



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:10 PM GMT

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 : 2009-01-27
Resolution : 3.49 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

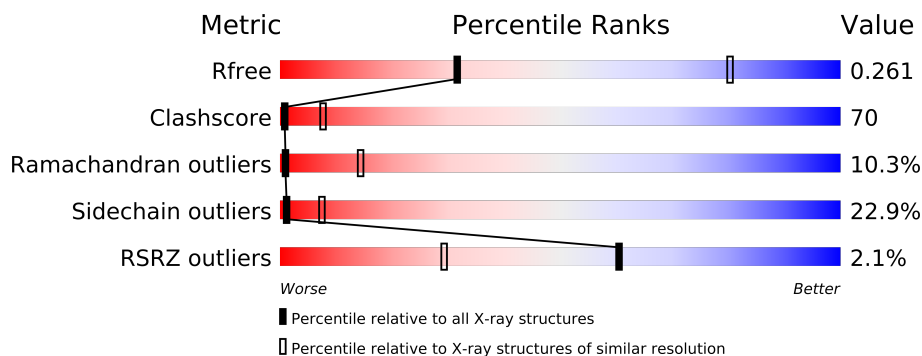
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8156 atoms, of which 0 are hydrogen and 0 are deuterium.

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-carboxymethylaminomethylmodification 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	B	1	Total	O	S	0	0
			5	4	1		
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		

E536	Q537	A538	A539	E540	Q541	V542	E543	I544	Q545	V546	K547	Y548	E549	G550	L103	Y104	R105	Q106	A107	V108	R109	T110	A111	L112	E113	N114	Q115	P116	N117	L118	M119	I120	F121	Q122	Q123	A124	V125	E126	L127	L128	I129	V130	E131	N132	V133	R134	V135	V136	G137	A138	V139	T140	Q141	L144	K145	F146	R147	A148	K149	A150	V151	V152	L153	T154	V155	G156	T157	F158	L159	D160	G161	K162	I163		
															H164	I165	G166	LEU	ASP	ASN	TYR	SER	GLY	GLY	ARG	ALA	GLY	ASP	PRO	S180	I181	P182	L183	S184	R185	R186	L187	R188	E189	L190	P191	L192	V193	V194	G195	R196	L197	K198	T199	G200	V139	T140	Q141	R204	L205	D206	A207	R208	T209	I210	D211	F212	V151	S213	V214	L215	A216	Q217	Q218	I219	N222	P223	M224	P225	
															V226	F227	A228	D229	R230	N231	Q232	A233	S234	Q235	H236	P237	Q238	Q239	V240	P241	C242	Y243	I244	T245	H246	T247	N248	E249	K250	R251	H252	V253	V254	I255	R256	L259	D260	R261	S262	PRO	MET	TYR	ALA	GLY	VAL	ILE	GLU	GLY	VAL	GLY	PRO	ARG	TYR	CYS	P278	S279	Q279	I280	E281	K283	V284	M285	R286		
															F287	F347	A288	D289	R290	N291	Q292	H293	Q294	F296	L297	E298	P299	E300	G301	L302	T303	S304	N305	E306	I307	Y308	P309	N310	G311	R312	S313	T314	S315	L316	P317	F318	D319	V320	Q321	N322	Q323	T324	V325	R326	N390	S327	N328	Q329	Q330	N331	E332	N333	A334	K335	I336	V337	R338	P339	G340	Y341	A342	T343	E344	Y345	D346
															F347	F348	D349	P350	R351	P355	T356	L357	E358	S359	K360	F361	I362	Q363	G364	F365	F366	F367	A368	Q369	Q370	I371	N372	G373	G376	Y377	E378	E379	A380	A381	A382	Q383	G384	L385	L386	A387	G388	L389	N390	A391	A392	R393	L394	S395	D396	D397	K398	E399	G400	W401	A402	P403	A404	R405	S406	Q407	A408	Y409			
															L410	G411	V412	L413	V414	D415	D416	L417	L420	G421	T422	K423	E424	P425	Y426	R427	M428	F429	T430	S431	R432	A433	E434	Y435	R436	L437	M438	L439	R440	E441	D442	M443	A444	D445	L446	R447	L448	T449	E450	I451	G452	R453	E454	L455	G456	L457	V458	D459	D460	E461	R462	W463	F466	N467	E468	K469	L470	E471			
															N472	I473	E474	R475	E476	R479	L480	K481	S482	T483	W484	V485	T486	P487	S488	A489	E490	A491	A492	A493	E494	V495	N496	L499	T500	A501	P502	L503	S504	R505	E506	A507	S508	D511	L512	L513	R514	R515	P516	E517	M518	T519	Y520	E521	K522	L523	T524	T525	L526	P527	P528	F529	A532	L533	T534	D535					

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 5.4.0069	Depositor
R, R_{free}	0.227 , 0.265 0.226 , 0.261	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 , 83.5	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42342 reflections	Xtriage
F_o, F_c correlation	0.90	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.

5 Model quality i

5.1 Standard geometry i

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 70.

All (1141) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(Å)
1:A:312:ILE:HG21	1:A:328:MET:HE1	1.29	1.14
1:B:12:ILE:O	1:B:154:THR:HG22	0.97	1.14
1:A:314:THR:HG22	1:A:316:LEU:H	1.05	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:404:ALA:CB	1:A:407:GLN:HG3	1.84	1.06
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: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:180:SER:O	1:B:181:ILE:CG2	2.07	1.02
1:B:156:GLY:O	1:B:157:THR:HG23	1.57	1.02
1:A:166:GLY:N	1:A:315:SER:O	1.93	1.02
1:A:205:ILE:HG21	1:A:210:ILE:HD11	1.42	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:230:MET:CE	1:B:230:MET:HA	1.89	1.01
1:A:262:SER:OG	1:A:263:PRO:HD2	1.57	1.01
1:B:252:HIS:HD2	1:B:284:VAL:HG11	1.26	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:448:LEU:CD2	1:A:451:ILE:HD11	1.92	0.98
1:A:108:VAL:O	1:A:112:LEU:HD12	1.63	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:424:GLU:OE2	1:A:436:ARG:NH2	2.01	0.94
1:A:247:THR:HG22	1:A:293:HIS:H	1.29	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:203:PRO:HB3	1:A:340:GLY:H	1.34	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:B:427:ARG:HH21	1:B:428:MET:HE1	1.37	0.89
1:A:530:ALA:HB1	1:A:531:PRO:HA	1.54	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:3:TYR:HD2	1:B:5:ASP:H	1.22	0.86
1:B:417:LEU:O	1:B:421:GLY:HA2	1.74	0.86
1:B:158:PHE:O	1:B:159:LEU:C	2.09	0.85
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:361:PHE:N	1:B:361:PHE:HD2	1.71	0.84
1:A:163:ILE:CG2	1:A:341:TYR:CD2	2.59	0.84
1:B:181:ILE:HG23	1:B:184:SER:HB2	1.58	0.84
1:A:440:ARG:HH21	1:A:544:ILE:CG2	1.90	0.84
1:A:351:ARG:HD2	1:A:421:GLY:HA3	1.60	0.84
1:A:262:SER:HB2	1:A:263:PRO:HD2	1.57	0.84
1:A:253:ASP:O	1:A:257:SER:OG	1.95	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: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:81:PHE:CB	1:A:225:PRO:HG2	2.07	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: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:A:440:ARG:NH2	1:A:544:ILE:HG21	1.94	0.81
1:A:159:LEU:HB3	1:A:160:ASP:CA	2.09	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:540:GLU:O	1:B:544:ILE:HG12	1.80	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:A:432:ARG:HB2	1:A:436:ARG:HH11	1.46	0.81
1:A:234:SER:O	1:A:236:HIS:N	2.14	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:541:GLN:HG3	1:B:545:GLN:NE2	1.97	0.78
1:A:382:ALA:HB1	1:A:410:LEU:HD23	1.64	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:209:THR:HG21	1:B:335:LYS:HB2	1.66	0.77
1:B:158:PHE:O	1:B:158:PHE:CG	2.37	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: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:A:199:THR:O	1:A:343:ILE:HD12	1.85	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:156:GLY:O	1:A:157:THR:CG2	2.29	0.76
1:A:139:VAL:CG1	1:A:145:LYS:HG2	2.15	0.76
1:B:247:THR:HG23	1:B:248:ASN:N	2.00	0.76
1:A:473:ILE:HG23	1:A:542:VAL:HG23	1.67	0.76
1:B:155:VAL:O	1:B:155:VAL:CG2	2.29	0.76
1:A:439:LEU:HD23	1:A:439:LEU:H	1.46	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:45:MET:HG2	1:B:377:TYR:HE2	1.51	0.76
1:B:165:ILE:HG22	1:B:341:TYR:HA	1.68	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:B:356:THR:O	1:B:357:LEU:HB2	1.87	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:CG	1:A:96:ARG:HH11	2.01	0.74
1:B:90:PRO:CB	1:B:440:ARG:HD2	2.14	0.74
1:A:389:LEU:HD22	1:A:457:LEU:HD11	1.69	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:B:72:LYS:O	1:B:73:ALA:C	2.25	0.74
1:A:465:ARG:NH1	1:A:535:ASP:OD2	2.17	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:B:241:PRO:HB2	1:B:243:TYR:HE2	1.52	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:389:LEU:HD13	1:A:457:LEU:HD21	1.69	0.73
1:A:103:LEU:O	1:A:106:GLN:HB3	1.87	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:B:20:GLU:HG3	1:B:381:ALA:HB1	1.71	0.72
1:A:404:ALA:CB	1:A:407:GLN:CG	2.55	0.72
1:A:129:ILE:HG22	1:A:136:VAL:HG13	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:B:27:ARG:HH11	1:B:27:ARG:HG2	1.55	0.72
1:A:385:LEU:HD23	1:A:385:LEU:C	2.09	0.72
1:B:190:LEU:HD11	1:B:362:ILE:HD11	1.70	0.72
1:A:28:MET:HE2	1:A:392:ALA:HB1	1.71	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:239:GLN:C	1:B:240:VAL:HG12	2.11	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:A:413:LEU:HD11	1:A:417:LEU:HD11	1.72	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:155:VAL:HG11	1:B:371:ILE:HB	1.73	0.70
1:B:191:PRO:HG2	1:B:361:PHE:CE1	2.26	0.70
1:B:126:GLU:O	1:B:182:PRO:HG2	1.90	0.70
1:A:209:THR:HB	1:A:334:ALA:CA	2.19	0.70
1:B:127:ASP:HB2	1:B:182:PRO:HG2	1.74	0.70
1:B:45:MET:CG	1:B:377:TYR:CE2	2.72	0.70
1:B:252:HIS:CD2	1:B:284:VAL:CG1	2.71	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: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:B:9:VAL:HG21	1:B:25:ALA:HB1	1.72	0.69
1:A:511:ASP:HA	1:A:514:ARG:HH21	1.57	0.69
1:B:309:PRO:HB2	1:B:312:ILE:HD11	1.74	0.69
1:B:78:GLY:CA	1:B:98:GLN:O	2.41	0.69
1:A:28:MET:HE1	1:A:392:ALA:HB3	1.74	0.69
1:A:468:GLU:O	1:A:472:ASN:HB2	1.92	0.69
1:B:470:LEU:O	1:B:473:ILE:N	2.19	0.69
1:A:222:ASN:HD22	1:A:223:PRO:HA	1.58	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:467:ASN:O	1:B:470:LEU:N	2.22	0.68
1:A:473:ILE:HG23	1:A:542:VAL:CG2	2.24	0.68
1:A:45:MET:HE1	1:A:49:PRO:HA	1.74	0.68
1:A:102:VAL:HG12	1:A:103:LEU:N	2.09	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: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:115:GLN:HG3	1:A:115:GLN:O	1.95	0.66
1:B:230:MET:CE	1:B:230:MET:CA	2.71	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: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:B:347:PHE:CE1	1:B:373:GLY:HA3	2.31	0.66
1:A:165:ILE:C	1:A:166:GLY:O	2.31	0.66
1:B:80:GLN:OE1	1:B:242:CYS:SG	2.54	0.66
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:217:GLN:NE2	1:A:219:HIS:NE2	2.44	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:292:GLN:CA	1:B:292:GLN:HE21	2.09	0.65
1:A:481:LYS:O	1:A:483:THR:N	2.29	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:B:356:THR:HG22	1:B:390:ASN:OD1	1.96	0.65
1:B:243:TYR:N	1:B:243:TYR:CD2	2.64	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:A:155:VAL:HG12	1:A:156:GLY:H	1.61	0.64
1:A:285:MET:N	1:A:285:MET:HE2	1.99	0.64
1:B:226:VAL:CG2	1:B:232:ASN:HA	2.26	0.64
1:A:417:LEU:N	1:A:417:LEU:HD23	2.11	0.64
1:A:244:ILE:HD13	1:A:296:PHE:CE1	2.32	0.64
1:B:154:THR:CG2	1:B:155:VAL:N	2.31	0.64
1:B:38:ASN:HD22	1:B:40:ASP:H	1.45	0.64
1:A:203:PRO:CB	1:A:340:GLY:H	2.06	0.64
1:B:251:THR:O	1:B:255:ILE:HG13	1.97	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:A:219:HIS:CE1	1:A:241:PRO:HB3	2.32	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:B:247:THR:CG2	1:B:248:ASN:N	2.60	0.64
1:A:405:ARG:HD2	1:A:415:ASP:OD2	1.97	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
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:432:ARG:O	1:A:434:GLU:N	2.32	0.63
1:A:314:THR:CG2	1:A:316:LEU:N	2.53	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:58:HIS:CE1	1:B:429:PHE:HZ	2.14	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:197:LEU:CD1	1:B:345:TYR:HB2	2.28	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: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:392:ALA:O	1:A:395:SER:N	2.31	0.63
1:A:430:THR:O	1:A:433:ALA:HB3	1.98	0.62
1:A:28:MET:CE	1:A:392:ALA:CB	2.77	0.62
1:A:48:ASN:HB2	1:A:49:PRO:CD	2.29	0.62
1:A:206:ASP:HB2	1:A:337:VAL:CG2	2.29	0.62
1:A:408:ALA:HB2	1:A:448:LEU:HD11	1.81	0.62
1:A:343:ILE:N	1:A:343:ILE:HD12	2.15	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:B:54:ILE:HD11	1:B:85:ASN:HD21	1.64	0.62
1:A:95:THR:HG22	1:A:227:PHE:HE2	1.63	0.62
1:B:126:GLU:HB3	1:B:139:VAL:O	2.00	0.62
1:A:209:THR:CB	1:A:334:ALA:HA	2.23	0.62
1:B:318:PHE:CE1	1:B:336:ILE:HG21	2.35	0.62
1:B:377:TYR:CD1	1:B:377:TYR:N	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:B:122:GLN:O	1:B:123:GLN:HG2	2.00	0.61
1:A:108:VAL:O	1:A:112:LEU:CD1	2.46	0.61
1:B:158:PHE:O	1:B:159:LEU:O	2.17	0.61
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:A:11:ILE:HG13	1:A:22:ALA:HB2	1.82	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:38:ASN:C	1:B:40:ASP:N	2.52	0.61
1:B:366:PHE:CD1	1:B:391:ALA:HB2	2.35	0.61
1:B:287:PHE:O	1:B:288:ALA:HB2	1.99	0.61
1:A:201:THR:HG22	1:A:202:PRO:CD	2.29	0.61
1:B:544:ILE:O	1:B:548:TYR:HD1	1.84	0.61
1:B:7:PHE:N	1:B:147:ARG:O	2.28	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:191:PRO:HG2	1:A:361:PHE:CE2	2.35	0.61
1:A:37:HIS:NE2	1:A:157:THR:HG23	2.15	0.61
1:A:312:ILE:HG21	1:A:328:MET:CE	2.19	0.61
1:A:210:ILE:HG22	1:A:212:PHE:CE2	2.36	0.61
1:A:341:TYR:N	1:A:341:TYR:HD1	1.99	0.61
1:A:247:THR:HG22	1:A:293:HIS:N	2.10	0.61
1:B:62:GLU:HG2	1:B:448:LEU:HD12	1.82	0.61
1:B:127:ASP:O	1:B:138:ALA:HB1	2.01	0.60
1:A:202:PRO:HA	1:A:313:SER:HA	1.81	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:B:79:ILE:O	1:B:79:ILE:CG1	2.49	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:A:491:ALA:C	1:A:493:ALA:H	2.02	0.60
1:B:318:PHE:HE1	1:B:336:ILE:HG21	1.65	0.60
1:A:96:ARG:CG	1:A:96:ARG:NH1	2.63	0.60
1:B:163:ILE:HD12	1:B:163:ILE:H	1.66	0.60
1:B:282:ASP:C	1:B:284:VAL:H	2.04	0.60
1:A:465:ARG:HD2	1:A:465:ARG:O	2.01	0.60
1:A:53:GLY:N	1:A:96:ARG:HB3	2.17	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:A:215:LEU:HD13	1:A:245:THR:HG22	1.81	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: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:96:ARG:HG3	1:A:96:ARG:HH11	1.66	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
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: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:A:139:VAL:HG13	1:A:145:LYS:CG	2.32	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:B:37:HIS:ND1	1:B:38:ASN:HB2	2.17	0.59
1:A:448:LEU:O	1:A:451:ILE:CG1	2.47	0.59
1:A:408:ALA:O	1:A:411:GLY:N	2.35	0.59
1:A:341:TYR:CD1	1:A:341:TYR:N	2.71	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:79:ILE:HA	1:B:239:GLN:HE21	1.65	0.59
1:A:240:VAL:HG23	1:A:241:PRO:N	2.18	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:247:THR:CG2	1:A:293:HIS:H	2.09	0.59
1:A:228:SER:OG	1:A:229:PHE:N	2.34	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:152:VAL:HG22	1:A:366:PHE:HB2	1.84	0.58
1:A:349:ASP:OD1	1:A:350:PRO:HD2	2.03	0.58
1:A:527:THR:N	1:A:528:PRO:CD	2.67	0.58
1:B:360:LYS:C	1:B:361:PHE:HD2	2.05	0.58
1:A:230:MET:CE	1:A:230:MET:HA	2.33	0.58
1:B:191:PRO:HB2	1:B:361:PHE:CZ	2.37	0.58
1:A:61:LYS:HG3	1:A:441:GLU:HG2	1.85	0.58
1:A:106:GLN:O	1:A:110:THR:HG23	2.03	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:B:443:ASN:OD1	1:B:447:ARG:NH1	2.37	0.58
1:A:17:ALA:HB2	1:A:380:ALA:HB1	1.85	0.58
1:B:158:PHE:C	1:B:159:LEU:O	2.40	0.58
1:B:110:THR:O	1:B:114:ASN:HB2	2.04	0.58
1:A:491:ALA:C	1:A:493:ALA:N	2.57	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:537:GLN:O	1:B:540:GLU:HB3	2.04	0.57
1:B:48:ASN:ND2	1:B:50:ALA:HB3	2.18	0.57
1:B:452:GLY:O	1:B:453:ARG:C	2.43	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:232:ASN:N	1:B:232:ASN:HD22	2.02	0.57
1:B:95:THR:N	1:B:441:GLU:OE2	2.37	0.57
1:B:70:MET:HG2	1:B:70:MET:O	2.03	0.57
1:A:389:LEU:HD21	1:A:455:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:12:ILE:HG22	1:B:12:ILE:O	2.04	0.57
1:A:448:LEU:HD23	1:A:451:ILE:CD1	2.20	0.57
1:B:243:TYR:N	1:B:243:TYR:HD2	2.01	0.57
1:A:10:ILE:HG13	1:A:148:ALA:HB2	1.87	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:45:MET:HE1	1:A:50:ALA:N	2.20	0.57
1:B:156:GLY:C	1:B:157:THR:HG22	2.25	0.57
1:A:453:ARG:HG2	1:A:463:TRP:CZ2	2.39	0.57
1:A:53:GLY:CA	1:A:96:ARG:HB3	2.35	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:194:VAL:HG22	1:B:348:PHE:CD1	2.41	0.56
1:B:314:THR:CG2	1:B:316:LEU:N	2.68	0.56
1:B:80:GLN:H	1:B:239:GLN:HE22	1.52	0.56
1:A:319:ASP:N	1:A:319:ASP:OD2	2.38	0.56
1:B:81:PHE:O	1:B:82:ARG:O	2.23	0.56
1:A:513:LEU:HD23	1:A:546:VAL:HG11	1.88	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:33:LEU:HD12	1:A:119:MET:O	2.05	0.56
1:A:45:MET:CE	1:A:49:PRO:CA	2.75	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:B:165:ILE:HG23	1:B:341:TYR:CB	2.36	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
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:127:ASP:HA	1:A:183:LEU:HB2	1.88	0.56
1:A:261:ARG:O	1:A:262:SER:O	2.23	0.56
1:B:191:PRO:HD2	1:B:361:PHE:CD1	2.41	0.55
1:B:306:GLU:OE1	1:B:338:ARG:NH1	2.39	0.55
1:B:279:SER:HB2	1:B:282:ASP:HB2	1.88	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:LEU:O	1:B:71:ALA:N	2.40	0.55
1:B:380:ALA:O	1:B:381:ALA:C	2.42	0.55
1:B:205:ILE:HD11	1:B:336:ILE:HG13	1.89	0.55
1:B:486:THR:C	1:B:488:SER:H	2.10	0.55
1:A:496:ASN:HD22	1:A:502:PRO:HB3	1.72	0.55
1:A:85:ASN:O	1:A:93:ARG:HD3	2.05	0.55
1:A:155:VAL:HG11	1:A:370:GLN:HE21	1.72	0.55
1:B:98:GLN:HE22	1:B:298:GLU:HG2	1.72	0.55
1:B:349:ASP:OD2	1:B:351:ARG:NH1	2.39	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: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:181:ILE:O	1:B:181:ILE:HG23	2.07	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: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:371:ILE:HG23	1:B:372:ASN:N	2.22	0.54
1:B:234:SER:O	1:B:236:HIS:N	2.40	0.54
1:B:320:VAL:HG12	1:B:324:ILE:HD11	1.89	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:A:209:THR:HG21	1:A:335:LYS:HG3	0.83	0.54
1:B:476:GLU:HG2	1:B:533:LEU:HD22	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
1:A:503:LEU:HD21	1:A:512:LEU:HD21	1.88	0.54
1:B:337:VAL:HG12	1:B:338:ARG:HG3	1.90	0.54
1:A:440:ARG:NH1	1:A:440:ARG:HG3	2.23	0.54
1:A:240:VAL:HG23	1:A:241:PRO:O	2.08	0.54
1:B:525:THR:HG22	1:B:526:LEU:HD23	1.88	0.54
1:B:162:LYS:O	1:B:343:ILE:HG22	2.06	0.54
1:A:211:ASP:C	1:A:213:SER:H	2.10	0.54
1:B:33:LEU:HD12	1:B:119:MET:HG2	1.89	0.54
1:A:278:PRO:CD	1:A:279:SER:H	2.21	0.54
1:B:252:HIS:CD2	1:B:284:VAL:HG13	2.43	0.54
1:A:72:LYS:O	1:A:73:ALA:C	2.46	0.54
1:B:35:LEU:CD1	1:B:125:VAL:HG23	2.38	0.54
1:B:241:PRO:HB3	1:B:243:TYR:CE2	2.43	0.54
1:A:469:LYS:HE3	1:A:537:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:436:ARG:O	1:A:437:LEU:CB	2.51	0.54
1:A:155:VAL:CG1	1:A:370:GLN:HE21	2.19	0.54
1:A:79:ILE:HD11	1:A:299:PRO:HB2	1.90	0.54
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.73	0.54
1:A:488:SER:O	1:A:492:ALA:HB2	2.08	0.54
1:B:139:VAL:CG1	1:B:145:LYS:HG2	2.19	0.54
1:A:408:ALA:HA	1:A:447:ARG:NH2	2.21	0.54
1:B:317:PRO:HD2	1:B:320:VAL:HG21	1.90	0.54
1:A:351:ARG:HD2	1:A:420:LEU:C	2.27	0.54
1:B:404:ALA:O	1:B:407:GLN:N	2.28	0.54
1:A:485:VAL:HG23	1:A:503:LEU:CD1	2.38	0.54
1:B:372:ASN:HD22	1:B:383:GLN:NE2	2.06	0.54
1:B:190:LEU:CB	1:B:191:PRO:HD2	2.38	0.54
1:A:437:LEU:HD12	1:A:437:LEU:C	2.29	0.53
1:A:293:HIS:CD2	1:A:293:HIS:N	2.75	0.53
1:A:127:ASP:OD1	1:A:186:ARG:NH1	2.42	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:B:190:LEU:HB3	1:B:191:PRO:CD	2.39	0.53
1:A:2:PHE:CE1	1:A:145:LYS:HB3	2.43	0.53
1:B:96:ARG:CG	1:B:96:ARG:O	2.47	0.53
1:B:292:GLN:HA	1:B:292:GLN:NE2	2.22	0.53
1:A:70:MET:HE3	1:A:381:ALA:HB2	1.90	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
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: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:187:LEU:O	1:A:190:LEU:HG	2.09	0.53
1:B:399:GLU:OE1	1:B:399:GLU:HA	2.09	0.53
1:A:413:LEU:CD1	1:A:417:LEU:HD11	2.39	0.53
1:B:62:GLU:CD	1:B:408:ALA:HB1	2.28	0.53
1:B:404:ALA:O	1:B:407:GLN:HB2	2.08	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:B:362:ILE:O	1:B:363:GLN:C	2.47	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:ALA:CB	1:A:407:GLN:CD	2.77	0.52
1:A:205:ILE:CG2	1:A:210:ILE:CD1	2.85	0.52
1:A:314:THR:CG2	1:A:315:SER:H	2.08	0.52
1:A:30:GLN:CA	1:A:30:GLN:NE2	2.70	0.52
1:B:62:GLU:HG2	1:B:448:LEU:CD1	2.38	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: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:B:37:HIS:ND1	1:B:37:HIS:O	2.41	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:238:GLN:HB3	1:B:302:LEU:HD11	1.92	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:A:11:ILE:HG13	1:A:22:ALA:CA	2.39	0.52
1:A:289:ASP:O	1:A:291:ASN:O	2.27	0.52
1:B:409:TYR:HA	1:B:412:VAL:HG23	1.92	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:A:49:PRO:HD2	1:A:298:GLU:OE1	2.09	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:B:226:VAL:HG12	1:B:227:PHE:N	2.24	0.52
1:A:393:ARG:NH1	1:A:455:LEU:CD2	2.73	0.52
1:B:2:PHE:CE2	1:B:145:LYS:HE3	2.45	0.52
1:A:13:GLY:CA	1:A:154:THR:HG21	2.39	0.52
1:B:385:LEU:HD21	1:B:457:LEU:CD1	2.40	0.52
1:A:385:LEU:HD23	1:A:385:LEU:O	2.10	0.52
1:B:35:LEU:HD12	1:B:125:VAL:HG23	1.92	0.51
1:B:385:LEU:HD21	1:B:457:LEU:HD13	1.91	0.51
1:A:8:ASP:HB3	1:A:395:SER:HB2	1.92	0.51
1:A:155:VAL:CG1	1:A:156:GLY:H	2.14	0.51
1:B:426:TYR:O	1:B:429:PHE:N	2.40	0.51
1:B:415:ASP:O	1:B:416:ASP:C	2.49	0.51
1:A:95:THR:HG21	1:A:227:PHE:CE2	2.46	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:B:205:ILE:HG23	1:B:206:ASP:H	1.75	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:539:ALA:O	1:B:540:GLU:C	2.49	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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: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:A:129:ILE:HB	1:A:137:GLY:O	2.11	0.51
1:B:30:GLN:HA	1:B:30:GLN:NE2	2.26	0.51
1:B:30:GLN:CA	1:B:30:GLN:NE2	2.74	0.51
1:B:130:VAL:HG21	1:B:186:ARG:HE	1.76	0.51
1:B:379:GLU:N	1:B:379:GLU:OE1	2.28	0.51
1:A:262:SER:CB	1:A:263:PRO:HD3	2.34	0.51
1:A:206:ASP:N	1:A:337:VAL:HG23	2.25	0.51
1:A:2:PHE:CE1	1:A:145:LYS:CB	2.94	0.51
1:B:259:LEU:C	1:B:261:ARG:H	2.14	0.51
1:A:154:THR:HG23	1:A:155:VAL:N	2.26	0.50
1:A:262:SER:OG	1:A:263:PRO:N	2.39	0.50
1:B:159:LEU:HB3	1:B:160:ASP:CA	2.41	0.50
1:A:460:ASP:O	1:A:461:GLU:C	2.48	0.50
1:B:56:LYS:O	1:B:60:VAL:HG23	2.11	0.50
1:A:161:GLY:O	1:A:162:LYS:O	2.29	0.50
1:B:437:LEU:HG	1:B:437:LEU:O	2.12	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
1:A:62:GLU:CD	1:A:447:ARG:HH22	2.15	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:A:471:GLU:O	1:A:472:ASN:C	2.46	0.50
1:A:185:ARG:O	1:A:186:ARG:C	2.49	0.50
1:A:429:PHE:CD2	1:A:429:PHE:C	2.84	0.50
1:B:393:ARG:O	1:B:394:LEU:C	2.50	0.50
1:B:19:THR:HG23	1:B:112:LEU:HD11	1.92	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:B:12:ILE:C	1:B:154:THR:CG2	2.75	0.50
1:A:155:VAL:O	1:A:156:GLY:O	2.30	0.50
1:A:62:GLU:CD	1:A:408:ALA:HB1	2.31	0.50
1:B:156:GLY:O	1:B:157:THR:O	2.30	0.50
1:A:199:THR:HG22	1:A:343:ILE:CD1	2.42	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:488:SER:O	1:A:489:ALA:O	2.30	0.49
1:B:83:ILE:HG22	1:B:83:ILE:O	2.11	0.49
1:A:101:ARG:HD2	1:A:300:GLU:OE2	2.12	0.49
1:A:255:ILE:HG21	1:A:281:GLU:HA	1.95	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:322:MET:O	1:B:326:ARG:HB2	2.13	0.49
1:B:106:GLN:O	1:B:106:GLN:HG3	2.12	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:B:331:MET:N	1:B:332:GLU:OE1	2.45	0.49
1:B:300:GLU:OE2	1:B:308:TYR:HD1	1.96	0.49
1:B:417:LEU:O	1:B:421:GLY:CA	2.53	0.49
1:A:479:ARG:HA	1:A:482:SER:HB2	1.95	0.49
1:A:423:LYS:HE3	1:A:424:GLU:O	2.12	0.49
1:A:165:ILE:O	1:A:166:GLY:O	2.30	0.49
1:B:292:GLN:CA	1:B:292:GLN:NE2	2.75	0.49
1:B:366:PHE:CE1	1:B:391:ALA:CB	2.90	0.49
1:B:165:ILE:HG22	1:B:341:TYR:CA	2.41	0.49
1:A:378:GLU:N	1:A:378:GLU:OE1	2.43	0.49
1:B:19:THR:O	1:B:23:MET:HB2	2.13	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:440:ARG:O	1:B:447:ARG:NH1	2.46	0.49
1:B:431:SER:C	1:B:433:ALA:N	2.65	0.49
1:B:200:GLY:HA2	1:B:342:ALA:HA	1.95	0.49
1:B:154:THR:C	1:B:155:VAL:CG1	2.52	0.48
1:A:379:GLU:OE2	1:A:426:TYR:OH	2.26	0.48
1:A:314:THR:CG2	1:A:316:LEU:CB	2.84	0.48
1:A:-3:GLN:O	1:A:-2:GLY:O	2.30	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:205:ILE:HD12	1:B:336:ILE:HA	1.87	0.48
1:A:469:LYS:HG2	1:A:473:ILE:HD11	1.95	0.48
1:A:458:VAL:HG12	1:A:459:ASP:N	2.29	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:385:LEU:C	1:A:385:LEU:CD2	2.81	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:B:194:VAL:CG2	1:B:348:PHE:CD1	2.97	0.48
1:A:432:ARG:O	1:A:433:ALA:C	2.51	0.48
1:B:520:TYR:HB3	1:B:543:GLU:OE2	2.13	0.48
1:A:365:LEU:HG	1:A:367:PHE:CE1	2.46	0.48
1:B:188:ARG:NH1	1:B:188:ARG:HB2	2.28	0.48
1:A:463:TRP:O	1:A:466:PHE:HB3	2.13	0.48
1:B:363:GLN:HE21	1:B:363:GLN:HB3	1.45	0.48
1:A:453:ARG:HA	1:A:453:ARG:HD2	1.65	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: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: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
1:B:473:ILE:HG23	1:B:542:VAL:HG23	1.95	0.47
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: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:393:ARG:HH21	1:A:398:LYS:HB3	1.79	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:B:128:LEU:HA	1:B:138:ALA:HB2	1.96	0.47
1:A:441:GLU:O	1:A:443:ASN:N	2.46	0.47
1:A:247:THR:O	1:A:248:ASN:HB3	2.14	0.47
1:A:64:ASP:O	1:A:67:GLY:N	2.39	0.47
1:A:230:MET:HE3	1:A:230:MET:HA	1.96	0.47
1:A:413:LEU:C	1:A:413:LEU:HD12	2.34	0.47
1:A:444:ALA:O	1:A:448:LEU:HB2	2.14	0.47
1:B:183:LEU:HG	1:B:183:LEU:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:LEU:HD22	1:A:154:THR:H	1.78	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:B:239:GLN:O	1:B:240:VAL:HG12	2.14	0.47
1:A:392:ALA:O	1:A:395:SER:OG	2.25	0.47
1:B:165:ILE:HG23	1:B:341:TYR:HB2	1.96	0.47
1:A:11:ILE:HD12	1:A:21:ALA:CB	2.44	0.47
1:A:89:GLY:CA	1:A:93:ARG:HE	2.28	0.47
1:B:450:GLU:C	1:B:452:GLY:N	2.65	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:299:PRO:HA	1:B:307:ILE:HD12	1.96	0.47
1:B:410:LEU:O	1:B:413:LEU:HB3	2.15	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: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:B:65:ALA:HA	1:B:462:ARG:NH1	2.29	0.46
1:A:526:LEU:C	1:A:528:PRO:HD2	2.35	0.46
1:A:412:VAL:O	1:A:413:LEU:C	2.54	0.46
1:B:51:ILE:HB	1:B:74:ILE:HG13	1.97	0.46
1:B:48:ASN:HA	1:B:49:PRO:HD3	1.66	0.46
1:B:542:VAL:CG1	1:B:543:GLU:N	2.75	0.46
1:B:518:MET:SD	1:B:523:LEU:HD12	2.55	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:A:11:ILE:HG13	1:A:22:ALA:CB	2.45	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:B:409:TYR:CE1	1:B:439:LEU:HB3	2.50	0.46
1:A:116:PRO:O	1:A:117:ASN:HB2	2.15	0.46
1:B:467:ASN:O	1:B:468:GLU:C	2.53	0.46
1:A:423:LYS:HE2	1:A:426:TYR:CE2	2.51	0.46
1:A:410:LEU:O	1:A:410:LEU:HD13	2.15	0.46
1:B:64:ASP:OD1	1:B:228:SER:HB2	2.15	0.46
1:A:81:PHE:HB3	1:A:225:PRO:CG	2.29	0.46
1:A:463:TRP:CE3	1:A:463:TRP:HA	2.50	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13:GLY:CA	1:B:154:THR:CG2	2.77	0.46
1:A:423:LYS:HG2	1:A:424:GLU:O	2.16	0.46
1:A:295:ILE:CD1	1:A:312:ILE:HG23	2.45	0.46
1:B:459:ASP:C	1:B:461:GLU:N	2.68	0.46
1:A:294:GLN:HB2	1:A:294:GLN:HE21	1.58	0.46
1:A:123:GLN:HG3	1:A:142:MET:CE	2.45	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:357:LEU:HA	1:B:357:LEU:HD23	1.77	0.46
1:B:459:ASP:O	1:B:460:ASP:C	2.54	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:2:PHE:HE2	1:B:145:LYS:HE3	1.82	0.46
1:B:444:ALA:HA	1:B:447:ARG:NH1	2.31	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:A:393:ARG:NH2	1:A:398:LYS:HB3	2.30	0.46
1:B:301:GLY:O	1:B:303:THR:N	2.49	0.46
1:B:290:ARG:HD2	1:B:291:ASN:ND2	2.28	0.46
1:A:338:ARG:NH2	1:B:39:ILE:HB	2.12	0.45
1:A:481:LYS:N	1:A:481:LYS:HD3	2.32	0.45
1:A:489:ALA:O	1:A:490:GLU:C	2.54	0.45
1:B:158:PHE:CD1	1:B:158:PHE:O	2.68	0.45
1:A:186:ARG:HH11	1:A:186:ARG:CB	2.30	0.45
1:A:289:ASP:CA	1:A:291:ASN:O	2.65	0.45
1:B:295:ILE:HA	1:B:295:ILE:HD13	1.62	0.45
1:A:70:MET:HE3	1:A:381:ALA:CB	2.46	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:B:367:PHE:CD1	1:B:367:PHE:N	2.84	0.45
1:B:445:ASP:O	1:B:449:THR:HB	2.16	0.45
1:B:427:ARG:NH2	1:B:428:MET:HE2	2.31	0.45
1:B:416:ASP:OD1	1:B:420:LEU:HD11	2.17	0.45
1:A:484:TRP:HA	1:A:508:SER:HA	1.98	0.45
1:A:287:PHE:HB3	1:A:288:ALA:O	2.16	0.45
1:A:92:VAL:HG21	1:A:430:THR:HG23	1.99	0.45
1:A:440:ARG:NH2	1:A:544:ILE:HG22	2.30	0.45
1:B:386:LEU:O	1:B:389:LEU:HB3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:ASP:OD2	1:B:462:ARG:NH1	2.46	0.45
1:B:31:GLN:HA	1:B:31:GLN:HE21	1.77	0.45
1:A:7:PHE:CD2	1:A:33:LEU:HB2	2.52	0.45
1:B:9:VAL:HA	1:B:150:ALA:O	2.16	0.45
1:B:116:PRO:O	1:B:117:ASN:HB2	2.17	0.45
1:A:354:LYS:C	1:A:356:THR:N	2.69	0.45
1:A:9:VAL:HG22	1:A:150:ALA:HB3	1.99	0.45
1:B:44:GLN:HB2	1:B:44:GLN:HE21	1.55	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: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:53:GLY:HA2	1:A:96:ARG:HB3	1.99	0.45
1:B:371:ILE:CG2	1:B:372:ASN:H	2.29	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:38:ASN:O	1:B:39:ILE:C	2.52	0.44
1:A:372:ASN:ND2	1:A:383:GLN:HE21	2.08	0.44
1:A:166:GLY:CA	1:A:317:PRO:HG3	2.33	0.44
1:A:474:GLU:HB3	1:A:475:ARG:H	1.57	0.44
1:B:206:ASP:HB3	1:B:209:THR:CG2	2.46	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:B:81:PHE:CD2	1:B:236:HIS:CD2	3.03	0.44
1:A:467:ASN:HA	1:A:470:LEU:HB3	1.99	0.44
1:B:124:ALA:HB3	1:B:141:GLN:HB3	1.99	0.44
1:A:310:ASN:HD22	1:A:311:GLY:N	2.15	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:450:GLU:O	1:B:451:ILE:C	2.54	0.44
1:B:303:THR:O	1:B:303:THR:OG1	2.36	0.44
1:A:52:GLY:N	1:A:378:GLU:OE2	2.43	0.44
1:B:222:ASN:C	1:B:223:PRO:O	2.55	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: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:202:PRO:CA	1:A:313:SER:HA	2.46	0.44
1:B:90:PRO:HG3	1:B:544:ILE:HG23	1.98	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:380:ALA:O	1:A:381:ALA:C	2.56	0.44
1:A:215:LEU:N	1:A:215:LEU:HD23	2.32	0.44
1:A:80:GLN:HE21	1:A:98:GLN:HG2	1.82	0.44
1:A:396:ASP:OD1	1:A:396:ASP:O	2.35	0.44
1:B:280:ILE:C	1:B:282:ASP:H	2.19	0.44
1:A:84:LEU:N	1:A:94:ALA:O	2.51	0.44
1:B:500:THR:HG23	1:B:501:ALA:N	2.32	0.44
1:B:81:PHE:HB3	1:B:225:PRO:HD2	2.00	0.44
1:A:232:ASN:N	1:A:235:GLN:OE1	2.44	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: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: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:B:191:PRO:CD	1:B:361:PHE:CE1	3.00	0.44
1:B:209:THR:OG1	1:B:334:ALA:CA	2.44	0.44
1:B:396:ASP:O	1:B:396:ASP:OD1	2.36	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:A:27:ARG:NH2	1:A:68:GLY:N	2.65	0.44
1:A:481:LYS:C	1:A:483:THR:N	2.67	0.44
1:B:290:ARG:CD	1:B:291:ASN:HD22	2.31	0.44
1:B:141:GLN:O	1:B:141:GLN:HG2	2.17	0.44
1:B:130:VAL:HG21	1:B:186:ARG:NE	2.32	0.43
1:A:211:ASP:O	1:A:212:PHE:C	2.54	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:A:246:HIS:CD2	1:A:246:HIS:N	2.84	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:399:GLU:OE1	1:B:399:GLU:CA	2.66	0.43
1:B:300:GLU:OE2	1:B:308:TYR:CD1	2.71	0.43
1:A:2:PHE:CD1	1:A:145:LYS:CB	2.98	0.43
1:B:59:LEU:HA	1:B:59:LEU:HD12	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:80:GLN:N	1:B:239:GLN:NE2	2.64	0.43
1:A:403:PRO:HG2	1:A:410:LEU:HD12	2.00	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:B:195:GLY:O	1:B:346:ASP:HA	2.19	0.43
1:A:479:ARG:HG2	1:A:479:ARG:O	2.19	0.43
1:B:371:ILE:CG2	1:B:372:ASN:N	2.82	0.43
1:A:425:PRO:HD2	1:A:428:MET:CE	2.49	0.43
1:A:212:PHE:HD1	1:A:243:TYR:CG	2.36	0.43
1:A:408:ALA:CA	1:A:447:ARG:HH21	2.31	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:A:413:LEU:CD1	1:A:417:LEU:HD21	2.49	0.43
1:B:115:GLN:HG3	1:B:115:GLN:O	2.19	0.43
1:B:139:VAL:HG13	1:B:145:LYS:CD	2.47	0.43
1:A:166:GLY:HA2	1:A:315:SER:O	2.16	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
1:A:89:GLY:O	1:A:91:ALA:N	2.51	0.43
1:A:243:TYR:HB2	1:A:297:LEU:HB2	2.00	0.43
1:A:81:PHE:CZ	1:A:236:HIS:CE1	3.07	0.43
1:A:80:GLN:O	1:A:97:ALA:HA	2.19	0.43
1:A:212:PHE:HD1	1:A:243:TYR:CD2	2.37	0.43
1:B:118:LEU:HD12	1:B:119:MET:N	2.34	0.43
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.87	0.43
1:A:56:LYS:HB3	1:A:378:GLU:HG2	2.01	0.43
1:A:38:ASN:C	1:A:38:ASN:ND2	2.70	0.43
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.52	0.43
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.63	0.43
1:B:10:ILE:HG12	1:B:33:LEU:HD23	2.01	0.43
1:B:238:GLN:HB3	1:B:302:LEU:CD1	2.49	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: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:B:302:LEU:HA	1:B:302:LEU:HD23	1.50	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:A:41:THR:O	1:A:42:LEU:C	2.58	0.42
1:A:31:GLN:OE1	1:A:117:ASN:ND2	2.52	0.42
1:B:448:LEU:HA	1:B:448:LEU:HD23	1.77	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:423:LYS:HB3	1:B:423:LYS:HE3	1.80	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:A:7:PHE:CD1	1:A:7:PHE:N	2.87	0.42
1:A:490:GLU:OE2	1:A:490:GLU:HA	2.19	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:B:38:ASN:ND2	1:B:40:ASP:H	2.15	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:100:ASP:OD2	1:B:302:LEU:HB2	2.19	0.42
1:B:485:VAL:HG11	1:B:528:PRO:HG3	2.02	0.42
1:B:299:PRO:HG2	1:B:299:PRO:O	2.18	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:539:ALA:O	1:B:541:GLN:N	2.52	0.42
1:B:-1:SER:OG	1:B:-1:SER:O	2.36	0.42
1:A:95:THR:HG21	1:A:227:PHE:CD2	2.54	0.42
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: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:242:CYS:HB3	1:B:297:LEU:O	2.19	0.42
1:B:439:LEU:HA	1:B:439:LEU:HD23	1.45	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:305:ASN:N	1:B:305:ASN:OD1	2.48	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: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:A:428:MET:SD	1:A:432:ARG:NH2	2.93	0.42
1:A:31:GLN:OE1	1:A:31:GLN:HA	2.19	0.42
1:B:316:LEU:HD22	1:B:320:VAL:HG11	2.02	0.42
1:A:393:ARG:HH11	1:A:455:LEU:HD23	1.83	0.42
1:A:27:ARG:NH2	1:A:67:GLY:CA	2.83	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:259:LEU:C	1:A:261:ARG:H	2.24	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:317:PRO:O	1:A:321:GLN:HG3	2.19	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:57:GLY:O	1:A:60:VAL:N	2.51	0.41
1:A:12:ILE:HG23	1:A:12:ILE:HD13	1.84	0.41
1:A:25:ALA:O	1:A:30:GLN:HB2	2.21	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:127:ASP:OD1	1:A:128:LEU:N	2.53	0.41
1:A:525:THR:HG23	1:A:525:THR:O	2.19	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:450:GLU:HB3	1:B:463:TRP:CH2	2.56	0.41
1:B:425:PRO:HB2	1:B:428:MET:HG2	2.01	0.41
1:A:106:GLN:O	1:A:109:ARG:N	2.54	0.41
1:B:524:THR:CG2	1:B:532:ALA:HA	2.51	0.41
1:B:487:PRO:HB3	1:B:503:LEU:O	2.20	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:B:434:GLU:O	1:B:437:LEU:HB2	2.20	0.41
1:A:307:ILE:HA	1:A:307:ILE:HD12	1.72	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:167:LEU:HG	1:A:167:LEU:H	1.39	0.41
1:B:449:THR:O	1:B:449:THR:CG2	2.69	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:129:ILE:N	1:A:137:GLY:O	2.42	0.41
1:B:24:ALA:HA	1:B:27:ARG:HG2	2.02	0.41
1:A:512:LEU:HD12	1:A:529:PHE:HE2	1.85	0.41
1:B:515:ARG:HA	1:B:516:PRO:HD3	1.93	0.41
1:B:362:ILE:O	1:B:363:GLN:O	2.38	0.41
1:A:224:MET:HA	1:A:225:PRO:HD2	1.62	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: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:104:TYR:CE1	1:A:108:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:247:THR:OG1	1:A:251:THR:HG21	2.21	0.41
1:B:446:LEU:HA	1:B:466:PHE:HZ	1.86	0.41
1:B:436:ARG:O	1:B:438:MET:N	2.48	0.41
1:A:289:ASP:H	1:A:291:ASN:HA	1.80	0.41
1:B:184:SER:O	1:B:185:ARG:C	2.59	0.41
1:A:370:GLN:C	1:A:372:ASN:N	2.70	0.41
1:A:203:PRO:HA	1:A:340:GLY:N	2.35	0.41
1:B:386:LEU:HD22	1:B:410:LEU:HD11	2.03	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: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: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: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:A:312:ILE:HD13	1:A:328:MET:HE1	2.03	0.40
1:A:206:ASP:OD1	1:A:208:ARG:N	2.49	0.40
1:A:159:LEU:CB	1:A:160:ASP:CA	2.92	0.40
1:B:417:LEU:HD23	1:B:422:THR:H	1.86	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:115:GLN:HA	1:A:116:PRO:HD2	1.08	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:B:210:ILE:CD1	1:B:331:MET:CE	2.99	0.40
1:A:419:THR:HB	1:A:420:LEU:HG	2.02	0.40
1:B:222:ASN:CA	1:B:223:PRO:O	2.69	0.40
1:A:230:MET:HE1	1:A:465:ARG:HG2	2.04	0.40
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.91	0.40
1:A:232:ASN:O	1:A:235:GLN:HB2	2.22	0.40
1:B:98:GLN:HE22	1:B:298:GLU:CD	2.24	0.40
1:B:246:HIS:O	1:B:328:MET:HB3	2.21	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	521/576 (90%)	383 (74%)	88 (17%)	50 (10%)	1	17
1	B	518/576 (90%)	363 (70%)	98 (19%)	57 (11%)	1	13
All	All	1039/1152 (90%)	746 (72%)	186 (18%)	107 (10%)	1	14

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	2	10
1	B	427/474 (90%)	320 (75%)	107 (25%)	1	6
All	All	853/948 (90%)	658 (77%)	195 (23%)	1	7

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

Mol	Chain	Res	Type
1	A	-3	GLN
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
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 chains 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	0.27	0	6,6,6	0.33	0
2	SO4	A	552	-	4,4,4	0.23	0	6,6,6	0.42	0
2	SO4	B	1	-	4,4,4	0.19	0	6,6,6	0.48	0
2	SO4	B	551	-	4,4,4	0.13	0	6,6,6	0.25	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.

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%)	0.16	8 (1%) 70 36	53, 73, 123, 136	0
1	B	524/576 (90%)	0.29	14 (2%) 52 24	55, 79, 130, 137	0
All	All	1051/1152 (91%)	0.23	22 (2%) 60 29	53, 75, 128, 137	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	HIS	3.3
1	A	503	LEU	3.2
1	B	507	ALA	3.2
1	B	506	GLU	3.2
1	B	289	ASP	3.0
1	A	485	VAL	2.7
1	B	475	ARG	2.6
1	B	503	LEU	2.6
1	A	486	THR	2.6
1	B	479	ARG	2.5
1	B	286	ARG	2.5
1	B	292	GLN	2.4
1	A	498	HIS	2.3
1	A	507	ALA	2.3
1	A	518	MET	2.3
1	B	250	LYS	2.3
1	A	506	GLU	2.3
1	B	499	LEU	2.2
1	B	285	MET	2.2
1	B	485	VAL	2.2
1	A	491	ALA	2.0
1	B	288	ALA	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	1	5/5	0.33	1.61	77,78,78,78	0
2	SO4	A	551	5/5	0.23	0.21	71,72,72,72	0
2	SO4	B	551	5/5	0.25	0.09	85,85,85,86	0
2	SO4	A	552	5/5	0.23	-0.60	79,79,79,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.