.57
1:A:404:ALA:HB3	1:A:407:GLN:CB	2.34	0.56
1:A:491:ALA:HB1	1:A:494:GLU:HB3	1.87	0.56
1:A:95:THR:HG22	1:A:227:PHE:CE2	2.39	0.56
1:B:183:LEU:O	1:B:187:LEU:HD22	2.04	0.56
1:B:314:THR:CG2	1:B:316:LEU:N	2.68	0.56
1:A:319:ASP:N	1:A:319:ASP:OD2	2.38	0.56
1:B:194:VAL:HG22	1:B:348:PHE:CD1	2.41	0.56
1:B:80:GLN:H	1:B:239:GLN:HE22	1.52	0.56
1:A:513:LEU:HD23	1:A:546:VAL:HG11	1.88	0.56
1:B:81:PHE:O	1:B:82:ARG:O	2.23	0.56
1:A:33:LEU:HD12	1:A:119:MET:O	2.05	0.56
1:A:45:MET:HE1	1:A:49:PRO:C	2.25	0.56
1:B:415:ASP:O	1:B:417:LEU:N	2.39	0.56
1:A:45:MET:CE	1:A:49:PRO:CA	2.75	0.56
1:B:165:ILE:HG23	1:B:341:TYR:CB	2.36	0.56
1:B:228:SER:OG	1:B:230:MET:N	2.37	0.56
1:B:81:PHE:HB3	1:B:225:PRO:CG	2.33	0.56
1:A:240:VAL:HG21	1:A:299:PRO:HG2	1.87	0.56
1:B:484:TRP:CE3	1:B:508:SER:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:HA	1:A:183:LEU:HB2	1.88	0.56
1:B:204:ARG:HD2	1:B:338:ARG:HD3	1.88	0.56
1:B:73:ALA:CB	1:B:104:TYR:CE2	2.89	0.56
1:A:261:ARG:O	1:A:262:SER:O	2.23	0.56
1:B:279:SER:HB2	1:B:282:ASP:HB2	1.88	0.55
1:B:306:GLU:OE1	1:B:338:ARG:NH1	2.39	0.55
1:B:191:PRO:HD2	1:B:361:PHE:CD1	2.41	0.55
1:B:427:ARG:NH2	1:B:428:MET:CE	2.68	0.55
1:B:127:ASP:OD2	1:B:186:ARG:NH1	2.40	0.55
1:B:356:THR:O	1:B:357:LEU:CB	2.52	0.55
1:A:45:MET:HE1	1:A:49:PRO:CA	2.36	0.55
1:B:190:LEU:CB	1:B:191:PRO:CD	2.84	0.55
1:B:64:ASP:OD2	1:B:462:ARG:NH2	2.37	0.55
1:B:69:LEU:O	1:B:71:ALA:N	2.40	0.55
1:A:496:ASN:HD22	1:A:502:PRO:HB3	1.72	0.55
1:B:205:ILE:HD11	1:B:336:ILE:HG13	1.89	0.55
1:B:380:ALA:O	1:B:381:ALA:C	2.42	0.55
1:B:486:THR:C	1:B:488:SER:H	2.10	0.55
1:A:155:VAL:HG11	1:A:370:GLN:HE21	1.72	0.55
1:A:85:ASN:O	1:A:93:ARG:HD3	2.05	0.55
1:B:349:ASP:OD2	1:B:351:ARG:NH1	2.39	0.55
1:B:98:GLN:HE22	1:B:298:GLU:HG2	1.72	0.55
1:A:123:GLN:HG3	1:A:142:MET:HE1	1.88	0.55
1:A:207:ALA:HB2	1:A:305:ASN:O	2.07	0.55
1:B:306:GLU:CD	1:B:338:ARG:NH1	2.61	0.55
1:B:48:ASN:CB	1:B:308:TYR:CE2	2.83	0.55
1:A:310:ASN:C	1:A:310:ASN:HD22	2.10	0.55
1:A:316:LEU:HD13	1:A:320:VAL:HG11	1.89	0.55
1:B:181:ILE:O	1:B:181:ILE:HG23	2.07	0.55
1:B:424:GLU:OE2	1:B:436:ARG:NH2	2.36	0.55
1:B:440:ARG:NH2	1:B:442:ASP:OD1	2.35	0.55
1:B:194:VAL:HG22	1:B:348:PHE:CE1	2.42	0.54
1:B:234:SER:O	1:B:236:HIS:N	2.40	0.54
1:B:371:ILE:HG23	1:B:372:ASN:N	2.22	0.54
1:A:38:ASN:ND2	1:A:40:ASP:H	2.04	0.54
1:B:140:THR:HG21	1:B:146:PHE:HE2	1.71	0.54
1:B:320:VAL:HG12	1:B:324:ILE:HD11	1.89	0.54
1:A:209:THR:HG21	1:A:335:LYS:HG3	0.83	0.54
1:A:503:LEU:HD21	1:A:512:LEU:HD21	1.88	0.54
1:A:70:MET:CE	1:A:381:ALA:HB2	2.37	0.54
1:B:524:THR:HG21	1:B:532:ALA:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:GLU:HG2	1:B:533:LEU:HD22	1.88	0.54
1:B:337:VAL:HG12	1:B:338:ARG:HG3	1.90	0.54
1:A:240:VAL:HG23	1:A:241:PRO:O	2.08	0.54
1:A:440:ARG:NH1	1:A:440:ARG:HG3	2.23	0.54
1:B:162:LYS:O	1:B:343:ILE:HG22	2.06	0.54
1:B:525:THR:HG22	1:B:526:LEU:HD23	1.88	0.54
1:A:211:ASP:C	1:A:213:SER:H	2.10	0.54
1:A:278:PRO:CD	1:A:279:SER:H	2.21	0.54
1:B:33:LEU:HD12	1:B:119:MET:HG2	1.89	0.54
1:A:469:LYS:HE3	1:A:537:GLN:HG2	1.90	0.54
1:A:72:LYS:O	1:A:73:ALA:C	2.46	0.54
1:B:241:PRO:HB3	1:B:243:TYR:CE2	2.43	0.54
1:B:252:HIS:CD2	1:B:284:VAL:HG13	2.43	0.54
1:B:35:LEU:CD1	1:B:125:VAL:HG23	2.38	0.54
1:A:79:ILE:HD11	1:A:299:PRO:HB2	1.90	0.54
1:A:155:VAL:CG1	1:A:370:GLN:HE21	2.19	0.54
1:A:436:ARG:O	1:A:437:LEU:CB	2.51	0.54
1:A:488:SER:O	1:A:492:ALA:HB2	2.08	0.54
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.73	0.54
1:A:351:ARG:HD2	1:A:420:LEU:C	2.27	0.54
1:A:408:ALA:HA	1:A:447:ARG:NH2	2.21	0.54
1:A:485:VAL:HG23	1:A:503:LEU:CD1	2.38	0.54
1:B:139:VAL:CG1	1:B:145:LYS:HG2	2.19	0.54
1:B:317:PRO:HD2	1:B:320:VAL:HG21	1.90	0.54
1:B:404:ALA:O	1:B:407:GLN:N	2.28	0.54
1:B:190:LEU:CB	1:B:191:PRO:HD2	2.38	0.54
1:B:372:ASN:HD22	1:B:383:GLN:NE2	2.06	0.54
1:A:437:LEU:HD12	1:A:437:LEU:C	2.29	0.53
1:A:127:ASP:OD1	1:A:186:ARG:NH1	2.42	0.53
1:A:293:HIS:CD2	1:A:293:HIS:N	2.75	0.53
1:A:536:GLU:OE1	1:A:536:GLU:HA	2.07	0.53
1:A:203:PRO:O	1:A:205:ILE:HD13	2.09	0.53
1:A:2:PHE:CE1	1:A:145:LYS:HB3	2.43	0.53
1:A:70:MET:HE3	1:A:381:ALA:HB2	1.90	0.53
1:B:190:LEU:HB3	1:B:191:PRO:CD	2.39	0.53
1:B:292:GLN:HA	1:B:292:GLN:NE2	2.22	0.53
1:B:96:ARG:CG	1:B:96:ARG:O	2.47	0.53
1:A:33:LEU:C	1:A:33:LEU:HD12	2.28	0.53
1:A:484:TRP:N	1:A:484:TRP:CD1	2.76	0.53
1:B:366:PHE:CD1	1:B:366:PHE:N	2.75	0.53
1:B:410:LEU:O	1:B:414:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:O	1:A:190:LEU:HG	2.09	0.53
1:A:297:LEU:HD11	1:A:331:MET:HE1	1.89	0.53
1:B:385:LEU:C	1:B:385:LEU:HD23	2.29	0.53
1:A:413:LEU:CD1	1:A:417:LEU:HD11	2.39	0.53
1:B:399:GLU:OE1	1:B:399:GLU:HA	2.09	0.53
1:B:404:ALA:O	1:B:407:GLN:HB2	2.08	0.53
1:B:62:GLU:CD	1:B:408:ALA:HB1	2.28	0.53
1:A:440:ARG:HH11	1:A:440:ARG:HG3	1.74	0.53
1:A:474:GLU:O	1:A:475:ARG:C	2.46	0.53
1:A:377:TYR:O	1:A:380:ALA:N	2.40	0.53
1:A:485:VAL:HG23	1:A:503:LEU:HD13	1.89	0.53
1:B:362:ILE:O	1:B:363:GLN:C	2.47	0.53
1:B:440:ARG:O	1:B:443:ASN:OD1	2.27	0.53
1:B:81:PHE:CD2	1:B:236:HIS:HD2	2.27	0.53
1:B:446:LEU:HD23	1:B:466:PHE:CE1	2.44	0.53
1:A:205:ILE:CG2	1:A:210:ILE:CD1	2.85	0.52
1:A:30:GLN:CA	1:A:30:GLN:NE2	2.70	0.52
1:A:314:THR:CG2	1:A:315:SER:H	2.08	0.52
1:A:196:ARG:NH2	1:A:344:GLU:HB3	2.25	0.52
1:A:354:LYS:C	1:A:356:THR:H	2.11	0.52
1:A:404:ALA:CB	1:A:407:GLN:CD	2.77	0.52
1:B:62:GLU:HG2	1:B:448:LEU:CD1	2.38	0.52
1:A:284:VAL:O	1:A:285:MET:C	2.42	0.52
1:B:318:PHE:HA	1:B:321:GLN:HG3	1.91	0.52
1:A:453:ARG:NH1	1:A:463:TRP:HB2	2.25	0.52
1:A:109:ARG:NH1	1:B:303:THR:O	2.41	0.52
1:B:37:HIS:ND1	1:B:37:HIS:O	2.41	0.52
1:A:11:ILE:HG13	1:A:22:ALA:CA	2.39	0.52
1:A:445:ASP:OD1	1:A:445:ASP:N	2.42	0.52
1:A:469:LYS:O	1:A:473:ILE:HD12	2.09	0.52
1:B:238:GLN:HB3	1:B:302:LEU:HD11	1.92	0.52
1:A:289:ASP:O	1:A:291:ASN:O	2.27	0.52
1:A:512:LEU:HD12	1:A:529:PHE:CE2	2.44	0.52
1:B:129:ILE:O	1:B:136:VAL:HG12	2.10	0.52
1:B:409:TYR:HA	1:B:412:VAL:HG23	1.92	0.52
1:A:49:PRO:HD2	1:A:298:GLU:OE1	2.09	0.52
1:A:393:ARG:NH1	1:A:455:LEU:CD2	2.73	0.52
1:B:226:VAL:HG12	1:B:227:PHE:N	2.24	0.52
1:B:255:ILE:HG23	1:B:316:LEU:HD11	1.90	0.52
1:B:470:LEU:O	1:B:471:GLU:C	2.47	0.52
1:A:13:GLY:CA	1:A:154:THR:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:PHE:CE2	1:B:145:LYS:HE3	2.45	0.52
1:B:385:LEU:HD21	1:B:457:LEU:CD1	2.40	0.52
1:A:385:LEU:O	1:A:385:LEU:HD23	2.10	0.52
1:B:35:LEU:HD12	1:B:125:VAL:HG23	1.92	0.51
1:A:8:ASP:HB3	1:A:395:SER:HB2	1.92	0.51
1:B:385:LEU:HD21	1:B:457:LEU:HD13	1.91	0.51
1:A:155:VAL:CG1	1:A:156:GLY:H	2.14	0.51
1:A:95:THR:HG21	1:A:227:PHE:CE2	2.46	0.51
1:B:415:ASP:O	1:B:416:ASP:C	2.49	0.51
1:B:426:TYR:O	1:B:429:PHE:N	2.40	0.51
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.43	0.51
1:B:295:ILE:CD1	1:B:311:GLY:O	2.58	0.51
1:A:248:ASN:O	1:A:251:THR:N	2.44	0.51
1:A:486:THR:O	1:A:488:SER:N	2.44	0.51
1:B:205:ILE:HG23	1:B:206:ASP:H	1.75	0.51
1:B:104:TYR:O	1:B:107:ALA:N	2.34	0.51
1:B:51:ILE:HD12	1:B:74:ILE:HG12	1.93	0.51
1:B:539:ALA:O	1:B:540:GLU:C	2.49	0.51
1:A:129:ILE:HB	1:A:137:GLY:O	2.11	0.51
1:A:153:LEU:CD2	1:A:154:THR:N	2.74	0.51
1:A:153:LEU:CD2	1:A:154:THR:H	2.23	0.51
1:A:316:LEU:HD13	1:A:320:VAL:CG1	2.41	0.51
1:B:30:GLN:HA	1:B:30:GLN:NE2	2.26	0.51
1:B:358:GLU:N	1:B:366:PHE:CD2	2.79	0.51
1:B:518:MET:HE2	1:B:519:THR:H	1.76	0.51
1:B:30:GLN:CA	1:B:30:GLN:NE2	2.74	0.51
1:A:206:ASP:N	1:A:337:VAL:HG23	2.25	0.51
1:A:262:SER:CB	1:A:263:PRO:HD3	2.34	0.51
1:A:2:PHE:CE1	1:A:145:LYS:CB	2.94	0.51
1:B:130:VAL:HG21	1:B:186:ARG:HE	1.76	0.51
1:B:259:LEU:C	1:B:261:ARG:H	2.14	0.51
1:B:379:GLU:N	1:B:379:GLU:OE1	2.28	0.51
1:A:154:THR:HG23	1:A:155:VAL:N	2.26	0.50
1:A:161:GLY:O	1:A:162:LYS:O	2.29	0.50
1:A:262:SER:OG	1:A:263:PRO:N	2.39	0.50
1:A:460:ASP:O	1:A:461:GLU:C	2.48	0.50
1:B:159:LEU:HB3	1:B:160:ASP:CA	2.41	0.50
1:B:437:LEU:HG	1:B:437:LEU:O	2.12	0.50
1:B:56:LYS:O	1:B:60:VAL:HG23	2.11	0.50
1:A:251:THR:O	1:A:255:ILE:HD12	2.11	0.50
1:B:422:THR:HG22	1:B:422:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:O	1:A:186:ARG:C	2.49	0.50
1:A:429:PHE:C	1:A:429:PHE:CD2	2.84	0.50
1:A:62:GLU:CD	1:A:447:ARG:HH22	2.15	0.50
1:A:471:GLU:O	1:A:472:ASN:C	2.46	0.50
1:B:228:SER:OG	1:B:229:PHE:N	2.45	0.50
1:B:284:VAL:HG12	1:B:284:VAL:O	2.11	0.50
1:B:19:THR:HG23	1:B:112:LEU:HD11	1.92	0.50
1:B:393:ARG:O	1:B:394:LEU:C	2.50	0.50
1:A:287:PHE:HD1	1:A:288:ALA:H	1.59	0.50
1:B:232:ASN:N	1:B:232:ASN:ND2	2.58	0.50
1:A:155:VAL:O	1:A:156:GLY:O	2.30	0.50
1:A:199:THR:HG22	1:A:343:ILE:CD1	2.42	0.50
1:A:62:GLU:CD	1:A:408:ALA:HB1	2.31	0.50
1:B:12:ILE:C	1:B:154:THR:CG2	2.75	0.50
1:B:156:GLY:O	1:B:157:THR:O	2.30	0.50
1:A:203:PRO:HB3	1:A:340:GLY:N	2.15	0.50
1:A:474:GLU:O	1:A:476:GLU:N	2.44	0.50
1:B:165:ILE:CG2	1:B:341:TYR:HA	2.41	0.50
1:A:234:SER:C	1:A:236:HIS:H	2.16	0.50
1:A:60:VAL:HG11	1:A:227:PHE:CE1	2.46	0.50
1:B:239:GLN:C	1:B:240:VAL:CG1	2.80	0.50
1:B:349:ASP:OD1	1:B:349:ASP:C	2.50	0.50
1:A:488:SER:O	1:A:489:ALA:O	2.30	0.49
1:A:90:PRO:HA	1:A:93:ARG:HG3	1.94	0.49
1:B:459:ASP:O	1:B:462:ARG:N	2.41	0.49
1:B:83:ILE:HG22	1:B:83:ILE:O	2.11	0.49
1:A:255:ILE:HG21	1:A:281:GLU:HA	1.95	0.49
1:A:101:ARG:HD2	1:A:300:GLU:OE2	2.12	0.49
1:B:159:LEU:HA	1:B:160:ASP:O	2.12	0.49
1:A:408:ALA:O	1:A:409:TYR:C	2.49	0.49
1:B:106:GLN:O	1:B:106:GLN:HG3	2.12	0.49
1:B:322:MET:O	1:B:326:ARG:HB2	2.13	0.49
1:A:289:ASP:CA	1:A:291:ASN:C	2.81	0.49
1:B:194:VAL:CG2	1:B:348:PHE:HE1	2.24	0.49
1:B:366:PHE:C	1:B:367:PHE:HD1	2.16	0.49
1:A:479:ARG:HA	1:A:482:SER:HB2	1.95	0.49
1:B:300:GLU:OE2	1:B:308:TYR:HD1	1.96	0.49
1:B:331:MET:N	1:B:332:GLU:OE1	2.45	0.49
1:B:417:LEU:O	1:B:421:GLY:CA	2.53	0.49
1:A:165:ILE:O	1:A:166:GLY:O	2.30	0.49
1:A:423:LYS:HE3	1:A:424:GLU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLN:CA	1:B:292:GLN:NE2	2.75	0.49
1:A:378:GLU:N	1:A:378:GLU:OE1	2.43	0.49
1:B:165:ILE:HG22	1:B:341:TYR:CA	2.41	0.49
1:B:19:THR:O	1:B:23:MET:HB2	2.13	0.49
1:B:366:PHE:CE1	1:B:391:ALA:CB	2.90	0.49
1:A:316:LEU:HD22	1:A:320:VAL:HG11	1.95	0.49
1:B:318:PHE:CE1	1:B:336:ILE:HD13	2.48	0.49
1:B:408:ALA:CB	1:B:448:LEU:HD11	2.43	0.49
1:A:43:GLY:HA3	1:A:105:ARG:HA	1.95	0.49
1:B:200:GLY:HA2	1:B:342:ALA:HA	1.95	0.49
1:B:431:SER:C	1:B:433:ALA:N	2.65	0.49
1:B:440:ARG:O	1:B:447:ARG:NH1	2.46	0.49
1:A:314:THR:CG2	1:A:316:LEU:CB	2.84	0.48
1:A:379:GLU:OE2	1:A:426:TYR:OH	2.26	0.48
1:A:-3:GLN:O	1:A:-2:GLY:O	2.30	0.48
1:B:154:THR:C	1:B:155:VAL:CG1	2.52	0.48
1:B:458:VAL:HG13	1:B:462:ARG:HD2	1.94	0.48
1:B:71:ALA:O	1:B:72:LYS:C	2.50	0.48
1:A:167:LEU:O	1:A:168:ASP:OD1	2.31	0.48
1:A:310:ASN:C	1:A:310:ASN:ND2	2.65	0.48
1:A:458:VAL:HG12	1:A:459:ASP:N	2.29	0.48
1:A:469:LYS:HG2	1:A:473:ILE:HD11	1.95	0.48
1:B:205:ILE:HD12	1:B:336:ILE:HA	1.87	0.48
1:A:385:LEU:C	1:A:385:LEU:CD2	2.81	0.48
1:A:430:THR:O	1:A:433:ALA:CB	2.61	0.48
1:A:53:GLY:N	1:A:96:ARG:CB	2.77	0.48
1:A:9:VAL:O	1:A:32:THR:HA	2.12	0.48
1:B:65:ALA:HB1	1:B:449:THR:OG1	2.13	0.48
1:A:289:ASP:HA	1:A:291:ASN:O	2.13	0.48
1:A:365:LEU:HG	1:A:367:PHE:CE1	2.46	0.48
1:A:432:ARG:O	1:A:433:ALA:C	2.51	0.48
1:B:188:ARG:NH1	1:B:188:ARG:HB2	2.28	0.48
1:B:194:VAL:CG2	1:B:348:PHE:CD1	2.97	0.48
1:B:520:TYR:HB3	1:B:543:GLU:OE2	2.13	0.48
1:A:463:TRP:O	1:A:466:PHE:HB3	2.13	0.48
1:A:453:ARG:HA	1:A:453:ARG:HD2	1.65	0.48
1:B:363:GLN:HE21	1:B:363:GLN:HB3	1.45	0.48
1:B:371:ILE:HG23	1:B:372:ASN:H	1.79	0.48
1:A:204:ARG:HD3	1:A:338:ARG:HD2	1.96	0.48
1:A:358:GLU:OE2	1:A:363:GLN:HB3	2.13	0.48
1:A:519:THR:O	1:A:520:TYR:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PHE:O	1:B:225:PRO:CG	2.62	0.48
1:B:81:PHE:CZ	1:B:236:HIS:NE2	2.82	0.48
1:B:24:ALA:HA	1:B:27:ARG:HH11	1.75	0.47
1:B:408:ALA:HB2	1:B:448:LEU:HD11	1.96	0.47
1:B:473:ILE:HG23	1:B:542:VAL:HG23	1.95	0.47
1:A:393:ARG:HH21	1:A:398:LYS:HB3	1.79	0.47
1:B:386:LEU:HD12	1:B:389:LEU:CD2	2.35	0.47
1:B:508:SER:O	1:B:512:LEU:CD2	2.62	0.47
1:A:295:ILE:CD1	1:A:311:GLY:HA3	2.44	0.47
1:A:314:THR:CG2	1:A:315:SER:N	2.48	0.47
1:A:448:LEU:CG	1:A:451:ILE:HD11	2.44	0.47
1:A:230:MET:HE3	1:A:230:MET:HA	1.96	0.47
1:A:247:THR:O	1:A:248:ASN:HB3	2.14	0.47
1:A:413:LEU:C	1:A:413:LEU:HD12	2.34	0.47
1:A:441:GLU:O	1:A:443:ASN:N	2.46	0.47
1:A:64:ASP:O	1:A:67:GLY:N	2.39	0.47
1:B:128:LEU:HA	1:B:138:ALA:HB2	1.96	0.47
1:A:444:ALA:O	1:A:448:LEU:HB2	2.14	0.47
1:A:392:ALA:O	1:A:395:SER:OG	2.25	0.47
1:B:239:GLN:O	1:B:240:VAL:HG12	2.14	0.47
1:A:153:LEU:HD22	1:A:154:THR:H	1.78	0.47
1:A:11:ILE:HD12	1:A:21:ALA:CB	2.44	0.47
1:B:165:ILE:HG23	1:B:341:TYR:HB2	1.96	0.47
1:B:183:LEU:HG	1:B:183:LEU:O	2.14	0.47
1:B:331:MET:HB2	1:B:334:ALA:HB2	1.96	0.47
1:B:393:ARG:NE	1:B:399:GLU:O	2.44	0.47
1:B:431:SER:HB2	1:B:432:ARG:H	1.43	0.47
1:A:89:GLY:CA	1:A:93:ARG:HE	2.28	0.47
1:B:201:THR:HG21	1:B:341:TYR:CD1	2.49	0.47
1:B:222:ASN:ND2	1:B:223:PRO:HA	2.21	0.47
1:B:450:GLU:C	1:B:452:GLY:N	2.65	0.47
1:B:299:PRO:HA	1:B:307:ILE:HD12	1.96	0.47
1:A:16:HIS:O	1:A:17:ALA:C	2.53	0.47
1:B:322:MET:O	1:B:323:GLN:C	2.54	0.47
1:B:410:LEU:O	1:B:413:LEU:HB3	2.15	0.47
1:A:154:THR:O	1:A:155:VAL:HB	2.12	0.46
1:A:541:GLN:HE21	1:A:545:GLN:HE21	1.62	0.46
1:B:357:LEU:O	1:B:358:GLU:C	2.53	0.46
1:B:385:LEU:O	1:B:385:LEU:HD23	2.15	0.46
1:A:412:VAL:O	1:A:413:LEU:C	2.54	0.46
1:A:526:LEU:C	1:A:528:PRO:HD2	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ALA:HA	1:B:462:ARG:NH1	2.29	0.46
1:B:51:ILE:HB	1:B:74:ILE:HG13	1.97	0.46
1:A:11:ILE:HG13	1:A:22:ALA:CB	2.45	0.46
1:A:24:ALA:O	1:A:25:ALA:C	2.53	0.46
1:B:197:LEU:HD12	1:B:345:TYR:CB	2.41	0.46
1:B:48:ASN:HA	1:B:49:PRO:HD3	1.66	0.46
1:B:518:MET:SD	1:B:523:LEU:HD12	2.55	0.46
1:B:542:VAL:CG1	1:B:543:GLU:N	2.75	0.46
1:B:56:LYS:HD3	1:B:378:GLU:CD	2.36	0.46
1:B:91:ALA:H	1:B:440:ARG:HD2	1.80	0.46
1:A:116:PRO:O	1:A:117:ASN:HB2	2.15	0.46
1:B:409:TYR:CE1	1:B:439:LEU:HB3	2.50	0.46
1:B:467:ASN:O	1:B:468:GLU:C	2.53	0.46
1:A:410:LEU:O	1:A:410:LEU:HD13	2.15	0.46
1:A:423:LYS:HE2	1:A:426:TYR:CE2	2.51	0.46
1:A:219:HIS:ND1	1:A:241:PRO:HB3	2.30	0.46
1:A:377:TYR:O	1:A:378:GLU:C	2.53	0.46
1:A:463:TRP:CE3	1:A:463:TRP:HA	2.50	0.46
1:A:81:PHE:HB3	1:A:225:PRO:CG	2.29	0.46
1:B:64:ASP:OD1	1:B:228:SER:HB2	2.15	0.46
1:A:123:GLN:HG3	1:A:142:MET:CE	2.45	0.46
1:A:294:GLN:HB2	1:A:294:GLN:HE21	1.58	0.46
1:A:295:ILE:CD1	1:A:312:ILE:HG23	2.45	0.46
1:A:423:LYS:HG2	1:A:424:GLU:O	2.16	0.46
1:B:13:GLY:CA	1:B:154:THR:CG2	2.77	0.46
1:B:459:ASP:C	1:B:461:GLU:N	2.68	0.46
1:A:460:ASP:O	1:A:462:ARG:N	2.49	0.46
1:B:215:LEU:HD21	1:B:329:GLN:HG2	1.98	0.46
1:B:357:LEU:HA	1:B:357:LEU:HD23	1.77	0.46
1:B:348:PHE:N	1:B:371:ILE:O	2.49	0.46
1:B:379:GLU:O	1:B:380:ALA:C	2.54	0.46
1:B:459:ASP:O	1:B:460:ASP:C	2.54	0.46
1:A:393:ARG:NH2	1:A:398:LYS:HB3	2.30	0.46
1:B:240:VAL:HA	1:B:241:PRO:HD2	1.62	0.46
1:B:287:PHE:O	1:B:288:ALA:HB3	2.13	0.46
1:B:290:ARG:HD2	1:B:291:ASN:ND2	2.28	0.46
1:B:2:PHE:HE2	1:B:145:LYS:HE3	1.82	0.46
1:B:301:GLY:O	1:B:303:THR:N	2.49	0.46
1:B:444:ALA:HA	1:B:447:ARG:NH1	2.31	0.46
1:A:481:LYS:N	1:A:481:LYS:HD3	2.32	0.45
1:A:338:ARG:NH2	1:B:39:ILE:HB	2.12	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ALA:O	1:A:490:GLU:C	2.54	0.45
1:A:186:ARG:HH11	1:A:186:ARG:CB	2.30	0.45
1:B:158:PHE:CD1	1:B:158:PHE:O	2.68	0.45
1:A:289:ASP:CA	1:A:291:ASN:O	2.65	0.45
1:A:70:MET:HE3	1:A:381:ALA:CB	2.46	0.45
1:B:295:ILE:HA	1:B:295:ILE:HD13	1.62	0.45
1:A:259:LEU:O	1:A:261:ARG:N	2.50	0.45
1:A:278:PRO:HG2	1:A:279:SER:H	1.79	0.45
1:B:215:LEU:CD2	1:B:329:GLN:HG2	2.46	0.45
1:B:77:ALA:O	1:B:99:ALA:HA	2.17	0.45
1:A:208:ARG:O	1:A:210:ILE:N	2.50	0.45
1:B:505:ARG:O	1:B:507:ALA:N	2.50	0.45
1:A:484:TRP:HA	1:A:508:SER:HA	1.98	0.45
1:B:367:PHE:CD1	1:B:367:PHE:N	2.84	0.45
1:B:416:ASP:OD1	1:B:420:LEU:HD11	2.17	0.45
1:B:427:ARG:NH2	1:B:428:MET:HE2	2.31	0.45
1:B:445:ASP:O	1:B:449:THR:HB	2.16	0.45
1:A:287:PHE:HB3	1:A:288:ALA:O	2.16	0.45
1:A:7:PHE:CD2	1:A:33:LEU:HB2	2.52	0.45
1:A:354:LYS:C	1:A:356:THR:N	2.69	0.45
1:A:440:ARG:NH2	1:A:544:ILE:HG22	2.30	0.45
1:A:92:VAL:HG21	1:A:430:THR:HG23	1.99	0.45
1:A:9:VAL:HG22	1:A:150:ALA:HB3	1.99	0.45
1:B:116:PRO:O	1:B:117:ASN:HB2	2.17	0.45
1:B:31:GLN:HA	1:B:31:GLN:HE21	1.77	0.45
1:B:386:LEU:O	1:B:389:LEU:HB3	2.17	0.45
1:B:44:GLN:HB2	1:B:44:GLN:HE21	1.55	0.45
1:B:64:ASP:OD2	1:B:462:ARG:NH1	2.46	0.45
1:B:9:VAL:HA	1:B:150:ALA:O	2.16	0.45
1:A:37:HIS:CD2	1:A:157:THR:HG23	2.52	0.45
1:A:312:ILE:HG13	1:A:312:ILE:O	2.17	0.45
1:A:53:GLY:HA2	1:A:96:ARG:HB3	1.99	0.45
1:B:321:GLN:HA	1:B:324:ILE:HD12	1.99	0.45
1:B:430:THR:CG2	1:B:431:SER:N	2.80	0.45
1:A:166:GLY:CA	1:A:317:PRO:HG3	2.33	0.44
1:A:372:ASN:ND2	1:A:383:GLN:HE21	2.08	0.44
1:A:467:ASN:HA	1:A:470:LEU:HB3	1.99	0.44
1:A:474:GLU:HB3	1:A:475:ARG:H	1.57	0.44
1:A:54:ILE:CD1	1:A:85:ASN:HD21	2.30	0.44
1:A:91:ALA:HB2	1:A:437:LEU:HD13	1.99	0.44
1:B:124:ALA:HB3	1:B:141:GLN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASP:HB3	1:B:209:THR:CG2	2.46	0.44
1:B:81:PHE:CD2	1:B:236:HIS:CD2	3.03	0.44
1:B:371:ILE:CG2	1:B:372:ASN:H	2.29	0.44
1:B:38:ASN:O	1:B:39:ILE:C	2.52	0.44
1:B:390:ASN:HA	1:B:390:ASN:HD22	1.41	0.44
1:B:28:MET:HG3	1:B:457:LEU:HD23	1.98	0.44
1:A:310:ASN:HD22	1:A:311:GLY:N	2.15	0.44
1:A:52:GLY:N	1:A:378:GLU:OE2	2.43	0.44
1:A:474:GLU:O	1:A:477:ARG:N	2.49	0.44
1:B:205:ILE:HD11	1:B:336:ILE:CG1	2.47	0.44
1:B:247:THR:O	1:B:248:ASN:HB3	2.18	0.44
1:B:303:THR:O	1:B:303:THR:OG1	2.36	0.44
1:B:450:GLU:O	1:B:451:ILE:C	2.54	0.44
1:A:11:ILE:HG21	1:A:18:GLY:O	2.17	0.44
1:A:59:LEU:HA	1:A:59:LEU:HD12	1.87	0.44
1:B:222:ASN:C	1:B:223:PRO:O	2.55	0.44
1:B:245:THR:HG23	1:B:246:HIS:N	2.33	0.44
1:B:495:VAL:HG11	1:B:503:LEU:HD11	1.99	0.44
1:A:215:LEU:N	1:A:215:LEU:HD23	2.32	0.44
1:A:202:PRO:CA	1:A:313:SER:HA	2.46	0.44
1:A:380:ALA:O	1:A:381:ALA:C	2.56	0.44
1:A:396:ASP:OD1	1:A:396:ASP:O	2.35	0.44
1:A:80:GLN:HE21	1:A:98:GLN:HG2	1.82	0.44
1:B:205:ILE:HD13	1:B:205:ILE:HA	1.47	0.44
1:B:484:TRP:HA	1:B:508:SER:HA	1.98	0.44
1:B:90:PRO:HG3	1:B:544:ILE:HG23	1.98	0.44
1:A:84:LEU:N	1:A:94:ALA:O	2.51	0.44
1:B:280:ILE:C	1:B:282:ASP:H	2.19	0.44
1:B:500:THR:HG23	1:B:501:ALA:N	2.32	0.44
1:A:232:ASN:N	1:A:235:GLN:OE1	2.44	0.44
1:B:81:PHE:HB3	1:B:225:PRO:HD2	2.00	0.44
1:A:207:ALA:CB	1:A:305:ASN:O	2.66	0.44
1:B:137:GLY:HA3	1:B:146:PHE:O	2.18	0.44
1:B:28:MET:CE	1:B:392:ALA:HB3	2.47	0.44
1:B:405:ARG:HG3	1:B:412:VAL:HA	2.00	0.44
1:B:495:VAL:O	1:B:499:LEU:HD23	2.18	0.44
1:A:41:THR:OG1	1:A:157:THR:OG1	2.34	0.44
1:A:27:ARG:HH22	1:A:68:GLY:N	2.15	0.44
1:B:496:ASN:HB3	1:B:502:PRO:HB3	2.00	0.44
1:A:202:PRO:HG3	1:A:308:TYR:CE2	2.53	0.44
1:A:27:ARG:NH2	1:A:68:GLY:N	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LYS:C	1:A:483:THR:N	2.67	0.44
1:A:473:ILE:HG13	1:A:538:ALA:HB1	2.00	0.44
1:A:542:VAL:HG12	1:A:543:GLU:N	2.33	0.44
1:B:141:GLN:O	1:B:141:GLN:HG2	2.17	0.44
1:B:209:THR:OG1	1:B:334:ALA:CA	2.44	0.44
1:B:290:ARG:CD	1:B:291:ASN:HD22	2.31	0.44
1:B:191:PRO:CD	1:B:361:PHE:CE1	3.00	0.44
1:B:396:ASP:O	1:B:396:ASP:OD1	2.36	0.44
1:A:211:ASP:O	1:A:212:PHE:C	2.54	0.43
1:A:246:HIS:CD2	1:A:246:HIS:N	2.84	0.43
1:A:248:ASN:O	1:A:251:THR:OG1	2.17	0.43
1:A:38:ASN:O	1:A:40:ASP:N	2.51	0.43
1:B:130:VAL:HG21	1:B:186:ARG:NE	2.32	0.43
1:A:2:PHE:CD1	1:A:145:LYS:CB	2.98	0.43
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.83	0.43
1:B:234:SER:O	1:B:235:GLN:C	2.55	0.43
1:B:300:GLU:OE2	1:B:308:TYR:CD1	2.71	0.43
1:B:399:GLU:OE1	1:B:399:GLU:CA	2.66	0.43
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.64	0.43
1:A:153:LEU:HA	1:A:153:LEU:HD23	1.58	0.43
1:A:317:PRO:HD2	1:A:320:VAL:HG21	2.00	0.43
1:A:403:PRO:HG2	1:A:410:LEU:HD12	2.00	0.43
1:B:80:GLN:N	1:B:239:GLN:NE2	2.64	0.43
1:B:366:PHE:H	1:B:366:PHE:HD1	1.66	0.43
1:B:7:PHE:CE1	1:B:33:LEU:HD13	2.53	0.43
1:B:369:GLY:C	1:B:371:ILE:H	2.19	0.43
1:B:7:PHE:O	1:B:148:ALA:CA	2.61	0.43
1:A:479:ARG:HG2	1:A:479:ARG:O	2.19	0.43
1:B:195:GLY:O	1:B:346:ASP:HA	2.19	0.43
1:A:212:PHE:HD1	1:A:243:TYR:CG	2.36	0.43
1:A:413:LEU:CD1	1:A:417:LEU:HD21	2.49	0.43
1:A:425:PRO:HD2	1:A:428:MET:CE	2.49	0.43
1:A:408:ALA:CA	1:A:447:ARG:HH21	2.31	0.43
1:B:115:GLN:HG3	1:B:115:GLN:O	2.19	0.43
1:B:331:MET:HE2	1:B:331:MET:HB3	1.83	0.43
1:B:367:PHE:HD1	1:B:367:PHE:N	2.17	0.43
1:B:371:ILE:CG2	1:B:372:ASN:N	2.82	0.43
1:A:166:GLY:HA2	1:A:315:SER:O	2.16	0.43
1:B:139:VAL:HG13	1:B:145:LYS:CD	2.47	0.43
1:B:204:ARG:O	1:B:205:ILE:HD13	2.18	0.43
1:B:526:LEU:C	1:B:528:PRO:HD2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PHE:CZ	1:A:236:HIS:CE1	3.07	0.43
1:A:243:TYR:HB2	1:A:297:LEU:HB2	2.00	0.43
1:A:80:GLN:O	1:A:97:ALA:HA	2.19	0.43
1:A:89:GLY:O	1:A:91:ALA:N	2.51	0.43
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.52	0.43
1:A:212:PHE:HD1	1:A:243:TYR:CD2	2.37	0.43
1:A:56:LYS:HB3	1:A:378:GLU:HG2	2.01	0.43
1:A:38:ASN:ND2	1:A:38:ASN:C	2.70	0.43
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.87	0.43
1:B:118:LEU:HD12	1:B:119:MET:N	2.34	0.43
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.63	0.43
1:A:230:MET:HA	1:A:230:MET:HE2	2.00	0.43
1:A:413:LEU:HD13	1:A:417:LEU:HD21	2.01	0.43
1:B:238:GLN:HB3	1:B:302:LEU:CD1	2.49	0.43
1:B:10:ILE:HG12	1:B:33:LEU:HD23	2.01	0.43
1:B:423:LYS:HG2	1:B:424:GLU:N	2.34	0.43
1:A:544:ILE:O	1:A:545:GLN:C	2.55	0.42
1:B:79:ILE:CA	1:B:239:GLN:NE2	2.71	0.42
1:A:34:LEU:HD12	1:A:34:LEU:C	2.39	0.42
1:A:519:THR:O	1:A:522:LYS:N	2.52	0.42
1:B:302:LEU:HA	1:B:302:LEU:HD23	1.50	0.42
1:A:31:GLN:OE1	1:A:117:ASN:ND2	2.52	0.42
1:A:41:THR:O	1:A:42:LEU:C	2.58	0.42
1:B:423:LYS:HB3	1:B:423:LYS:HE3	1.80	0.42
1:B:448:LEU:HA	1:B:448:LEU:HD23	1.77	0.42
1:A:354:LYS:O	1:A:356:THR:N	2.52	0.42
1:A:429:PHE:O	1:A:429:PHE:CD2	2.72	0.42
1:A:490:GLU:OE2	1:A:490:GLU:HA	2.19	0.42
1:A:7:PHE:CD1	1:A:7:PHE:N	2.87	0.42
1:B:386:LEU:HB3	1:B:387:ALA:H	1.70	0.42
1:B:98:GLN:HE22	1:B:298:GLU:CG	2.30	0.42
1:B:219:HIS:CE1	1:B:241:PRO:HD3	2.54	0.42
1:B:241:PRO:CB	1:B:243:TYR:HE2	2.17	0.42
1:B:299:PRO:HG2	1:B:299:PRO:O	2.18	0.42
1:B:100:ASP:OD2	1:B:302:LEU:HB2	2.19	0.42
1:B:38:ASN:ND2	1:B:40:ASP:H	2.15	0.42
1:B:485:VAL:HG11	1:B:528:PRO:HG3	2.02	0.42
1:A:95:THR:HG21	1:A:227:PHE:CD2	2.54	0.42
1:B:126:GLU:HA	1:B:126:GLU:OE1	2.20	0.42
1:B:181:ILE:HA	1:B:182:PRO:HD2	1.79	0.42
1:B:-1:SER:OG	1:B:-1:SER:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:MET:CE	1:B:115:GLN:OE1	2.67	0.42
1:B:493:ALA:HA	1:B:496:ASN:HD22	1.84	0.42
1:B:539:ALA:O	1:B:541:GLN:N	2.52	0.42
1:A:33:LEU:CD1	1:A:119:MET:O	2.68	0.42
1:A:278:PRO:CD	1:A:279:SER:N	2.82	0.42
1:B:242:CYS:HB3	1:B:297:LEU:O	2.19	0.42
1:B:305:ASN:N	1:B:305:ASN:OD1	2.48	0.42
1:B:365:LEU:CD2	1:B:367:PHE:HE1	2.32	0.42
1:B:413:LEU:O	1:B:414:VAL:C	2.58	0.42
1:B:439:LEU:HA	1:B:439:LEU:HD23	1.45	0.42
1:A:463:TRP:HE3	1:A:463:TRP:HA	1.85	0.42
1:B:131:GLU:N	1:B:134:ARG:O	2.53	0.42
1:B:190:LEU:N	1:B:190:LEU:HD23	2.35	0.42
1:B:314:THR:HG23	1:B:316:LEU:CA	2.49	0.42
1:A:31:GLN:OE1	1:A:31:GLN:HA	2.19	0.42
1:A:428:MET:SD	1:A:432:ARG:NH2	2.93	0.42
1:A:27:ARG:NH2	1:A:67:GLY:CA	2.83	0.42
1:A:393:ARG:HH11	1:A:455:LEU:HD23	1.83	0.42
1:B:316:LEU:HD22	1:B:320:VAL:HG11	2.02	0.42
1:B:446:LEU:HD23	1:B:446:LEU:HA	1.89	0.42
1:B:251:THR:O	1:B:254:VAL:HB	2.20	0.41
1:B:314:THR:CG2	1:B:316:LEU:CB	2.84	0.41
1:B:79:ILE:O	1:B:79:ILE:HG13	2.20	0.41
1:B:80:GLN:H	1:B:239:GLN:CD	2.24	0.41
1:A:12:ILE:HG23	1:A:12:ILE:HD13	1.84	0.41
1:A:259:LEU:C	1:A:261:ARG:H	2.24	0.41
1:A:317:PRO:O	1:A:321:GLN:HG3	2.19	0.41
1:A:57:GLY:O	1:A:60:VAL:N	2.51	0.41
1:B:428:MET:O	1:B:429:PHE:C	2.57	0.41
1:B:508:SER:O	1:B:511:ASP:HB2	2.20	0.41
1:A:127:ASP:OD1	1:A:128:LEU:N	2.53	0.41
1:A:25:ALA:O	1:A:30:GLN:HB2	2.21	0.41
1:A:525:THR:HG23	1:A:525:THR:O	2.19	0.41
1:A:7:PHE:CE2	1:A:33:LEU:HB2	2.55	0.41
1:B:115:GLN:O	1:B:116:PRO:C	2.56	0.41
1:A:106:GLN:O	1:A:109:ARG:N	2.54	0.41
1:A:376:GLY:HA3	1:A:379:GLU:OE1	2.20	0.41
1:A:443:ASN:OD1	1:A:447:ARG:CD	2.54	0.41
1:B:425:PRO:HB2	1:B:428:MET:HG2	2.01	0.41
1:B:450:GLU:HB3	1:B:463:TRP:CH2	2.56	0.41
1:B:487:PRO:HB3	1:B:503:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:THR:CG2	1:B:532:ALA:HA	2.51	0.41
1:A:295:ILE:HA	1:A:295:ILE:HD13	1.92	0.41
1:A:443:ASN:O	1:A:446:LEU:HB2	2.21	0.41
1:B:210:ILE:HG21	1:B:210:ILE:HD13	1.76	0.41
1:A:252:HIS:HD2	1:A:284:VAL:CG2	2.33	0.41
1:A:307:ILE:HD12	1:A:307:ILE:HA	1.72	0.41
1:B:434:GLU:O	1:B:437:LEU:HB2	2.20	0.41
1:A:129:ILE:N	1:A:137:GLY:O	2.42	0.41
1:A:167:LEU:HG	1:A:167:LEU:H	1.39	0.41
1:A:81:PHE:HB2	1:A:225:PRO:HG2	1.98	0.41
1:A:230:MET:HB3	1:A:230:MET:HE2	1.71	0.41
1:A:280:ILE:O	1:A:284:VAL:HG23	2.21	0.41
1:A:422:THR:HG23	1:A:423:LYS:O	2.20	0.41
1:A:512:LEU:HD12	1:A:529:PHE:HE2	1.85	0.41
1:B:24:ALA:HA	1:B:27:ARG:HG2	2.02	0.41
1:B:449:THR:O	1:B:449:THR:CG2	2.69	0.41
1:B:515:ARG:HA	1:B:516:PRO:HD3	1.93	0.41
1:A:224:MET:HA	1:A:225:PRO:HD2	1.62	0.41
1:B:362:ILE:O	1:B:363:GLN:O	2.38	0.41
1:B:396:ASP:CG	1:B:398:LYS:HE3	2.41	0.41
1:B:426:TYR:O	1:B:427:ARG:O	2.38	0.41
1:B:470:LEU:HD12	1:B:470:LEU:HA	1.65	0.41
1:A:104:TYR:CE1	1:A:108:VAL:HG21	2.56	0.41
1:B:436:ARG:O	1:B:438:MET:N	2.48	0.41
1:B:446:LEU:HA	1:B:466:PHE:HZ	1.86	0.41
1:A:247:THR:OG1	1:A:251:THR:HG21	2.21	0.41
1:B:127:ASP:HB2	1:B:182:PRO:CG	2.46	0.41
1:B:325:VAL:O	1:B:331:MET:HG3	2.20	0.41
1:B:390:ASN:HD21	1:B:401:TRP:H	1.67	0.41
1:A:11:ILE:HD12	1:A:21:ALA:HB3	2.03	0.41
1:A:120:ILE:HG22	1:A:121:PHE:N	2.36	0.41
1:A:203:PRO:HA	1:A:340:GLY:N	2.35	0.41
1:A:289:ASP:H	1:A:291:ASN:HA	1.80	0.41
1:A:370:GLN:C	1:A:372:ASN:N	2.70	0.41
1:A:392:ALA:O	1:A:395:SER:CB	2.69	0.41
1:A:466:PHE:C	1:A:466:PHE:CD1	2.94	0.41
1:B:184:SER:O	1:B:185:ARG:C	2.59	0.41
1:B:81:PHE:CB	1:B:225:PRO:HD2	2.51	0.41
1:B:284:VAL:CG1	1:B:284:VAL:O	2.69	0.41
1:B:386:LEU:HD22	1:B:410:LEU:HD11	2.03	0.41
1:A:159:LEU:CB	1:A:160:ASP:CA	2.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASP:OD1	1:A:208:ARG:N	2.49	0.40
1:A:312:ILE:HD13	1:A:328:MET:HE1	2.03	0.40
1:A:426:TYR:O	1:A:427:ARG:C	2.60	0.40
1:A:90:PRO:HG2	1:A:548:TYR:CD1	2.56	0.40
1:B:38:ASN:C	1:B:38:ASN:HD22	2.25	0.40
1:B:417:LEU:HD23	1:B:422:THR:H	1.86	0.40
1:A:115:GLN:HA	1:A:116:PRO:HD2	1.08	0.40
1:A:166:GLY:O	1:A:168:ASP:N	2.54	0.40
1:B:392:ALA:O	1:B:395:SER:OG	2.38	0.40
1:A:202:PRO:HB2	1:A:203:PRO:CD	2.51	0.40
1:A:212:PHE:HD2	1:A:212:PHE:H	1.67	0.40
1:A:419:THR:HB	1:A:420:LEU:HG	2.02	0.40
1:A:230:MET:HE1	1:A:465:ARG:HG2	2.04	0.40
1:B:222:ASN:CA	1:B:223:PRO:O	2.69	0.40
1:B:210:ILE:CD1	1:B:331:MET:CE	2.99	0.40
1:A:232:ASN:O	1:A:235:GLN:HB2	2.22	0.40
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.91	0.40
1:B:246:HIS:O	1:B:328:MET:HB3	2.21	0.40
1:B:98:GLN:HE22	1:B:298:GLU:CD	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/576 (90%)	383 (74%)	88 (17%)	50 (10%)	1	9
1	B	518/576 (90%)	363 (70%)	98 (19%)	57 (11%)	0	7
All	All	1039/1152 (90%)	746 (72%)	186 (18%)	107 (10%)	0	8

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLY
1	A	142	MET
1	A	160	ASP
1	A	167	LEU
1	A	212	PHE
1	A	235	GLN
1	A	237	PRO
1	A	260	ASP
1	A	262	SER
1	A	285	MET
1	A	289	ASP
1	A	433	ALA
1	A	437	LEU
1	A	474	GLU
1	A	475	ARG
1	A	482	SER
1	A	490	GLU
1	B	39	ILE
1	B	80	GLN
1	B	82	ARG
1	B	90	PRO
1	B	91	ALA
1	B	155	VAL
1	B	158	PHE
1	B	159	LEU
1	B	160	ASP
1	B	235	GLN
1	B	241	PRO
1	B	283	LYS
1	B	287	PHE
1	B	288	ALA
1	B	357	LEU
1	B	363	GLN
1	B	405	ARG
1	B	432	ARG
1	B	460	ASP
1	B	490	GLU
1	B	502	PRO
1	B	506	GLU
1	B	535	ASP
1	B	540	GLU
1	A	-2	GLY
1	A	136	VAL

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Mol	Chain	Res	Type
1	A	156	GLY
1	A	159	LEU
1	A	162	LYS
1	A	166	GLY
1	A	397	ASP
1	A	487	PRO
1	A	489	ALA
1	A	494	GLU
1	A	502	PRO
1	B	-2	GLY
1	B	68	GLY
1	B	70	MET
1	B	110	THR
1	B	157	THR
1	B	279	SER
1	B	302	LEU
1	B	305	ASN
1	B	389	LEU
1	B	415	ASP
1	B	416	ASP
1	B	422	THR
1	B	427	ARG
1	B	431	SER
1	B	447	ARG
1	A	24	ALA
1	A	103	LEU
1	A	116	PRO
1	A	294	GLN
1	B	132	ASN
1	B	260	ASP
1	B	358	GLU
1	B	376	GLY
1	B	394	LEU
1	B	406	SER
1	B	539	ALA
1	A	209	THR
1	A	464	ALA
1	A	535	ASP
1	A	536	GLU
1	B	181	ILE
1	B	289	ASP
1	B	312	ILE

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Mol	Chain	Res	Type
1	A	17	ALA
1	A	141	GLN
1	A	181	ILE
1	A	436	ARG
1	A	442	ASP
1	A	517	GLU
1	B	144	LEU
1	B	254	VAL
1	B	499	LEU
1	B	536	GLU
1	A	4	PRO
1	A	39	ILE
1	A	106	GLN
1	A	107	ALA
1	A	155	VAL
1	A	161	GLY
1	A	412	VAL
1	B	3	TYR
1	B	386	LEU
1	B	487	PRO
1	A	54	ILE
1	B	452	GLY

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	426/474 (90%)	338 (79%)	88 (21%)	1	7
1	B	427/474 (90%)	320 (75%)	107 (25%)	0	4
All	All	853/948 (90%)	658 (77%)	195 (23%)	1	5

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	GLN

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Mol	Chain	Res	Type
1	A	-1	SER
1	A	2	PHE
1	A	5	ASP
1	A	12	ILE
1	A	31	GLN
1	A	39	ILE
1	A	44	GLN
1	A	49	PRO
1	A	54	ILE
1	A	69	LEU
1	A	70	MET
1	A	76	GLN
1	A	82	ARG
1	A	92	VAL
1	A	93	ARG
1	A	96	ARG
1	A	100	ASP
1	A	106	GLN
1	A	110	THR
1	A	115	GLN
1	A	125	VAL
1	A	136	VAL
1	A	139	VAL
1	A	153	LEU
1	A	155	VAL
1	A	167	LEU
1	A	181	ILE
1	A	184	SER
1	A	187	LEU
1	A	190	LEU
1	A	197	LEU
1	A	199	THR
1	A	209	THR
1	A	217	GLN
1	A	221	ASP
1	A	222	ASN
1	A	227	PHE
1	A	230	MET
1	A	244	ILE
1	A	245	THR
1	A	251	THR
1	A	257	SER

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Mol	Chain	Res	Type
1	A	262	SER
1	A	279	SER
1	A	280	ILE
1	A	282	ASP
1	A	285	MET
1	A	287	PHE
1	A	294	GLN
1	A	302	LEU
1	A	307	ILE
1	A	310	ASN
1	A	313	SER
1	A	319	ASP
1	A	322	MET
1	A	341	TYR
1	A	343	ILE
1	A	347	PHE
1	A	354	LYS
1	A	363	GLN
1	A	371	ILE
1	A	394	LEU
1	A	397	ASP
1	A	413	LEU
1	A	422	THR
1	A	428	MET
1	A	431	SER
1	A	432	ARG
1	A	434	GLU
1	A	437	LEU
1	A	438	MET
1	A	439	LEU
1	A	440	ARG
1	A	445	ASP
1	A	448	LEU
1	A	450	GLU
1	A	453	ARG
1	A	461	GLU
1	A	481	LYS
1	A	484	TRP
1	A	485	VAL
1	A	488	SER
1	A	502	PRO
1	A	527	THR

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Mol	Chain	Res	Type
1	A	534	THR
1	A	540	GLU
1	A	549	GLU
1	B	-3	GLN
1	B	2	PHE
1	B	9	VAL
1	B	27	ARG
1	B	30	GLN
1	B	33	LEU
1	B	35	LEU
1	B	37	HIS
1	B	38	ASN
1	B	39	ILE
1	B	44	GLN
1	B	46	SER
1	B	54	ILE
1	B	59	LEU
1	B	69	LEU
1	B	72	LYS
1	B	74	ILE
1	B	79	ILE
1	B	82	ARG
1	B	106	GLN
1	B	110	THR
1	B	114	ASN
1	B	119	MET
1	B	120	ILE
1	B	122	GLN
1	B	133	ASP
1	B	139	VAL
1	B	141	GLN
1	B	149	LYS
1	B	153	LEU
1	B	157	THR
1	B	163	ILE
1	B	180	SER
1	B	184	SER
1	B	186	ARG
1	B	187	LEU
1	B	190	LEU
1	B	193	ARG
1	B	197	LEU

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Mol	Chain	Res	Type
1	B	199	THR
1	B	205	ILE
1	B	208	ARG
1	B	209	THR
1	B	214	VAL
1	B	222	ASN
1	B	227	PHE
1	B	228	SER
1	B	230	MET
1	B	232	ASN
1	B	234	SER
1	B	238	GLN
1	B	240	VAL
1	B	243	TYR
1	B	245	THR
1	B	247	THR
1	B	251	THR
1	B	259	LEU
1	B	282	ASP
1	B	286	ARG
1	B	289	ASP
1	B	290	ARG
1	B	292	GLN
1	B	295	ILE
1	B	303	THR
1	B	304	SER
1	B	306	GLU
1	B	307	ILE
1	B	310	ASN
1	B	312	ILE
1	B	313	SER
1	B	314	THR
1	B	319	ASP
1	B	323	GLN
1	B	326	ARG
1	B	336	ILE
1	B	338	ARG
1	B	339	PRO
1	B	343	ILE
1	B	351	ARG
1	B	355	PRO
1	B	356	THR

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Mol	Chain	Res	Type
1	B	361	PHE
1	B	363	GLN
1	B	377	TYR
1	B	389	LEU
1	B	399	GLU
1	B	420	LEU
1	B	422	THR
1	B	430	THR
1	B	431	SER
1	B	432	ARG
1	B	470	LEU
1	B	471	GLU
1	B	474	GLU
1	B	476	GLU
1	B	481	LYS
1	B	484	TRP
1	B	499	LEU
1	B	502	PRO
1	B	512	LEU
1	B	513	LEU
1	B	518	MET
1	B	519	THR
1	B	534	THR
1	B	542	VAL
1	B	547	LYS
1	B	548	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	31	GLN
1	A	38	ASN
1	A	80	GLN
1	A	117	ASN
1	A	217	GLN
1	A	218	GLN
1	A	222	ASN
1	A	232	ASN
1	A	252	HIS
1	A	294	GLN
1	A	310	ASN

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Mol	Chain	Res	Type
1	A	363	GLN
1	A	370	GLN
1	A	383	GLN
1	A	390	ASN
1	A	541	GLN
1	B	30	GLN
1	B	31	GLN
1	B	38	ASN
1	B	44	GLN
1	B	85	ASN
1	B	98	GLN
1	B	117	ASN
1	B	217	GLN
1	B	222	ASN
1	B	232	ASN
1	B	236	HIS
1	B	239	GLN
1	B	252	HIS
1	B	291	ASN
1	B	292	GLN
1	B	310	ASN
1	B	363	GLN
1	B	383	GLN
1	B	390	ASN
1	B	545	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

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	A	551	-	4,4,4	0.17	0	6,6,6	0.50	0
2	SO4	A	552	-	4,4,4	0.19	0	6,6,6	0.56	0
2	SO4	B	1	-	4,4,4	0.25	0	6,6,6	0.52	0
2	SO4	B	551	-	4,4,4	0.24	0	6,6,6	0.31	0

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
2	SO4	A	551	-	-	0/0/0/0	0/0/0/0
2	SO4	A	552	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	551	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	551	SO4	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	527/576 (91%)	0.36	26 (4%)	30 24	53, 73, 123, 136	0
1	B	524/576 (90%)	0.60	49 (9%)	9 9	55, 79, 130, 137	0
All	All	1051/1152 (91%)	0.48	75 (7%)	17 15	53, 75, 128, 137	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	LEU	5.6
1	A	485	VAL	5.5
1	B	507	ALA	5.4
1	B	289	ASP	5.3
1	B	164	HIS	5.1
1	A	486	THR	4.8
1	B	506	GLU	4.6
1	A	507	ALA	4.4
1	B	485	VAL	4.3
1	B	486	THR	4.0
1	B	503	LEU	4.0
1	A	498	HIS	3.9
1	A	491	ALA	3.8
1	B	498	HIS	3.8
1	B	286	ARG	3.8
1	B	499	LEU	3.7
1	A	504	SER	3.7
1	B	525	THR	3.7
1	B	285	MET	3.6
1	A	506	GLU	3.6
1	A	518	MET	3.6
1	B	292	GLN	3.4
1	B	475	ARG	3.4
1	B	484	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	214	VAL	3.3
1	A	532	ALA	3.3
1	A	180	SER	3.3
1	B	472	ASN	3.2
1	B	529	PHE	3.2
1	A	501	ALA	3.1
1	B	288	ALA	3.1
1	A	499	LEU	3.1
1	B	500	THR	3.1
1	A	483	THR	3.0
1	B	523	LEU	3.0
1	B	479	ARG	3.0
1	A	512	LEU	2.9
1	B	480	LEU	2.9
1	A	529	PHE	2.9
1	B	491	ALA	2.9
1	A	527	THR	2.9
1	A	493	ALA	2.9
1	B	483	THR	2.8
1	B	505	ARG	2.8
1	A	484	TRP	2.8
1	B	284	VAL	2.7
1	A	215	LEU	2.7
1	B	180	SER	2.7
1	B	495	VAL	2.7
1	A	482	SER	2.6
1	A	526	LEU	2.6
1	B	250	LYS	2.5
1	A	495	VAL	2.5
1	B	527	THR	2.5
1	A	505	ARG	2.5
1	A	550	GLY	2.5
1	B	512	LEU	2.5
1	B	493	ALA	2.5
1	B	533	LEU	2.4
1	B	526	LEU	2.4
1	B	528	PRO	2.4
1	B	256	ARG	2.4
1	A	244	ILE	2.4
1	B	287	PHE	2.3
1	B	290	ARG	2.3
1	B	504	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	215	LEU	2.2
1	B	316	LEU	2.2
1	B	490	GLU	2.2
1	B	518	MET	2.1
1	B	474	GLU	2.1
1	B	261	ARG	2.1
1	B	510	GLU	2.0
1	B	476	GLU	2.0
1	B	291	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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
2	SO4	B	1	5/5	0.96	0.33	1.36	77,78,78,78	0
2	SO4	A	551	5/5	0.97	0.23	-0.02	71,72,72,72	0
2	SO4	A	552	5/5	0.93	0.26	-	79,79,79,80	0
2	SO4	B	551	5/5	0.91	0.25	-	85,85,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.