



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:33 PM GMT

PDB ID : 3IBJ
Title : X-ray structure of PDE2A
Authors : Pandit, J.
Deposited on : 2009-07-16
Resolution : 3.02 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>

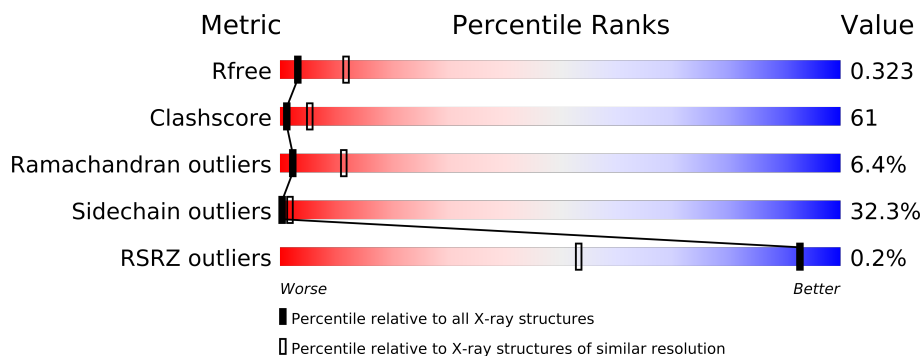
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.02 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	1332 (3.04-3.00)
Clashscore	79885	1732 (3.04-3.00)
Ramachandran outliers	78287	1669 (3.04-3.00)
Sidechain outliers	78261	1672 (3.04-3.00)
RSRZ outliers	66119	1333 (3.04-3.00)

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	691	
1	B	691	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	905	-	X
3	MG	B	905	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10650 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 cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5291	3360	890	1000	41			
1	B	643	Total	C	N	O	S	0	0	0
			5164	3278	874	970	42			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	INITIATING METHIONINE	UNP O00408
A	901	LEU	-	EXPRESSION TAG	UNP O00408
A	902	VAL	-	EXPRESSION TAG	UNP O00408
A	903	PRO	-	EXPRESSION TAG	UNP O00408
A	904	ARG	-	EXPRESSION TAG	UNP O00408
B	214	MET	-	INITIATING METHIONINE	UNP O00408
B	901	LEU	-	EXPRESSION TAG	UNP O00408
B	902	VAL	-	EXPRESSION TAG	UNP O00408
B	903	PRO	-	EXPRESSION TAG	UNP O00408
B	904	ARG	-	EXPRESSION TAG	UNP O00408

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

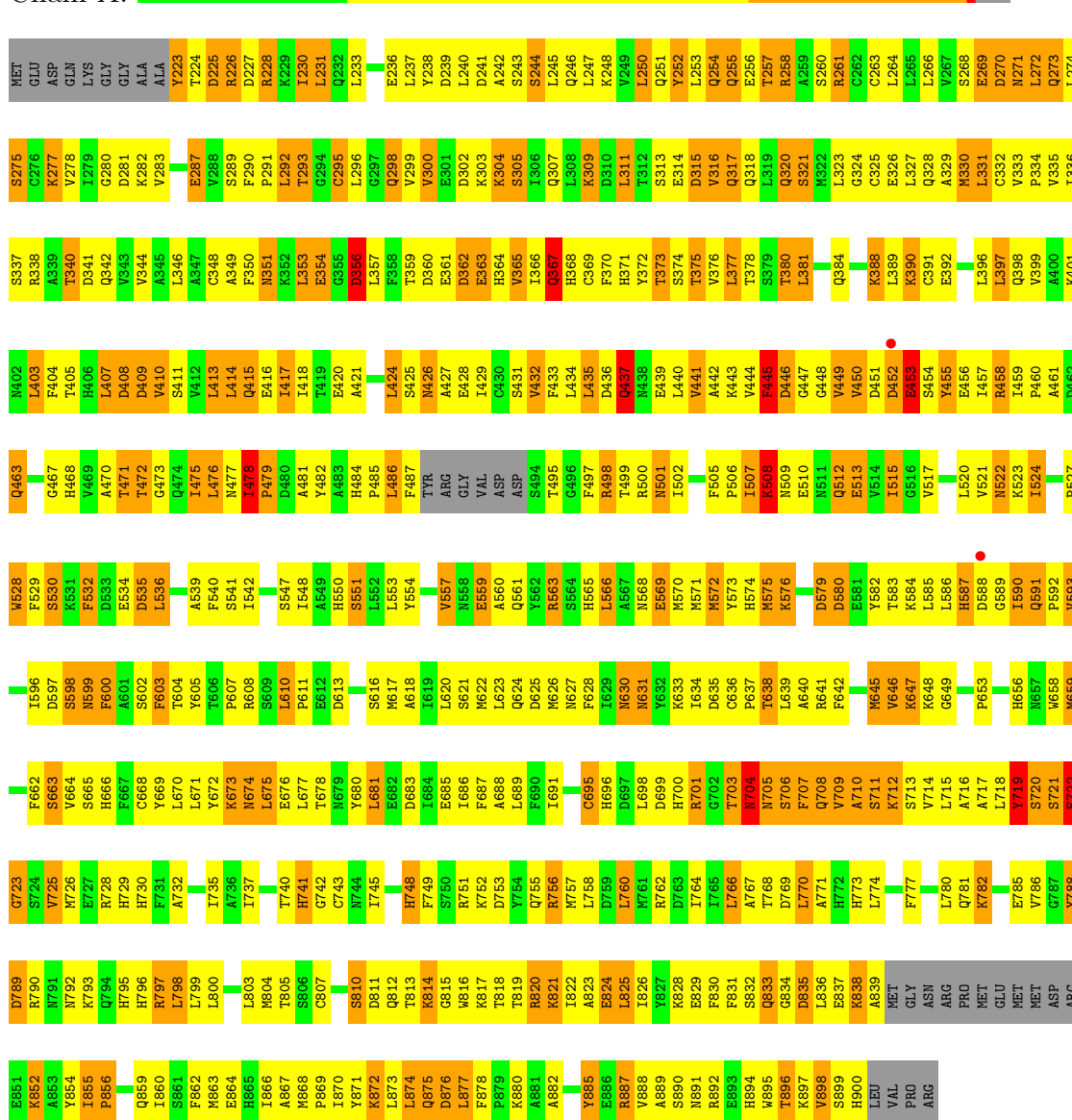
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	95	Total	O	0	0
			95	95		

3 Residue-property plots

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

- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain A:



- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain B:

M848	M849	D849	G787	V766	S724	H656	V693	P527	G464	K401	R338	S275	MET
D850	R850	E851	D789	Y788	W726	W658	I596	W528	I465	M402	A339	C276	GLU
K852	R852	R728	E727	D789	W728	W658	D597	F529	A466	L403	T340	K277	ASP
A853	R853	H729	S728	R790	S728	S663	S598	S530	H468	H406	Q341	V278	GLN
Y854	R854	H730	R729	R791	H729	S663	N599	K531	V469	H406	Q342	I279	LYS
I855	R855	H731	H730	R792	H730	H666	F600	F532	A470	D408	V344	D281	GLY
P856	R856	F731	F731	K793	F731	F667	A601	D533	T471	D409	A346	K282	ALA
				G794	F731	G668	S602	E534	T472	V410	L346	V283	ALA
Q859	I860	H736	I736	H796	A736	F667	S602	A537	G473	S411	A349	E287	Y223
S861	F861	L738	L738	L798	L738	L670	F603	D535	G474	V412	F350	V288	T224
F862	M863	W739	K673	L799	W739	L672	Y605	A537	L476	L413	R351	S289	D225
M864	R864	H741	M674	L675	H741	M674	R608	S541	N477	Q415	K352	F290	R226
							S609		I478	E416	L353	P291	R228
H865	I866	G742	E676	L610	G742	E676	P611	I546	A481	I418	G355	T293	T230
A867	T805	C743	T678	P612	C743	T678	P612	I548	Y482	A421	L357	L286	L231
M868	S868	I745	W679	D613	I745	W679	D613	A549	ALA	R422	F368	G287	G232
I870	R870	D747	L681	D614	D747	L681	D614	H550	HIS	M423	T358	Q298	L233
K872	S810	H749	D683	S616	H749	D683	S616	L553	PRO	L424	D360	V299	C234
L873	D811	S750	I684	A618	S750	I684	A618	Y554	LEU	S425	E361	V300	G236
L874	Q812	R751	E685	T619	R751	E685	T619	K555	TVR	N426	D362	E301	E237
Q875	T813	K752	F686	L620	K752	F686	L620	A567	ARG	E428	R364	K303	Y238
D876	K814	D753	F687	S621	D753	F687	S621	N558	GLY	I429	V365	K304	
L877	Y754	W754	A688	L699	Y754	W754	L699	Y562	VAL	V432	L366	S305	A242
									ASP	F430	Q367	I306	S243
A882	T818	R756	L699	Q624	T818	R756	Q624	Q561	SER	L434	C369	K308	S244
								Y562	THR	L435	F370	L246	L245
E885	R820	L758	H696	D625	R820	L758	D625	H565	GLY	D436	H371	D310	L247
R886	R821	D759	D697	N627	R821	D759	N627	L566	PHE	Q437	T372	L311	K248
V888	A823	M761	L698	F628	A823	M761	F628	A567	R498	E439	T373	T312	V249
A889	R824	R762	D699	I629	R824	R762	I629	N501	T499	L440	S374	S313	L250
S890	L825	D763	R701	N630	S890	D763	N630	M570	R500	L451	T375	E314	Q251
N891	R826	I764	G702	T632	N891	I764	T632	M571	N502	V441	V376	D315	Y252
E893	K828	L766	N704	L634	E893	L766	L634	Y573	C504	K443	L377	V316	L253
H894	E829	R768	ASN	D635	H894	E829	D635	H574	F505	V444	T380	Q317	Q254
W895	F830	D769	SER	C636	W895	F830	C636	M575	P506	PHE	L381	Q318	Q255
T896	R831	D769	PHE	P637	T896	R831	P637	K576	ASP	GLY	A382	Q320	T257
R897	S832	L770	GLN	T638	R897	S832	T638	Y577	ASP	GLY	F383	S321	R258
V898	Q833	A771	VAL	L639	V898	Q833	L639	S578	VAL	VAL	E386	K322	A259
S899	D835	H772	ALA	A640	S899	D835	A640	D579	VAL	VAL	Q387	L323	S260
H900	L836	L774	SER	R641	H900	L836	R641	D580	ASP	ASP	C325	G324	R261
L901	E837	R775	K712	F642	L901	E837	F642	E581	ASP	GLY	L389	E326	C262
Y902	R838	I776	S713	M645	Y902	R838	M645	Y582	S494	GLU	K390	L327	C263
R904	A839	I777	L714	V646	R904	A839	V646	T583	Y485	ASP	C392	Q328	L265
	MET	K778	L715	K647	MET	K778	L715	L585	E456	GLY	E392	Q329	L266
	GLY	D779	A717	K648	GLY	D779	A717	G516	E456	GLY	C393	M330	S267
ASN	ASN	L780	Y719	R651	ASN	L780	Y719	L586	I457	ASP	L396	L331	S268
ARG	ARG	Q781	L718	D652	ARG	Q781	L718	H587	R458	GLY	A395	C332	C269
PRO	PRO	K782	S720	D652	PRO	K782	S720	G589	I459	GLY	L397	V333	D270
MET	MET	M783	S721	P653	MET	M783	S721	G590	P460	GLY	L397	P334	I271
GLU	GLU	A784	E722	P654	GLU	A784	E722	Q591	A461	GLY	Q399	V335	L272
									Q463			I336	Q273
												S337	L274

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.23Å 89.70Å 264.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.26 – 3.02 18.17 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.5 (18.26-3.02) 99.6 (18.17-3.02)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.03Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.210 , 0.311 0.218 , 0.323	Depositor DCC
R_{free} test set	1598 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 31511 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10650	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.66	0/5394	0.86	4/7292 (0.1%)
1	B	0.68	1/5260 (0.0%)	0.88	7/7105 (0.1%)
All	All	0.67	1/10654 (0.0%)	0.87	11/14397 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	722	GLU	CG-CD	5.25	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	855	ILE	C-N-CD	-8.18	102.61	120.60
1	A	478	ILE	C-N-CD	-7.99	103.03	120.60
1	B	902	VAL	C-N-CD	-7.13	104.91	120.60
1	B	478	ILE	C-N-CD	-6.90	105.43	120.60
1	B	723	GLY	N-CA-C	-6.66	96.44	113.10
1	B	312	THR	N-CA-C	-6.38	93.76	111.00
1	B	636	CYS	CA-CB-SG	-6.02	103.17	114.00
1	B	766	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	723	GLY	N-CA-C	-5.77	98.68	113.10
1	A	264	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	B	403	LEU	CA-CB-CG	5.54	128.04	115.30

There are no chirality outliers.

There are no planarity outliers.

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	5291	0	5225	671	0
1	B	5164	0	5128	656	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	96	0	0	10	0
4	B	95	0	0	7	0
All	All	10650	0	10353	1263	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 61.

All (1263) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:704:ASN:ND2	1:A:705:ASN:H	1.41	1.17
1:B:312:THR:HG22	1:B:314:GLU:H	1.06	1.14
1:A:774:LEU:HD12	1:B:838:LYS:HG3	1.27	1.14
1:B:320:GLN:HG2	1:B:327:LEU:HD13	1.14	1.14
1:B:460:PRO:HG2	1:B:463:GLN:HB3	1.30	1.12
1:B:499:THR:HG22	1:B:500:ARG:H	1.11	1.12
1:A:672:TYR:HA	1:A:677:LEU:HD12	1.28	1.12
1:A:399:VAL:HG21	1:A:424:LEU:HD11	1.34	1.09
1:B:672:TYR:HA	1:B:677:LEU:HD12	1.35	1.08
1:B:789:ASP:HB3	1:B:792:ASN:HB2	1.10	1.07
1:A:303:LYS:HD3	1:A:336:ILE:HD13	1.32	1.06
1:A:440:LEU:HD12	1:A:459:ILE:HD11	1.29	1.05
1:B:223:TYR:HD2	1:B:225:ASP:HB2	1.19	1.04
1:A:458:ARG:HG2	1:A:458:ARG:HH11	1.16	1.03
1:A:566:LEU:HD11	1:B:755:GLN:HG2	1.37	1.03
1:A:704:ASN:HD22	1:A:705:ASN:N	1.55	1.02
1:A:309:LYS:HD2	1:A:309:LYS:H	1.20	1.02
1:A:789:ASP:HB3	1:A:792:ASN:HB2	1.42	1.01
1:B:330:MET:HE1	1:B:332:CYS:HB2	1.42	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:695:CYS:HB3	1:A:698:LEU:HD12	1.39	1.00
1:A:484:HIS:NE2	1:A:486:LEU:HD12	1.75	1.00
1:B:290:PHE:HB2	1:B:291:PRO:HD2	1.44	0.99
1:B:303:LYS:HB3	1:B:336:ILE:HD11	1.44	0.98
1:A:460:PRO:HG2	1:A:463:GLN:HB3	1.46	0.95
1:A:444:VAL:HG21	1:A:455:TYR:HD2	1.31	0.95
1:B:309:LYS:H	1:B:309:LYS:HD2	1.30	0.93
1:A:311:LEU:HD23	1:A:315:ASP:HB3	1.50	0.93
1:B:223:TYR:CD2	1:B:225:ASP:HB2	2.04	0.93
1:A:484:HIS:CD2	1:A:486:LEU:HD12	2.05	0.92
1:B:789:ASP:CB	1:B:792:ASN:HB2	1.99	0.92
1:B:270:ASP:HB2	1:B:272:LEU:CD2	2.00	0.91
1:A:270:ASP:HB2	1:A:272:LEU:CD2	2.01	0.90
1:A:799:LEU:O	1:A:803:LEU:HD12	1.71	0.90
1:B:700:HIS:HD2	1:B:702:GLY:H	1.19	0.90
1:B:270:ASP:HB2	1:B:272:LEU:HD21	1.50	0.90
1:B:623:LEU:HA	1:B:626:MET:HE2	1.51	0.90
1:A:445:PHE:HZ	1:A:450:VAL:HG22	1.37	0.89
1:A:571:MET:HA	1:A:571:MET:HE2	1.54	0.89
1:B:323:LEU:CD1	1:B:327:LEU:HD11	2.03	0.88
1:A:303:LYS:HB3	1:A:336:ILE:HD11	1.53	0.88
1:A:672:TYR:CA	1:A:677:LEU:HD12	2.03	0.88
1:A:695:CYS:HB3	1:A:698:LEU:CD1	2.03	0.87
1:A:774:LEU:HD12	1:B:838:LYS:CG	2.04	0.87
1:B:337:SER:O	1:B:341:ASP:HA	1.72	0.87
1:B:370:PHE:HA	1:B:373:THR:HG22	1.56	0.87
1:A:487:PHE:HZ	1:A:499:THR:HB	1.40	0.87
1:B:312:THR:HG22	1:B:314:GLU:N	1.89	0.86
1:A:304:LYS:HA	1:A:304:LYS:HE3	1.56	0.86
1:A:835:ASP:HA	1:A:838:LYS:CD	2.05	0.86
1:A:223:TYR:HE1	1:A:364:HIS:HE2	1.23	0.86
1:A:241:ASP:OD2	1:A:243:SER:HB2	1.76	0.85
1:B:460:PRO:HG2	1:B:463:GLN:CB	2.04	0.85
1:A:421:ALA:HB2	1:A:540:PHE:CE2	2.11	0.85
1:B:792:ASN:HB3	1:B:795:HIS:HB2	1.58	0.85
1:A:231:LEU:HD21	1:B:230:ILE:HG22	1.56	0.85
1:A:388:LYS:O	1:A:392:GLU:HG3	1.76	0.85
1:B:672:TYR:CA	1:B:677:LEU:HD12	2.07	0.84
1:B:314:GLU:HG3	1:B:315:ASP:N	1.92	0.84
1:B:499:THR:CG2	1:B:500:ARG:H	1.90	0.84
1:B:320:GLN:HG2	1:B:327:LEU:CD1	2.04	0.84
1:B:887:ARG:HH11	1:B:887:ARG:HG3	1.43	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:LEU:HD23	1:A:536:LEU:HD11	1.61	0.83
1:A:550:HIS:NE2	1:B:550:HIS:NE2	2.27	0.83
1:A:811:ASP:HB2	1:A:822:ILE:HD13	1.60	0.82
1:B:323:LEU:HD13	1:B:327:LEU:HD11	1.58	0.82
1:B:304:LYS:HE3	1:B:304:LYS:HA	1.60	0.82
1:B:579:ASP:O	1:B:583:THR:HG23	1.78	0.82
1:A:647:LYS:HD2	1:A:658:TRP:CD1	2.14	0.82
1:B:902:VAL:CG2	1:B:903:PRO:HD2	2.09	0.82
1:B:312:THR:HB	1:B:315:ASP:OD2	1.80	0.82
1:A:792:ASN:HB3	1:A:795:HIS:HB2	1.60	0.81
1:B:432:VAL:HG12	1:B:518:ALA:HB2	1.62	0.81
1:A:638:THR:HG22	1:A:745:ILE:HG22	1.60	0.81
1:A:330:MET:CE	1:A:332:CYS:HB2	2.10	0.81
1:A:711:SER:HB3	1:A:854:TYR:CE2	2.16	0.81
1:B:507:ILE:HG22	1:B:515:ILE:HG22	1.61	0.81
1:A:311:LEU:HD23	1:A:315:ASP:CB	2.11	0.81
1:A:290:PHE:HB2	1:A:291:PRO:HD2	1.61	0.81
1:A:666:HIS:CE1	1:A:670:LEU:HD21	2.16	0.80
1:B:656:HIS:HD2	1:B:829:GLU:OE2	1.62	0.80
1:A:399:VAL:HG21	1:A:424:LEU:CD1	2.10	0.80
1:B:638:THR:HG22	1:B:745:ILE:HG22	1.63	0.80
1:B:499:THR:HG22	1:B:500:ARG:N	1.93	0.80
1:A:875:GLN:HE21	1:A:882:ALA:HA	1.45	0.80
1:A:314:GLU:HB2	4:A:93:HOH:O	1.81	0.79
1:A:630:ASN:HD22	1:A:631:ASN:H	1.29	0.79
1:B:630:ASN:HD22	1:B:631:ASN:H	1.29	0.79
1:B:320:GLN:NE2	1:B:327:LEU:HB2	1.96	0.79
1:A:653:PRO:HB2	1:A:829:GLU:OE1	1.83	0.79
1:A:292:LEU:HD11	1:A:300:VAL:HG21	1.65	0.79
1:A:838:LYS:HD2	1:A:838:LYS:H	1.47	0.79
1:A:320:GLN:HG3	1:A:327:LEU:HD13	1.65	0.79
1:A:270:ASP:HB2	1:A:272:LEU:HD21	1.63	0.79
1:A:669:TYR:HD2	1:A:670:LEU:HD23	1.46	0.78
1:B:576:LYS:O	1:B:648:LYS:HE2	1.81	0.78
1:A:251:GLN:NE2	1:A:281:ASP:HA	1.98	0.78
1:A:837:GLU:HB2	1:A:838:LYS:HE3	1.65	0.78
1:A:789:ASP:CB	1:A:792:ASN:HB2	2.13	0.78
1:B:307:GLN:HG2	1:B:330:MET:O	1.83	0.78
1:A:238:TYR:HA	1:B:375:THR:OG1	1.84	0.78
1:B:330:MET:CE	1:B:332:CYS:HB2	2.14	0.77
1:A:835:ASP:HA	1:A:838:LYS:HD2	1.64	0.77
1:A:630:ASN:ND2	1:A:631:ASN:H	1.82	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:320:GLN:HE21	1:B:327:LEU:HB2	1.49	0.77
1:B:329:ALA:HB2	1:B:356:ASP:OD2	1.84	0.77
1:B:399:VAL:HG21	1:B:540:PHE:HE1	1.48	0.77
1:A:405:THR:HG22	1:B:546:ILE:HD12	1.65	0.77
1:A:819:THR:HG21	1:A:891:ASN:ND2	1.99	0.77
1:A:307:GLN:HG2	1:A:330:MET:O	1.85	0.77
1:B:396:LEU:HA	1:B:399:VAL:HG13	1.65	0.77
1:A:401:LYS:O	1:A:405:THR:HG23	1.84	0.77
1:A:224:THR:HG22	1:A:228:ARG:NH2	1.99	0.77
1:A:309:LYS:HD2	1:A:309:LYS:N	1.99	0.76
1:A:605:TYR:CE2	1:A:610:LEU:HD11	2.21	0.76
1:A:749:PHE:HB3	1:A:753:ASP:HB2	1.67	0.76
1:B:479:PRO:HG3	1:B:528:TRP:CZ3	2.19	0.76
1:B:299:VAL:HG12	1:B:334:PRO:HG3	1.68	0.76
1:A:711:SER:HB3	1:A:854:TYR:CD2	2.20	0.76
1:A:337:SER:OG	1:A:340:THR:HG23	1.85	0.76
1:A:340:THR:OG1	1:A:342:GLN:HG3	1.85	0.76
1:A:610:LEU:H	1:A:610:LEU:HD12	1.51	0.76
1:A:326:GLU:O	1:A:327:LEU:HD12	1.85	0.76
1:B:718:LEU:O	1:B:720:SER:N	2.17	0.76
1:A:748:HIS:CD2	1:A:748:HIS:H	2.03	0.76
1:A:250:LEU:HD21	1:A:263:CYS:HA	1.68	0.76
1:B:789:ASP:HB3	1:B:792:ASN:CB	2.04	0.75
1:B:508:LYS:HA	1:B:513:GLU:O	1.86	0.75
1:A:864:GLU:OE2	1:A:892:ARG:HD3	1.85	0.75
1:B:500:ARG:HG2	1:B:522:ASN:OD1	1.87	0.75
1:A:356:ASP:O	1:A:357:LEU:HG	1.87	0.75
1:B:605:TYR:O	1:B:814:LYS:HE3	1.86	0.75
1:B:224:THR:HG22	1:B:228:ARG:NH2	2.02	0.75
1:B:902:VAL:HG22	1:B:903:PRO:HD2	1.68	0.75
1:B:561:GLN:HE21	1:B:561:GLN:HA	1.51	0.75
1:A:508:LYS:HA	1:A:513:GLU:O	1.86	0.75
1:B:837:GLU:HB2	1:B:838:LYS:HZ3	1.51	0.75
1:A:576:LYS:HD3	1:A:576:LYS:O	1.85	0.75
1:B:799:LEU:O	1:B:803:LEU:HD12	1.87	0.75
1:B:340:THR:OG1	1:B:342:GLN:HG3	1.86	0.75
1:A:410:VAL:O	1:A:414:LEU:HB2	1.87	0.75
1:A:342:GLN:O	1:A:344:VAL:HG23	1.88	0.74
1:A:270:ASP:O	1:A:272:LEU:HD23	1.87	0.74
1:A:370:PHE:HA	1:A:373:THR:HG22	1.68	0.74
1:A:671:LEU:HD13	1:A:803:LEU:HD23	1.69	0.74
1:A:303:LYS:HD3	1:A:336:ILE:CD1	2.16	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:468:HIS:O	1:A:472:THR:HG23	1.88	0.74
1:A:242:ALA:O	1:A:246:GLN:HG3	1.88	0.73
1:B:381:LEU:O	1:B:381:LEU:HD12	1.87	0.73
1:A:247:LEU:HD22	1:A:251:GLN:HE22	1.53	0.73
1:A:664:VAL:HG22	1:A:807:CYS:O	1.88	0.73
1:A:484:HIS:CG	1:A:485:PRO:HD2	2.24	0.73
1:A:507:ILE:HG22	1:A:515:ILE:HG22	1.69	0.73
1:B:440:LEU:HG	1:B:461:ALA:HA	1.71	0.73
1:B:242:ALA:O	1:B:246:GLN:HG3	1.89	0.73
1:B:764:ILE:O	1:B:767:ALA:HB3	1.88	0.73
1:B:443:LYS:HD2	1:B:456:GLU:CB	2.19	0.73
1:A:458:ARG:HG2	1:A:458:ARG:NH1	1.93	0.73
1:A:705:ASN:O	1:A:707:PHE:N	2.22	0.72
1:A:700:HIS:HD2	1:A:701:ARG:H	1.36	0.72
1:A:354:GLU:HA	1:A:354:GLU:OE1	1.89	0.72
1:B:562:TYR:CZ	1:B:566:LEU:HD21	2.25	0.72
1:A:337:SER:CB	1:A:340:THR:HG23	2.19	0.72
1:A:330:MET:HE1	1:A:332:CYS:HB2	1.71	0.72
1:A:704:ASN:HD22	1:A:705:ASN:H	0.74	0.72
1:A:410:VAL:CG1	1:A:551:SER:HB3	2.19	0.72
1:A:530:SER:C	1:A:532:PHE:H	1.93	0.72
1:B:671:LEU:HD13	1:B:803:LEU:HD23	1.71	0.72
1:A:333:VAL:HB	1:A:366:ILE:HG21	1.72	0.72
1:B:468:HIS:O	1:B:472:THR:HG23	1.90	0.71
1:B:863:MET:HA	1:B:867:ALA:HB3	1.71	0.71
1:B:303:LYS:HB3	1:B:336:ILE:CD1	2.20	0.71
1:B:599:ASN:HD21	1:B:602:SER:HB3	1.54	0.71
1:A:799:LEU:O	1:A:799:LEU:HD12	1.90	0.71
1:B:714:VAL:HG12	1:B:716:ALA:H	1.56	0.71
1:B:622:MET:HE3	1:B:666:HIS:HA	1.72	0.71
1:A:299:VAL:HG13	1:A:304:LYS:O	1.90	0.71
1:A:835:ASP:HA	1:A:838:LYS:HD3	1.72	0.71
1:A:675:LEU:HD13	1:A:878:PHE:CB	2.21	0.71
1:B:875:GLN:HA	1:B:878:PHE:O	1.90	0.71
1:A:460:PRO:HG2	1:A:463:GLN:CB	2.21	0.71
1:B:299:VAL:CG1	1:B:334:PRO:HG3	2.20	0.71
1:B:642:PHE:O	1:B:646:VAL:HG12	1.90	0.71
1:A:527:PRO:HG2	1:A:528:TRP:CD1	2.26	0.71
1:B:740:THR:HG22	1:B:743:CYS:SG	2.31	0.71
1:B:309:LYS:N	1:B:309:LYS:HD2	2.04	0.70
1:B:681:LEU:HD13	1:B:800:LEU:HD21	1.72	0.70
1:B:572:MET:C	1:B:574:HIS:H	1.93	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:864:GLU:OE2	1:B:892:ARG:HD3	1.92	0.70
1:B:320:GLN:HA	1:B:323:LEU:HB2	1.73	0.70
1:A:895:TRP:HA	1:A:898:VAL:CG2	2.21	0.70
1:A:674:ASN:H	1:A:674:ASN:ND2	1.88	0.70
1:A:330:MET:HG3	1:A:350:PHE:CD1	2.27	0.70
1:A:311:LEU:CD2	1:A:315:ASP:HB3	2.21	0.70
1:A:782:LYS:O	1:A:786:VAL:HG22	1.91	0.70
1:B:799:LEU:HD12	1:B:799:LEU:O	1.90	0.70
1:B:605:TYR:OH	1:B:610:LEU:HD11	1.91	0.70
1:B:827:TYR:CD2	1:B:855:ILE:HD13	2.27	0.70
1:B:720:SER:OG	1:B:721:SER:N	2.25	0.69
1:A:329:ALA:HB2	1:A:356:ASP:OD2	1.91	0.69
1:A:410:VAL:HG12	1:A:551:SER:HB3	1.73	0.69
1:B:780:LEU:HD23	1:B:798:LEU:HB3	1.73	0.69
1:A:720:SER:CA	1:A:770:LEU:HB2	2.23	0.69
1:A:822:ILE:HA	1:A:825:LEU:HD12	1.73	0.69
1:A:223:TYR:CE2	1:A:226:ARG:HG3	2.27	0.69
1:A:669:TYR:CD2	1:A:670:LEU:HD23	2.27	0.69
1:A:311:LEU:HB3	1:A:316:VAL:HG23	1.74	0.69
1:B:479:PRO:HG3	1:B:528:TRP:HZ3	1.58	0.69
1:A:484:HIS:CD2	1:A:485:PRO:HG2	2.28	0.69
1:A:444:VAL:HG21	1:A:455:TYR:CD2	2.23	0.69
1:A:231:LEU:HD12	1:B:372:TYR:CE1	2.27	0.69
1:B:675:LEU:HD13	1:B:878:PHE:CB	2.23	0.69
1:B:261:ARG:HD3	1:B:280:GLY:HA3	1.75	0.69
1:B:829:GLU:O	1:B:831:PHE:N	2.25	0.69
1:A:666:HIS:HE1	1:A:670:LEU:HD11	1.58	0.69
1:B:433:PHE:CD2	1:B:442:ALA:HB2	2.27	0.69
1:A:720:SER:CB	1:A:770:LEU:HB2	2.23	0.68
1:B:859:GLN:NE2	1:B:859:GLN:HA	2.07	0.68
1:A:675:LEU:HD13	1:A:878:PHE:HB3	1.75	0.68
1:B:901:LEU:HD23	1:B:901:LEU:N	2.07	0.68
1:B:313:SER:O	1:B:316:VAL:HG12	1.92	0.68
1:A:721:SER:HA	1:A:769:ASP:OD2	1.93	0.68
1:A:704:ASN:ND2	1:A:705:ASN:N	2.27	0.68
1:B:313:SER:C	1:B:316:VAL:HG12	2.14	0.68
1:A:223:TYR:OH	1:A:364:HIS:NE2	2.25	0.68
1:B:315:ASP:O	1:B:319:LEU:HB2	1.93	0.68
1:A:698:LEU:O	1:A:730:HIS:HD2	1.76	0.68
1:B:461:ALA:O	1:B:467:GLY:HA2	1.94	0.68
1:B:523:LYS:NZ	1:B:533:ASP:OD2	2.26	0.68
1:B:622:MET:HE1	1:B:666:HIS:HB2	1.74	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:481:ALA:O	1:A:487:PHE:HB2	1.94	0.68
1:B:313:SER:HA	1:B:316:VAL:HG12	1.73	0.68
1:A:445:PHE:HZ	1:A:450:VAL:CG2	2.07	0.68
1:A:445:PHE:CZ	1:A:450:VAL:HG22	2.26	0.68
1:B:749:PHE:HB3	1:B:753:ASP:HB2	1.76	0.68
1:B:507:ILE:CG2	1:B:515:ILE:HG22	2.24	0.68
1:A:587:HIS:O	1:A:589:GLY:N	2.27	0.68
1:A:456:GLU:HG2	1:A:458:ARG:HE	1.58	0.67
1:B:623:LEU:HA	1:B:626:MET:CE	2.24	0.67
1:A:872:LYS:HD2	1:A:885:TYR:HE1	1.59	0.67
1:B:443:LYS:HD2	1:B:456:GLU:CG	2.24	0.67
1:B:354:GLU:HA	1:B:354:GLU:OE1	1.93	0.67
1:A:797:ARG:HD3	4:A:59:HOH:O	1.95	0.67
1:B:667:PHE:CD2	1:B:807:CYS:HA	2.29	0.67
1:A:875:GLN:HA	1:A:878:PHE:O	1.95	0.67
1:A:241:ASP:HB3	1:A:244:SER:OG	1.94	0.67
1:B:627:ASN:OD1	1:B:630:ASN:ND2	2.28	0.67
1:B:599:ASN:ND2	1:B:602:SER:HB3	2.10	0.67
1:B:313:SER:CA	1:B:316:VAL:HG12	2.25	0.67
1:A:837:GLU:HB2	1:A:838:LYS:CE	2.24	0.67
1:B:591:GLN:HG3	1:B:592:PRO:N	2.09	0.67
1:A:428:GLU:OE2	1:A:500:ARG:NH2	2.28	0.67
1:A:456:GLU:OE1	1:A:458:ARG:NH2	2.28	0.67
1:A:569:GLU:HG2	1:A:570:MET:N	2.10	0.67
1:B:741:HIS:HB2	4:B:146:HOH:O	1.95	0.67
1:B:399:VAL:HG21	1:B:540:PHE:CE1	2.29	0.67
1:A:605:TYR:HE2	1:A:610:LEU:HD11	1.58	0.67
1:A:895:TRP:O	1:A:898:VAL:HG23	1.94	0.67
1:A:528:TRP:N	1:A:528:TRP:CD1	2.61	0.66
1:B:774:LEU:HD21	1:B:866:ILE:CD1	2.24	0.66
1:B:292:LEU:HD11	1:B:300:VAL:HG21	1.75	0.66
1:A:542:ILE:HG21	1:B:401:LYS:NZ	2.10	0.66
1:B:622:MET:CE	1:B:666:HIS:HA	2.25	0.66
1:A:331:LEU:HD22	1:A:333:VAL:HG23	1.77	0.66
1:B:695:CYS:HB3	1:B:698:LEU:HD12	1.77	0.66
1:A:828:LYS:HE2	4:A:122:HOH:O	1.95	0.66
1:A:397:LEU:HD13	1:B:397:LEU:CD1	2.25	0.66
1:B:838:LYS:HB2	4:B:4:HOH:O	1.95	0.66
1:B:530:SER:O	1:B:533:ASP:N	2.28	0.66
1:A:487:PHE:CZ	1:A:499:THR:HB	2.27	0.66
1:A:231:LEU:HD12	1:B:372:TYR:CZ	2.29	0.66
1:A:709:VAL:HB	1:A:712:LYS:H	1.59	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:576:LYS:H	1:A:576:LYS:CD	2.08	0.66
1:B:320:GLN:CG	1:B:327:LEU:HD13	2.09	0.66
1:B:837:GLU:HB2	1:B:838:LYS:NZ	2.10	0.66
1:B:439:GLU:HB2	1:B:459:ILE:O	1.95	0.66
1:B:443:LYS:HD2	1:B:456:GLU:HG2	1.78	0.66
1:A:330:MET:HG3	1:A:350:PHE:CE1	2.31	0.66
1:B:807:CYS:O	1:B:810:SER:HB3	1.95	0.66
1:B:899:SER:O	1:B:902:VAL:HG12	1.95	0.66
1:A:829:GLU:O	1:A:831:PHE:N	2.29	0.66
1:A:337:SER:O	1:A:341:ASP:HA	1.96	0.66
1:B:308:LEU:O	1:B:311:LEU:HB3	1.96	0.66
1:A:307:GLN:HB3	1:A:309:LYS:HD3	1.77	0.66
1:B:418:ILE:HD11	1:B:432:VAL:CG2	2.26	0.66
1:A:375:THR:HG22	1:A:376:VAL:N	2.11	0.66
1:A:821:LYS:O	1:A:824:GLU:HG3	1.96	0.66
1:A:535:ASP:N	1:A:535:ASP:OD1	2.28	0.66
1:A:444:VAL:CG2	1:A:455:TYR:HD2	2.06	0.65
1:A:479:PRO:HB3	1:A:528:TRP:CE3	2.30	0.65
1:A:572:MET:CE	1:A:737:ILE:HG12	2.26	0.65
1:B:630:ASN:ND2	1:B:631:ASN:H	1.93	0.65
1:A:897:LYS:HA	1:A:900:HIS:CD2	2.31	0.65
1:A:602:SER:O	1:A:604:THR:N	2.29	0.65
1:B:260:SER:OG	1:B:351:ASN:HB2	1.96	0.65
1:B:470:ALA:HB2	1:B:517:VAL:HG21	1.78	0.65
1:B:528:TRP:N	1:B:528:TRP:CD1	2.64	0.65
1:A:405:THR:CG2	1:B:546:ILE:HD12	2.25	0.65
1:B:578:SER:N	1:B:581:GLU:OE1	2.28	0.65
1:A:330:MET:HA	1:A:349:ALA:O	1.96	0.65
1:B:258:ARG:HD3	1:B:352:LYS:NZ	2.12	0.65
1:B:780:LEU:CD2	1:B:798:LEU:HB3	2.27	0.65
1:A:225:ASP:O	1:A:228:ARG:HB2	1.96	0.65
1:B:498:ARG:O	1:B:522:ASN:ND2	2.29	0.65
1:A:226:ARG:C	1:A:228:ARG:H	1.99	0.65
1:A:278:VAL:HG22	1:A:283:VAL:HG22	1.78	0.65
1:B:527:PRO:HG2	1:B:528:TRP:CD1	2.32	0.64
1:B:653:PRO:HB2	1:B:829:GLU:OE1	1.96	0.64
1:B:580:ASP:O	1:B:584:LYS:HG3	1.96	0.64
1:A:436:ASP:HB3	1:A:441:VAL:HG21	1.79	0.64
1:B:270:ASP:O	1:B:272:LEU:HD23	1.96	0.64
1:A:320:GLN:HG2	1:A:325:CYS:O	1.97	0.64
1:B:266:LEU:HD11	1:B:277:LYS:HE2	1.78	0.64
1:A:255:GLN:O	1:A:257:THR:N	2.30	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:450:VAL:HG12	1:A:453:GLU:HA	1.79	0.64
1:B:786:VAL:O	1:B:786:VAL:HG23	1.97	0.64
1:B:313:SER:HA	1:B:316:VAL:CG1	2.28	0.64
1:B:328:GLN:HG2	1:B:351:ASN:OD1	1.97	0.64
1:B:827:TYR:CG	1:B:855:ILE:HD13	2.32	0.64
1:A:645:MET:HG2	1:A:737:ILE:HG23	1.80	0.64
1:A:436:ASP:HB3	1:A:441:VAL:CG2	2.27	0.64
1:A:307:GLN:HB3	1:A:309:LYS:CD	2.27	0.64
1:A:476:LEU:HD23	1:A:478:ILE:HD12	1.80	0.64
1:A:370:PHE:O	1:A:372:TYR:N	2.31	0.64
1:A:630:ASN:HD22	1:A:631:ASN:N	1.96	0.64
1:B:531:LYS:HA	1:B:534:GLU:OE1	1.98	0.64
1:A:680:TYR:HB3	1:A:788:TYR:CE2	2.33	0.64
1:A:700:HIS:CD2	1:A:701:ARG:H	2.15	0.64
1:A:856:PRO:O	1:A:860:ILE:HG12	1.98	0.64
1:A:399:VAL:HG11	1:A:540:PHE:CE1	2.33	0.64
1:B:460:PRO:CG	1:B:463:GLN:HB3	2.20	0.63
1:B:500:ARG:HG2	1:B:522:ASN:CG	2.18	0.63
1:B:648:LYS:HB2	1:B:648:LYS:NZ	2.12	0.63
1:A:260:SER:OG	1:A:351:ASN:HB2	1.98	0.63
1:A:269:GLU:O	1:A:271:ASN:ND2	2.30	0.63
1:A:838:LYS:CD	1:A:838:LYS:H	2.10	0.63
1:A:852:LYS:O	1:A:855:ILE:HG13	1.98	0.63
1:B:822:ILE:HA	1:B:825:LEU:CD1	2.29	0.63
1:B:768:THR:HG22	1:B:804:MET:CG	2.28	0.63
1:A:813:THR:O	1:A:887:ARG:HD2	1.97	0.63
1:A:863:MET:HA	1:A:867:ALA:HB3	1.80	0.63
1:A:720:SER:HB2	1:A:770:LEU:HB2	1.79	0.63
1:B:303:LYS:HD3	1:B:336:ILE:HD13	1.80	0.63
1:B:887:ARG:HG3	1:B:887:ARG:NH1	2.08	0.63
1:B:630:ASN:HD22	1:B:631:ASN:N	1.96	0.63
1:A:436:ASP:CB	1:A:441:VAL:HG21	2.28	0.63
1:B:265:LEU:HD13	1:B:274:LEU:HD12	1.80	0.63
1:A:330:MET:HE3	1:A:332:CYS:HB2	1.80	0.63
1:B:330:MET:HG3	1:B:350:PHE:CD1	2.33	0.63
1:B:433:PHE:CG	1:B:442:ALA:HB2	2.33	0.63
1:A:768:THR:HG22	1:A:804:MET:HG3	1.80	0.63
1:B:875:GLN:HG2	1:B:875:GLN:O	1.98	0.62
1:A:708:GLN:O	1:A:709:VAL:HG23	1.98	0.62
1:B:458:ARG:CG	1:B:458:ARG:HH11	2.13	0.62
1:B:376:VAL:HG13	1:B:377:LEU:N	2.14	0.62
1:B:434:LEU:HD21	1:B:548:ILE:HG21	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:561:GLN:CA	1:B:561:GLN:HE21	2.10	0.62
1:B:510:GLU:OE1	1:B:510:GLU:HA	1.99	0.62
1:A:456:GLU:HG2	1:A:458:ARG:NE	2.13	0.62
1:A:627:ASN:OD1	1:A:630:ASN:ND2	2.30	0.62
1:B:680:TYR:N	1:B:680:TYR:CD1	2.67	0.62
1:B:630:ASN:HD22	1:B:630:ASN:N	1.97	0.62
1:B:762:ARG:O	1:B:766:LEU:HD22	2.00	0.62
1:B:230:ILE:HG22	1:B:231:LEU:N	2.14	0.62
1:A:634:ILE:CG2	1:A:639:LEU:HB2	2.30	0.62
1:B:527:PRO:HB2	1:B:528:TRP:CD1	2.35	0.62
1:A:252:TYR:O	1:A:255:GLN:HB2	1.99	0.62
1:B:333:VAL:HB	1:B:366:ILE:HG21	1.82	0.62
1:B:328:GLN:HG3	4:B:9:HOH:O	2.00	0.62
1:A:814:LYS:HB3	1:A:818:THR:HG21	1.81	0.62
1:B:410:VAL:O	1:B:414:LEU:HB2	2.00	0.62
1:A:714:VAL:HG12	1:A:716:ALA:H	1.65	0.62
1:B:354:GLU:O	1:B:356:ASP:N	2.32	0.62
1:A:887:ARG:HG2	4:A:142:HOH:O	1.98	0.61
1:A:572:MET:HE1	1:A:737:ILE:HG12	1.82	0.61
1:A:408:ASP:OD1	1:A:408:ASP:N	2.28	0.61
1:B:596:ILE:HG21	1:B:600:PHE:CD1	2.35	0.61
1:B:837:GLU:CB	1:B:838:LYS:HZ3	2.13	0.61
1:B:475:ILE:HD13	1:B:506:PRO:HD3	1.83	0.61
1:B:762:ARG:HG2	1:B:766:LEU:CD2	2.29	0.61
1:B:417:ILE:HD13	1:B:548:ILE:HD11	1.81	0.61
1:A:223:TYR:CE2	1:A:226:ARG:HB2	2.36	0.61
1:A:610:LEU:HB3	1:A:611:PRO:HD2	1.82	0.61
1:B:875:GLN:HE21	1:B:882:ALA:CB	2.14	0.61
1:B:330:MET:HG3	1:B:350:PHE:CE1	2.36	0.61
1:B:630:ASN:ND2	1:B:630:ASN:H	1.98	0.61
1:A:484:HIS:HD2	1:A:486:LEU:H	1.47	0.61
1:B:435:LEU:HD11	1:B:437:GLN:O	2.01	0.61
1:A:579:ASP:O	1:A:583:THR:HG23	2.01	0.61
1:B:441:VAL:HG21	1:B:458:ARG:CZ	2.31	0.61
1:B:666:HIS:O	1:B:669:TYR:HB3	2.00	0.61
1:A:397:LEU:HD13	1:B:397:LEU:HD12	1.82	0.61
1:B:440:LEU:HD13	1:B:466:ALA:HB1	1.83	0.61
1:B:353:LEU:O	1:B:354:GLU:HB2	2.00	0.61
1:A:755:GLN:HG2	1:B:566:LEU:CD1	2.31	0.61
1:B:475:ILE:HD13	1:B:506:PRO:CD	2.31	0.60
1:B:675:LEU:HD23	1:B:675:LEU:N	2.16	0.60
1:A:648:LYS:HB2	1:A:648:LYS:NZ	2.15	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:530:SER:C	1:B:532:PHE:H	2.04	0.60
1:B:677:LEU:HD21	1:B:803:LEU:HD21	1.82	0.60
1:B:855:ILE:HB	1:B:856:PRO:HD3	1.83	0.60
1:B:611:PRO:HG2	1:B:614:ASP:OD2	2.01	0.60
1:A:399:VAL:CG1	1:A:540:PHE:HE1	2.14	0.60
1:A:859:GLN:O	1:A:863:MET:HG3	2.02	0.60
1:B:458:ARG:HG2	1:B:458:ARG:HH11	1.65	0.60
1:B:527:PRO:HG2	1:B:528:TRP:HD1	1.65	0.60
1:B:355:GLY:O	1:B:357:LEU:N	2.34	0.60
1:B:381:LEU:HD12	1:B:381:LEU:C	2.21	0.60
1:B:303:LYS:CD	1:B:336:ILE:HD13	2.31	0.60
1:A:270:ASP:HB2	1:A:272:LEU:HD23	1.82	0.60
1:A:630:ASN:ND2	1:A:631:ASN:N	2.48	0.60
1:B:805:THR:CG2	1:B:870:ILE:HD13	2.32	0.60
1:A:470:ALA:HB2	1:A:517:VAL:HG21	1.83	0.60
1:A:718:LEU:O	1:A:720:SER:N	2.32	0.60
1:B:399:VAL:HG11	1:B:424:LEU:HD11	1.84	0.60
1:A:251:GLN:HE22	1:A:281:ASP:HA	1.67	0.60
1:A:576:LYS:H	1:A:576:LYS:HD2	1.67	0.60
1:A:688:ALA:HA	1:A:757:MET:HE1	1.83	0.60
1:B:234:CYS:HA	1:B:237:LEU:HD12	1.83	0.60
1:B:443:LYS:HD2	1:B:456:GLU:HB3	1.83	0.59
1:B:356:ASP:OD1	4:B:9:HOH:O	2.17	0.59
1:B:678:THR:O	1:B:790:ARG:NH2	2.34	0.59
1:B:821:LYS:O	1:B:824:GLU:HG3	2.02	0.59
1:A:439:GLU:OE2	1:A:458:ARG:HB3	2.03	0.59
1:A:835:ASP:HB2	1:B:771:ALA:HB2	1.84	0.59
1:A:298:GLN:NE2	1:A:302:ASP:OD2	2.35	0.59
1:B:257:THR:O	1:B:352:LYS:HE3	2.03	0.59
1:B:459:ILE:HG13	1:B:463:GLN:OE1	2.02	0.59
1:A:566:LEU:CD1	1:B:755:GLN:HG2	2.21	0.59
1:A:237:LEU:O	1:B:375:THR:HG21	2.01	0.59
1:A:732:ALA:HB2	1:B:571:MET:HE1	1.83	0.59
1:A:507:ILE:CG2	1:A:515:ILE:HG22	2.32	0.59
1:A:570:MET:HE2	1:B:762:ARG:HH11	1.68	0.59
1:A:475:ILE:HG23	1:A:505:PHE:HB3	1.83	0.59
1:A:431:SER:HG	1:A:433:PHE:HE1	1.51	0.59
1:A:770:LEU:O	1:A:770:LEU:HD12	2.02	0.59
1:B:241:ASP:OD2	1:B:243:SER:HB2	2.02	0.59
1:B:700:HIS:CD2	1:B:702:GLY:H	2.09	0.59
1:A:333:VAL:CB	1:A:366:ILE:HG21	2.33	0.59
1:A:656:HIS:CD2	1:A:700:HIS:CE1	2.90	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:799:LEU:HD11	1:A:803:LEU:HD11	1.85	0.59
1:B:337:SER:OG	1:B:340:THR:HG23	2.03	0.59
1:B:432:VAL:CG1	1:B:518:ALA:HB2	2.33	0.59
1:A:720:SER:HB2	1:A:770:LEU:CB	2.33	0.59
1:A:576:LYS:N	1:A:576:LYS:CD	2.65	0.59
1:A:418:ILE:HG12	1:A:432:VAL:HG22	1.84	0.59
1:A:435:LEU:HD11	1:A:437:GLN:O	2.03	0.58
1:A:363:GLU:HG3	1:A:367:GLN:HE22	1.68	0.58
1:B:675:LEU:HD13	1:B:878:PHE:HB3	1.83	0.58
1:A:815:GLY:O	1:A:818:THR:HB	2.03	0.58
1:B:720:SER:CB	1:B:770:LEU:HB2	2.33	0.58
1:A:637:PRO:O	1:A:641:ARG:NE	2.36	0.58
1:A:774:LEU:HB2	1:B:838:LYS:HD2	1.84	0.58
1:A:575:MET:HG2	1:A:648:LYS:CD	2.33	0.58
1:A:364:HIS:HA	1:A:367:GLN:HE21	1.68	0.58
1:B:637:PRO:O	1:B:641:ARG:NE	2.29	0.58
1:B:535:ASP:OD1	1:B:535:ASP:N	2.27	0.58
1:B:471:THR:HG22	1:B:472:THR:N	2.19	0.58
1:B:509:ASN:OD1	1:B:513:GLU:HG3	2.03	0.58
1:A:860:ILE:CD1	1:A:895:TRP:HB3	2.34	0.58
1:A:872:LYS:HA	1:A:885:TYR:HD1	1.68	0.58
1:B:476:LEU:HD23	1:B:478:ILE:HD12	1.85	0.58
1:B:720:SER:CA	1:B:770:LEU:HB2	2.34	0.58
1:A:473:GLY:O	1:A:508:LYS:NZ	2.31	0.58
1:A:872:LYS:HD2	1:A:885:TYR:CE1	2.39	0.58
1:B:720:SER:HB2	1:B:770:LEU:HB2	1.85	0.58
1:A:482:TYR:CZ	1:A:487:PHE:HE2	2.22	0.58
1:B:721:SER:HB2	1:B:769:ASP:OD2	2.02	0.58
1:B:241:ASP:HB3	1:B:244:SER:OG	2.04	0.58
1:A:505:PHE:HB2	1:A:506:PRO:HD2	1.85	0.57
1:A:554:TYR:HD1	1:B:554:TYR:HD1	1.52	0.57
1:B:475:ILE:HG23	1:B:505:PHE:HB3	1.85	0.57
1:B:398:GLN:HE22	1:B:401:LYS:HD3	1.69	0.57
1:B:309:LYS:H	1:B:309:LYS:CD	2.10	0.57
1:B:304:LYS:HE3	1:B:304:LYS:CA	2.23	0.57
1:A:875:GLN:O	1:A:875:GLN:HG2	2.03	0.57
1:B:872:LYS:HE2	1:B:876:ASP:OD1	2.03	0.57
1:A:715:LEU:C	1:A:717:ALA:H	2.08	0.57
1:B:698:LEU:O	1:B:730:HIS:HD2	1.86	0.57
1:B:502:ILE:HG21	1:B:519:GLU:OE1	2.05	0.57
1:B:587:HIS:O	1:B:589:GLY:N	2.38	0.57
1:B:279:ILE:HD11	1:B:322:MET:SD	2.44	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:459:ILE:HD12	1:B:460:PRO:CD	2.35	0.57
1:A:416:GLU:HA	1:A:416:GLU:OE1	2.03	0.57
1:A:223:TYR:CE2	1:A:226:ARG:CG	2.88	0.57
1:A:475:ILE:HD13	1:A:506:PRO:CD	2.34	0.57
1:B:833:GLN:HG2	1:B:834:GLY:H	1.70	0.57
1:B:895:TRP:HA	1:B:898:VAL:HG22	1.87	0.56
1:A:885:TYR:CD2	1:A:885:TYR:C	2.78	0.56
1:A:415:GLN:O	1:A:418:ILE:HB	2.05	0.56
1:A:416:GLU:O	1:A:420:GLU:HB2	2.05	0.56
1:A:231:LEU:HD22	1:B:231:LEU:HD22	1.86	0.56
1:A:565:HIS:O	1:A:569:GLU:HB3	2.04	0.56
1:A:723:GLY:N	4:A:35:HOH:O	2.38	0.56
1:B:528:TRP:N	1:B:528:TRP:HD1	2.03	0.56
1:B:443:LYS:HA	1:B:456:GLU:HA	1.85	0.56
1:B:471:THR:HG22	1:B:472:THR:HG22	1.88	0.56
1:B:500:ARG:NE	1:B:522:ASN:HB3	2.20	0.56
1:A:223:TYR:HE2	1:A:226:ARG:CB	2.18	0.56
1:A:231:LEU:HD23	1:B:231:LEU:HB2	1.87	0.56
1:B:875:GLN:HE21	1:B:882:ALA:HB1	1.71	0.56
1:B:715:LEU:HD23	1:B:862:PHE:CD2	2.40	0.56
1:B:895:TRP:HA	1:B:898:VAL:CG2	2.35	0.56
1:A:253:LEU:O	1:A:257:THR:OG1	2.23	0.56
1:A:590:ILE:HG22	1:A:624:GLN:NE2	2.20	0.56
1:A:780:LEU:CD2	1:A:798:LEU:HB3	2.34	0.56
1:B:607:PRO:HG2	1:B:663:SER:HB3	1.87	0.56
1:A:417:ILE:HD13	1:A:548:ILE:HD11	1.87	0.56
1:A:868:MET:HG2	1:A:888:VAL:HG12	1.86	0.56
1:A:421:ALA:HB2	1:A:540:PHE:HE2	1.64	0.56
1:B:326:GLU:HB3	1:B:328:GLN:HE22	1.70	0.56
1:A:590:ILE:HG21	1:A:624:GLN:OE1	2.05	0.56
1:A:573:TYR:HE1	1:A:699:ASP:OD1	1.89	0.56
1:B:312:THR:HG21	1:B:314:GLU:HB3	1.88	0.56
1:A:810:SER:HA	1:A:871:TYR:OH	2.05	0.56
1:A:780:LEU:HD23	1:A:798:LEU:HB3	1.88	0.56
1:A:812:GLN:HB3	1:A:888:VAL:HG22	1.87	0.56
1:B:312:THR:CG2	1:B:314:GLU:HB3	2.36	0.56
1:A:399:VAL:HG11	1:A:540:PHE:HE1	1.69	0.56
1:B:258:ARG:HB2	1:B:352:LYS:HE2	1.87	0.56
1:B:822:ILE:HA	1:B:825:LEU:HD12	1.87	0.56
1:B:273:GLN:HE22	1:B:289:SER:HB2	1.71	0.56
1:A:550:HIS:CD2	1:B:550:HIS:HE2	2.21	0.56
1:A:674:ASN:O	1:A:880:LYS:HD3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:610:LEU:H	1:A:610:LEU:CD1	2.17	0.56
1:B:471:THR:HG22	1:B:472:THR:CG2	2.36	0.56
1:B:505:PHE:HB2	1:B:506:PRO:HD2	1.88	0.55
1:A:757:MET:O	1:A:757:MET:HG3	2.06	0.55
1:A:894:HIS:O	1:A:898:VAL:HG22	2.05	0.55
1:A:715:LEU:HD22	1:A:859:GLN:HE22	1.70	0.55
1:A:479:PRO:HB3	1:A:528:TRP:CZ3	2.42	0.55
1:A:764:ILE:O	1:A:767:ALA:HB3	2.07	0.55
1:A:550:HIS:CD2	1:B:550:HIS:NE2	2.75	0.55
1:A:610:LEU:N	1:A:610:LEU:HD12	2.21	0.55
1:A:748:HIS:N	1:A:748:HIS:CD2	2.73	0.55
1:A:403:LEU:HD13	1:A:417:ILE:HG13	1.87	0.55
1:A:427:ALA:HB2	1:A:520:LEU:HD22	1.89	0.55
1:B:586:LEU:CD1	1:B:640:ALA:HB3	2.36	0.55
1:B:718:LEU:HG	1:B:719:TYR:N	2.21	0.55
1:B:827:TYR:OH	1:B:859:GLN:NE2	2.38	0.55
1:A:261:ARG:HD3	1:A:280:GLY:HA3	1.89	0.55
1:A:838:LYS:HB2	1:B:774:LEU:HD12	1.89	0.55
1:B:505:PHE:HB2	1:B:506:PRO:CD	2.37	0.55
1:A:239:ASP:HB2	1:A:245:LEU:HD23	1.89	0.55
1:B:837:GLU:C	1:B:838:LYS:HZ3	2.10	0.55
1:A:440:LEU:O	1:A:458:ARG:HA	2.07	0.55
1:A:445:PHE:CZ	1:A:450:VAL:HG13	2.42	0.55
1:A:648:LYS:HB2	1:A:648:LYS:HZ2	1.72	0.55
1:A:295:CYS:HB3	1:A:315:ASP:OD2	2.07	0.55
1:B:666:HIS:CE1	1:B:670:LEU:HD21	2.42	0.55
1:B:593:VAL:HG22	1:B:621:SER:O	2.06	0.55
1:A:709:VAL:HB	1:A:712:LYS:HB2	1.87	0.55
1:B:439:GLU:CA	1:B:461:ALA:HB2	2.37	0.55
1:B:439:GLU:HA	1:B:461:ALA:HB2	1.88	0.55
1:B:530:SER:O	1:B:533:ASP:HB2	2.07	0.55
1:B:506:PRO:O	1:B:507:ILE:HD12	2.06	0.55
1:B:311:LEU:O	1:B:311:LEU:HG	2.07	0.55
1:A:668:CYS:SG	1:A:689:LEU:HD23	2.47	0.54
1:A:680:TYR:HB3	1:A:788:TYR:HE2	1.72	0.54
1:A:476:LEU:HD23	1:A:478:ILE:CD1	2.37	0.54
1:A:224:THR:HG22	1:A:228:ARG:CZ	2.36	0.54
1:A:607:PRO:O	1:A:610:LEU:HD13	2.07	0.54
1:B:500:ARG:NH2	1:B:523:LYS:O	2.39	0.54
1:A:223:TYR:HE2	1:A:226:ARG:CG	2.19	0.54
1:B:723:GLY:C	1:B:725:VAL:H	2.11	0.54
1:A:452:ASP:O	1:A:453:GLU:O	2.25	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:645:MET:HE1	1:B:740:THR:HG21	1.88	0.54
1:A:587:HIS:C	1:A:589:GLY:H	2.10	0.54
1:A:278:VAL:CG2	1:A:283:VAL:HG22	2.36	0.54
1:A:665:SER:O	1:A:668:CYS:HB3	2.07	0.54
1:B:418:ILE:CD1	1:B:444:VAL:HG21	2.37	0.54
1:B:630:ASN:N	1:B:630:ASN:ND2	2.53	0.54
1:B:721:SER:HA	1:B:769:ASP:OD2	2.07	0.54
1:A:468:HIS:CE1	1:A:472:THR:HG21	2.42	0.54
1:B:403:LEU:HD22	1:B:417:ILE:HG13	1.87	0.54
1:B:805:THR:HG22	1:B:870:ILE:HD13	1.90	0.54
1:A:275:SER:HB2	1:A:287:GLU:OE2	2.08	0.54
1:A:659:MET:O	1:A:663:SER:OG	2.24	0.54
1:A:477:ASN:HD21	1:A:529:PHE:HB2	1.72	0.54
1:A:363:GLU:O	1:A:367:GLN:NE2	2.41	0.54
1:B:593:VAL:HG12	1:B:600:PHE:CD2	2.42	0.54
1:B:361:GLU:O	1:B:365:VAL:HG12	2.08	0.54
1:A:309:LYS:CD	1:A:309:LYS:H	2.04	0.54
1:A:331:LEU:HD22	1:A:333:VAL:CG2	2.38	0.54
1:A:771:ALA:HB2	1:B:835:ASP:HB2	1.89	0.54
1:B:283:VAL:O	1:B:283:VAL:HG12	2.07	0.54
1:B:687:PHE:CE1	1:B:746:PHE:HE1	2.25	0.54
1:A:542:ILE:HG21	1:B:401:LYS:HZ1	1.73	0.54
1:A:231:LEU:CD2	1:B:231:LEU:HD22	2.38	0.54
1:B:444:VAL:O	1:B:444:VAL:HG13	2.08	0.54
1:A:376:VAL:HG21	1:B:375:THR:HG22	1.90	0.54
1:A:569:GLU:O	1:A:572:MET:HB2	2.07	0.54
1:B:821:LYS:HD3	1:B:824:GLU:OE1	2.07	0.54
1:B:499:THR:O	1:B:500:ARG:HD3	2.08	0.54
1:B:398:GLN:OE1	1:B:398:GLN:HA	2.06	0.54
1:B:789:ASP:N	1:B:795:HIS:ND1	2.53	0.54
1:A:458:ARG:CG	1:A:458:ARG:NH1	2.66	0.54
1:A:453:GLU:HA	1:A:453:GLU:OE1	2.07	0.54
1:A:575:MET:HG2	1:A:648:LYS:HD2	1.88	0.54
1:A:788:TYR:OH	1:A:799:LEU:HD23	2.08	0.54
1:A:815:GLY:O	1:A:818:THR:N	2.39	0.54
1:A:709:VAL:HG12	1:A:711:SER:H	1.73	0.53
1:A:720:SER:HA	1:A:770:LEU:HB2	1.89	0.53
1:B:593:VAL:HG12	1:B:600:PHE:CE2	2.44	0.53
1:B:606:THR:OG1	1:B:609:SER:HB3	2.07	0.53
1:A:666:HIS:O	1:A:669:TYR:HB3	2.07	0.53
1:B:593:VAL:CG1	1:B:600:PHE:CE2	2.91	0.53
1:A:440:LEU:HD12	1:A:459:ILE:CD1	2.20	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:835:ASP:CA	1:A:838:LYS:HD2	2.38	0.53
1:B:877:LEU:HB2	1:B:878:PHE:CD2	2.43	0.53
1:B:859:GLN:HE21	1:B:859:GLN:HA	1.71	0.53
1:A:860:ILE:HD11	1:A:895:TRP:C	2.29	0.53
1:A:642:PHE:O	1:A:646:VAL:HG12	2.08	0.53
1:B:443:LYS:CD	1:B:456:GLU:HB3	2.38	0.53
1:B:457:ILE:HG22	1:B:457:ILE:O	2.07	0.53
1:B:366:ILE:HG22	1:B:367:GLN:N	2.23	0.53
1:A:231:LEU:CD2	1:B:231:LEU:HB2	2.38	0.53
1:A:599:ASN:OD1	1:A:602:SER:HB2	2.08	0.53
1:B:596:ILE:HG21	1:B:600:PHE:CE1	2.43	0.53
1:A:719:TYR:O	1:A:770:LEU:HD23	2.09	0.53
1:B:331:LEU:HD22	1:B:333:VAL:HG23	1.91	0.53
1:A:335:VAL:HG22	1:A:370:PHE:CD2	2.44	0.53
1:A:550:HIS:NE2	1:B:550:HIS:CD2	2.77	0.53
1:A:495:THR:HG22	1:A:495:THR:O	2.09	0.53
1:B:521:VAL:HG12	1:B:522:ASN:OD1	2.08	0.53
1:A:420:GLU:OE2	1:A:420:GLU:HA	2.09	0.53
1:A:230:ILE:HG22	1:B:231:LEU:HD21	1.91	0.53
1:A:875:GLN:HE21	1:A:882:ALA:CA	2.20	0.53
1:B:530:SER:C	1:B:532:PHE:N	2.62	0.53
1:A:675:LEU:HD13	1:A:878:PHE:CG	2.44	0.53
1:B:255:GLN:O	1:B:257:THR:N	2.41	0.53
1:A:570:MET:C	1:A:572:MET:H	2.12	0.53
1:A:501:ASN:ND2	1:A:527:PRO:O	2.42	0.53
1:B:586:LEU:HD21	1:B:636:CYS:HB3	1.91	0.53
1:A:547:SER:O	1:A:551:SER:HB2	2.09	0.53
1:A:786:VAL:HG23	1:A:786:VAL:O	2.08	0.53
1:B:258:ARG:CG	1:B:258:ARG:HH11	2.22	0.53
1:B:768:THR:HG22	1:B:804:MET:HG3	1.91	0.52
1:A:439:GLU:HA	1:A:461:ALA:N	2.23	0.52
1:B:702:GLY:HA2	1:B:829:GLU:OE2	2.09	0.52
1:A:838:LYS:HB3	1:B:774:LEU:HB2	1.90	0.52
1:B:342:GLN:O	1:B:344:VAL:HG23	2.10	0.52
1:B:252:TYR:O	1:B:256:GLU:HG2	2.09	0.52
1:A:566:LEU:HD22	1:B:755:GLN:HE21	1.75	0.52
1:B:755:GLN:OE1	1:B:759:ASP:OD2	2.28	0.52
1:A:872:LYS:HA	1:A:885:TYR:CD1	2.44	0.52
1:B:278:VAL:HG22	1:B:283:VAL:HG22	1.91	0.52
1:B:619:ILE:O	1:B:623:LEU:HD12	2.09	0.52
1:A:433:PHE:CD2	1:A:442:ALA:HB2	2.44	0.52
1:A:270:ASP:OD2	1:A:270:ASP:N	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:231:LEU:HD12	1:B:231:LEU:O	2.10	0.52
1:B:715:LEU:C	1:B:717:ALA:H	2.13	0.52
1:B:435:LEU:HD13	1:B:436:ASP:N	2.24	0.52
1:A:688:ALA:HB2	1:A:760:LEU:HD12	1.92	0.52
1:A:530:SER:C	1:A:532:PHE:N	2.61	0.52
1:B:762:ARG:HG2	1:B:766:LEU:HD22	1.90	0.52
1:B:606:THR:O	1:B:609:SER:HB3	2.10	0.52
1:B:458:ARG:O	1:B:459:ILE:HB	2.09	0.52
1:A:789:ASP:N	1:A:795:HIS:ND1	2.57	0.52
1:B:307:GLN:HB3	1:B:309:LYS:CD	2.40	0.52
1:B:861:SER:O	1:B:865:HIS:HB2	2.10	0.52
1:A:721:SER:HB2	1:A:769:ASP:OD2	2.09	0.52
1:A:721:SER:OG	1:A:722:GLU:N	2.39	0.52
1:A:721:SER:O	1:A:722:GLU:OE1	2.27	0.52
1:A:770:LEU:O	1:A:774:LEU:HG	2.10	0.52
1:B:455:TYR:CD2	1:B:455:TYR:N	2.76	0.52
1:B:467:GLY:O	1:B:471:THR:HB	2.10	0.52
1:B:369:CYS:O	1:B:373:THR:HB	2.10	0.52
1:A:376:VAL:HG13	1:A:377:LEU:N	2.25	0.52
1:A:258:ARG:O	1:A:353:LEU:N	2.40	0.52
1:A:447:GLY:HA2	4:A:17:HOH:O	2.10	0.52
1:A:330:MET:CG	1:A:350:PHE:CE1	2.93	0.51
1:B:375:THR:HB	4:B:186:HOH:O	2.09	0.51
1:A:885:TYR:C	1:A:885:TYR:HD2	2.13	0.51
1:B:479:PRO:HB3	1:B:528:TRP:CE3	2.45	0.51
1:A:698:LEU:O	1:A:730:HIS:CD2	2.62	0.51
1:A:270:ASP:OD1	1:A:272:LEU:HG	2.10	0.51
1:A:434:LEU:O	1:A:441:VAL:HG23	2.10	0.51
1:A:634:ILE:HG21	1:A:639:LEU:HB2	1.92	0.51
1:A:854:TYR:N	1:A:854:TYR:CD1	2.77	0.51
1:A:348:CYS:HB3	1:A:350:PHE:CZ	2.45	0.51
1:A:715:LEU:CD2	1:A:859:GLN:HE22	2.23	0.51
1:A:439:GLU:N	1:A:461:ALA:HB2	2.25	0.51
1:B:307:GLN:O	1:B:310:ASP:HB2	2.10	0.51
1:B:236:GLU:O	1:B:248:LYS:NZ	2.39	0.51
1:B:273:GLN:HG2	1:B:291:PRO:HA	1.92	0.51
1:A:833:GLN:HG2	1:A:837:GLU:OE2	2.11	0.51
1:B:627:ASN:ND2	1:B:631:ASN:OD1	2.43	0.51
1:A:597:ASP:HB3	1:A:600:PHE:HB2	1.91	0.51
1:A:591:GLN:HG3	1:A:592:PRO:N	2.25	0.51
1:B:634:ILE:CG2	1:B:639:LEU:HB2	2.39	0.51
1:B:799:LEU:HG	1:B:803:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:290:PHE:CB	1:A:291:PRO:HD2	2.29	0.51
1:B:236:GLU:O	1:B:238:TYR:CD2	2.64	0.51
1:A:501:ASN:C	1:A:502:ILE:HG13	2.30	0.51
1:A:586:LEU:CD1	1:A:640:ALA:HB3	2.41	0.51
1:B:628:PHE:O	1:B:634:ILE:HD12	2.11	0.51
1:B:757:MET:HE3	1:B:761:MET:HG3	1.92	0.51
1:A:223:TYR:CZ	1:A:364:HIS:NE2	2.78	0.51
1:A:341:ASP:O	1:A:342:GLN:HG2	2.10	0.51
1:B:319:LEU:O	1:B:323:LEU:HB2	2.10	0.51
1:B:465:ILE:HG22	1:B:466:ALA:N	2.25	0.51
1:A:268:SER:HB3	1:A:273:GLN:O	2.11	0.51
1:A:820:ARG:O	1:A:824:GLU:HG2	2.11	0.51
1:B:233:LEU:O	1:B:236:GLU:N	2.36	0.51
1:B:421:ALA:HB2	1:B:540:PHE:CE2	2.45	0.50
1:A:816:TRP:CG	1:A:894:HIS:CD2	2.99	0.50
1:A:484:HIS:CD2	1:A:486:LEU:H	2.28	0.50
1:A:838:LYS:O	1:A:839:ALA:O	2.29	0.50
1:A:700:HIS:CD2	1:A:701:ARG:N	2.79	0.50
1:B:782:LYS:O	1:B:786:VAL:HG22	2.11	0.50
1:A:418:ILE:CG1	1:A:432:VAL:HG22	2.41	0.50
1:A:728:ARG:NE	1:B:701:ARG:NH2	2.59	0.50
1:B:307:GLN:HB3	1:B:309:LYS:HD3	1.93	0.50
1:A:482:TYR:CE1	1:A:487:PHE:CE2	2.99	0.50
1:A:762:ARG:O	1:A:766:LEU:HD22	2.11	0.50
1:B:608:ARG:HH22	1:B:655:TYR:HE1	1.60	0.50
1:A:688:ALA:CB	1:A:757:MET:HE3	2.41	0.50
1:A:317:GLN:O	1:A:321:SER:HB3	2.12	0.50
1:B:320:GLN:CA	1:B:323:LEU:HB2	2.41	0.50
1:B:477:ASN:OD1	1:B:478:ILE:N	2.44	0.50
1:B:776:ILE:HG13	1:B:780:LEU:HG	1.93	0.50
1:B:651:ARG:HB2	1:B:700:HIS:O	2.11	0.50
1:B:667:PHE:HD2	1:B:807:CYS:HA	1.73	0.50
1:B:299:VAL:HG13	1:B:304:LYS:O	2.10	0.50
1:B:507:ILE:O	1:B:508:LYS:O	2.30	0.50
1:B:735:ILE:HD13	1:B:735:ILE:N	2.25	0.50
1:B:441:VAL:HG22	1:B:458:ARG:HG3	1.94	0.50
1:A:523:LYS:HD3	1:A:528:TRP:O	2.12	0.50
1:B:418:ILE:CG1	1:B:432:VAL:HG22	2.41	0.50
1:A:239:ASP:OD1	1:A:248:LYS:HE3	2.12	0.50
1:B:320:GLN:HE21	1:B:327:LEU:N	2.10	0.50
1:A:435:LEU:HD22	1:A:440:LEU:HD23	1.94	0.50
1:A:743:CYS:O	1:A:745:ILE:HG23	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:666:HIS:CE1	1:A:670:LEU:HD11	2.43	0.50
1:B:719:TYR:OH	1:B:811:ASP:OD1	2.29	0.50
1:B:252:TYR:CD2	1:B:252:TYR:C	2.85	0.50
1:B:318:GLN:O	1:B:318:GLN:OE1	2.29	0.50
1:A:399:VAL:HG22	1:A:420:GLU:OE2	2.12	0.50
1:A:571:MET:CE	1:A:571:MET:HA	2.36	0.50
1:B:695:CYS:HB3	1:B:698:LEU:CD1	2.42	0.50
1:B:607:PRO:CG	1:B:663:SER:HB3	2.41	0.50
1:A:580:ASP:O	1:A:584:LYS:HG3	2.12	0.50
1:B:536:LEU:O	1:B:536:LEU:HD22	2.12	0.50
1:B:441:VAL:HG11	1:B:443:LYS:HE3	1.93	0.50
1:A:561:GLN:HE22	1:B:561:GLN:HA	1.77	0.50
1:B:572:MET:C	1:B:574:HIS:N	2.64	0.50
1:B:587:HIS:C	1:B:589:GLY:H	2.14	0.50
1:B:270:ASP:OD1	1:B:272:LEU:HG	2.12	0.49
1:A:528:TRP:N	1:A:528:TRP:HD1	2.09	0.49
1:A:666:HIS:CE1	1:A:670:LEU:CD2	2.93	0.49
1:B:721:SER:O	1:B:722:GLU:CD	2.51	0.49
1:B:305:SER:HB3	1:B:333:VAL:HA	1.93	0.49
1:B:265:LEU:HB3	1:B:274:LEU:HD13	1.94	0.49
1:A:628:PHE:O	1:A:634:ILE:HD12	2.13	0.49
1:A:688:ALA:HA	1:A:757:MET:CE	2.42	0.49
1:A:475:ILE:HD13	1:A:506:PRO:HD2	1.93	0.49
1:B:416:GLU:HA	1:B:416:GLU:OE1	2.12	0.49
1:A:409:ASP:C	1:A:411:SER:H	2.14	0.49
1:A:370:PHE:HD1	1:A:373:THR:HG22	1.75	0.49
1:A:571:MET:CA	1:A:571:MET:HE2	2.35	0.49
1:B:376:VAL:CG1	1:B:377:LEU:N	2.75	0.49
1:A:500:ARG:NH2	1:A:522:ASN:HB3	2.27	0.49
1:A:570:MET:CE	1:B:762:ARG:HH11	2.26	0.49
1:B:852:LYS:NZ	1:B:852:LYS:CB	2.76	0.49
1:A:668:CYS:O	1:A:671:LEU:HB2	2.13	0.49
1:A:811:ASP:HB2	1:A:822:ILE:CD1	2.37	0.49
1:B:428:GLU:O	1:B:429:ILE:HG23	2.12	0.49
1:B:795:HIS:HA	1:B:798:LEU:HD12	1.94	0.49
1:B:277:LYS:HB3	1:B:287:GLU:HG3	1.95	0.49
1:B:417:ILE:CD1	1:B:548:ILE:HD11	2.42	0.49
1:B:417:ILE:HD13	1:B:548:ILE:CD1	2.43	0.49
1:B:872:LYS:HE2	1:B:876:ASP:CG	2.33	0.49
1:A:822:ILE:O	1:A:825:LEU:N	2.45	0.49
1:B:602:SER:O	1:B:604:THR:N	2.45	0.49
1:B:882:ALA:O	1:B:886:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:265:LEU:CB	1:B:274:LEU:HD13	2.41	0.49
1:A:715:LEU:HD22	1:A:859:GLN:NE2	2.27	0.49
1:A:767:ALA:C	1:A:769:ASP:H	2.15	0.49
1:A:675:LEU:N	1:A:675:LEU:HD23	2.28	0.49
1:A:572:MET:HE3	1:A:737:ILE:HG12	1.93	0.49
1:A:390:LYS:HE2	1:B:386:GLU:OE1	2.12	0.49
1:A:709:VAL:HG12	1:A:710:ALA:N	2.28	0.49
1:A:445:PHE:O	1:A:446:ASP:HB2	2.12	0.49
1:A:478:ILE:HG21	1:A:481:ALA:HA	1.95	0.49
1:A:872:LYS:HB2	1:A:885:TYR:CE1	2.48	0.49
1:B:848:MET:HA	1:B:851:GLU:HB2	1.94	0.49
1:B:439:GLU:HA	1:B:461:ALA:N	2.27	0.49
1:A:460:PRO:HG2	1:A:463:GLN:NE2	2.28	0.49
1:A:337:SER:HB3	1:A:340:THR:HG23	1.92	0.49
1:A:709:VAL:HG21	1:A:712:LYS:HG3	1.95	0.48
1:B:788:TYR:HA	1:B:795:HIS:ND1	2.28	0.48
1:A:332:CYS:SG	1:A:346:LEU:HD13	2.53	0.48
1:A:484:HIS:CD2	1:A:485:PRO:HD2	2.47	0.48
1:A:226:ARG:O	1:A:228:ARG:N	2.46	0.48
1:B:714:VAL:HG12	1:B:716:ALA:N	2.25	0.48
1:B:572:MET:CE	1:B:645:MET:CE	2.91	0.48
1:A:569:GLU:HG3	1:A:574:HIS:CD2	2.48	0.48
1:B:473:GLY:HA2	1:B:514:VAL:HG21	1.93	0.48
1:A:441:VAL:HA	1:A:457:ILE:O	2.13	0.48
1:A:590:ILE:HG21	1:A:624:GLN:CD	2.33	0.48
1:B:885:TYR:CD2	1:B:885:TYR:C	2.86	0.48
1:A:873:LEU:O	1:A:877:LEU:HD12	2.12	0.48
1:B:777:PHE:CE2	1:B:781:GLN:NE2	2.81	0.48
1:B:799:LEU:HG	1:B:803:LEU:HD11	1.95	0.48
1:A:440:LEU:HB2	1:A:459:ILE:HG13	1.93	0.48
1:A:223:TYR:CD2	1:A:226:ARG:HB2	2.48	0.48
1:B:590:ILE:O	1:B:591:GLN:HB3	2.13	0.48
1:B:821:LYS:O	1:B:825:LEU:HD12	2.12	0.48
1:A:810:SER:O	1:A:813:THR:OG1	2.28	0.48
1:B:852:LYS:HG3	1:B:852:LYS:O	2.13	0.48
1:B:402:ASN:O	1:B:406:HIS:HD2	1.95	0.48
1:A:559:GLU:O	1:A:561:GLN:N	2.47	0.48
1:B:433:PHE:CD2	1:B:442:ALA:CB	2.96	0.48
1:B:768:THR:HG22	1:B:804:MET:HG2	1.95	0.48
1:A:510:GLU:OE1	1:A:510:GLU:HA	2.14	0.48
1:A:527:PRO:HB2	1:A:528:TRP:CD1	2.49	0.48
1:A:829:GLU:C	1:A:831:PHE:H	2.16	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:648:LYS:HE3	4:B:168:HOH:O	2.13	0.48
1:A:341:ASP:C	1:A:342:GLN:HG2	2.34	0.48
1:A:353:LEU:O	1:A:354:GLU:O	2.32	0.48
1:A:570:MET:CE	1:B:762:ARG:NH1	2.77	0.48
1:A:231:LEU:CD1	1:B:372:TYR:CE1	2.97	0.48
1:B:718:LEU:CG	1:B:719:TYR:N	2.76	0.48
1:A:732:ALA:HB2	1:B:571:MET:CE	2.44	0.48
1:A:476:LEU:CD2	1:A:478:ILE:HD11	2.44	0.48
1:A:305:SER:HB3	1:A:333:VAL:HA	1.94	0.48
1:A:247:LEU:CD2	1:A:251:GLN:HE22	2.22	0.48
1:B:353:LEU:HD23	1:B:353:LEU:HA	1.71	0.48
1:B:645:MET:HG2	1:B:737:ILE:HG23	1.95	0.48
1:B:330:MET:CG	1:B:350:PHE:CD1	2.97	0.48
1:B:667:PHE:O	1:B:670:LEU:HB2	2.14	0.48
1:B:579:ASP:HA	1:B:582:TYR:CD2	2.49	0.48
1:B:720:SER:HB2	1:B:770:LEU:CB	2.43	0.48
1:A:246:GLN:O	1:A:250:LEU:HB2	2.13	0.48
1:A:258:ARG:CB	1:A:258:ARG:HH11	2.26	0.48
1:B:559:GLU:O	1:B:562:TYR:HB3	2.14	0.48
1:A:770:LEU:CD1	1:A:773:HIS:HB3	2.44	0.48
1:B:501:ASN:C	1:B:502:ILE:HG13	2.35	0.48
1:B:226:ARG:C	1:B:228:ARG:H	2.18	0.48
1:B:341:ASP:O	1:B:342:GLN:HG2	2.14	0.48
1:B:261:ARG:HD3	1:B:280:GLY:CA	2.44	0.48
1:A:428:GLU:HA	1:A:524:ILE:HD11	1.96	0.48
1:A:688:ALA:HB3	1:A:760:LEU:HD13	1.96	0.48
1:B:607:PRO:HB2	1:B:663:SER:HB3	1.95	0.48
1:B:890:SER:O	1:B:893:GLU:N	2.47	0.48
1:A:258:ARG:HH11	1:A:258:ARG:HB3	1.78	0.47
1:B:393:CYS:O	1:B:397:LEU:N	2.34	0.47
1:A:591:GLN:HG3	1:A:592:PRO:CD	2.43	0.47
1:B:253:LEU:O	1:B:255:GLN:N	2.47	0.47
1:B:261:ARG:CD	1:B:280:GLY:HA3	2.43	0.47
1:B:479:PRO:CB	1:B:528:TRP:CE3	2.97	0.47
1:B:799:LEU:C	1:B:799:LEU:HD12	2.28	0.47
1:B:433:PHE:CE2	1:B:442:ALA:HB3	2.49	0.47
1:B:596:ILE:CG2	1:B:600:PHE:CD1	2.97	0.47
1:A:360:ASP:HB3	4:A:110:HOH:O	2.14	0.47
1:A:668:CYS:SG	1:A:689:LEU:CD2	3.03	0.47
1:A:527:PRO:CG	1:A:528:TRP:CD1	2.96	0.47
1:A:593:VAL:CG1	1:A:600:PHE:CE2	2.98	0.47
1:B:698:LEU:O	1:B:730:HIS:CD2	2.67	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:590:ILE:HG22	1:A:624:GLN:HE22	1.78	0.47
1:B:478:ILE:HG23	1:B:480:ASP:O	2.14	0.47
1:B:527:PRO:CB	1:B:528:TRP:CD1	2.97	0.47
1:B:330:MET:CG	1:B:350:PHE:CE1	2.97	0.47
1:A:273:GLN:HG2	1:A:291:PRO:HA	1.94	0.47
1:B:318:GLN:HA	1:B:321:SER:OG	2.15	0.47
1:A:563:ARG:HD3	4:A:57:HOH:O	2.14	0.47
1:A:838:LYS:HB3	1:B:774:LEU:CB	2.45	0.47
1:B:352:LYS:HB3	1:B:356:ASP:HA	1.96	0.47
1:A:565:HIS:HA	1:A:568:ASN:HB3	1.96	0.47
1:A:570:MET:HE3	1:B:762:ARG:NH1	2.29	0.47
1:B:868:MET:HG2	1:B:888:VAL:HG12	1.95	0.47
1:B:312:THR:HG22	1:B:313:SER:N	2.29	0.47
1:B:459:ILE:HD12	1:B:460:PRO:HD3	1.97	0.47
1:B:508:LYS:H	1:B:514:VAL:HA	1.79	0.47
1:A:630:ASN:N	1:A:630:ASN:HD22	2.11	0.47
1:B:253:LEU:C	1:B:255:GLN:N	2.68	0.47
1:A:605:TYR:O	1:A:814:LYS:HE3	2.14	0.47
1:A:605:TYR:CZ	1:A:610:LEU:HD11	2.50	0.47
1:A:814:LYS:HB3	1:A:818:THR:CG2	2.45	0.47
1:A:610:LEU:HB3	1:A:611:PRO:CD	2.44	0.47
1:A:602:SER:C	1:A:604:THR:H	2.18	0.47
1:A:648:LYS:CB	1:A:648:LYS:NZ	2.78	0.47
1:A:575:MET:HG2	1:A:648:LYS:HG2	1.96	0.47
1:A:425:SER:OG	1:A:520:LEU:HD22	2.14	0.47
1:B:567:ALA:O	1:B:570:MET:HB2	2.14	0.47
1:B:617:MET:O	1:B:620:LEU:N	2.48	0.47
1:A:874:LEU:HD23	1:A:874:LEU:HA	1.74	0.47
1:B:441:VAL:HG21	1:B:458:ARG:NH2	2.29	0.47
1:A:440:LEU:HG	1:A:461:ALA:HA	1.97	0.47
1:B:375:THR:HG22	1:B:376:VAL:N	2.29	0.47
1:B:460:PRO:HG2	1:B:463:GLN:CG	2.44	0.47
1:B:672:TYR:N	1:B:677:LEU:HD12	2.29	0.47
1:A:460:PRO:CG	1:A:463:GLN:NE2	2.77	0.47
1:A:476:LEU:CD2	1:A:478:ILE:CD1	2.92	0.47
1:A:224:THR:CG2	1:A:228:ARG:NH2	2.74	0.47
1:B:636:CYS:N	1:B:637:PRO:HD2	2.30	0.47
1:B:314:GLU:O	1:B:317:GLN:N	2.48	0.47
1:B:330:MET:HA	1:B:349:ALA:O	2.15	0.47
1:A:230:ILE:HA	1:A:230:ILE:HD13	1.48	0.47
1:A:656:HIS:HD2	1:A:829:GLU:OE2	1.98	0.47
1:B:597:ASP:HB3	1:B:600:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:641:ARG:NH1	1:A:742:GLY:HA3	2.30	0.47
1:A:566:LEU:HD13	1:B:755:GLN:HE21	1.80	0.46
1:A:223:TYR:HD2	1:A:223:TYR:O	1.98	0.46
1:A:681:LEU:HB3	1:A:685:GLU:OE1	2.15	0.46
1:B:458:ARG:CG	1:B:458:ARG:NH1	2.73	0.46
1:A:331:LEU:HD13	1:A:366:ILE:HD12	1.96	0.46
1:B:508:LYS:N	1:B:514:VAL:HA	2.31	0.46
1:A:860:ILE:HD11	1:A:895:TRP:HB3	1.96	0.46
1:A:575:MET:CE	1:A:649:GLY:HA2	2.45	0.46
1:A:403:LEU:CD1	1:A:417:ILE:HG13	2.45	0.46
1:B:460:PRO:CG	1:B:463:GLN:NE2	2.78	0.46
1:A:311:LEU:HD23	1:A:315:ASP:HB2	1.97	0.46
1:A:852:LYS:HB2	1:A:852:LYS:NZ	2.30	0.46
1:B:820:ARG:O	1:B:824:GLU:HG2	2.16	0.46
1:B:503:LEU:HD12	1:B:504:CYS:N	2.30	0.46
1:B:268:SER:HB3	1:B:273:GLN:O	2.15	0.46
1:B:270:ASP:N	1:B:270:ASP:OD2	2.48	0.46
1:B:260:SER:HG	1:B:351:ASN:HB2	1.78	0.46
1:A:593:VAL:HG12	1:A:600:PHE:CE2	2.49	0.46
1:B:561:GLN:CA	1:B:561:GLN:NE2	2.79	0.46
1:A:223:TYR:CE1	1:A:364:HIS:NE2	2.65	0.46
1:A:816:TRP:O	1:A:820:ARG:HB2	2.14	0.46
1:A:586:LEU:HD11	1:A:636:CYS:O	2.15	0.46
1:A:591:GLN:HG3	1:A:592:PRO:HD2	1.97	0.46
1:B:674:ASN:H	1:B:674:ASN:ND2	2.13	0.46
1:B:748:HIS:H	1:B:748:HIS:CD2	2.33	0.46
1:B:532:PHE:C	1:B:532:PHE:CD1	2.89	0.46
1:B:622:MET:HE1	1:B:666:HIS:CB	2.44	0.46
1:B:630:ASN:ND2	1:B:631:ASN:N	2.59	0.46
1:A:732:ALA:HB1	1:B:571:MET:HE2	1.98	0.46
1:B:320:GLN:HE21	1:B:327:LEU:CB	2.23	0.46
1:B:465:ILE:CD1	1:B:502:ILE:HD13	2.46	0.46
1:A:484:HIS:CD2	1:A:485:PRO:CG	2.99	0.46
1:B:333:VAL:CB	1:B:366:ILE:HG21	2.46	0.46
1:B:508:LYS:HA	1:B:513:GLU:C	2.37	0.46
1:A:521:VAL:O	1:A:522:ASN:HB2	2.16	0.46
1:B:837:GLU:CB	1:B:838:LYS:NZ	2.77	0.46
1:B:671:LEU:HB3	1:B:677:LEU:HD11	1.96	0.46
1:A:370:PHE:CD1	1:A:373:THR:HG22	2.50	0.46
1:A:388:LYS:HE3	1:A:388:LYS:HB3	1.45	0.46
1:B:818:THR:O	1:B:822:ILE:HD12	2.16	0.46
1:A:274:LEU:HD23	1:A:274:LEU:N	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:854:TYR:HE1	4:A:75:HOH:O	1.98	0.46
1:A:223:TYR:HH	1:A:364:HIS:CE1	2.32	0.46
1:A:700:HIS:CD2	1:A:701:ARG:O	2.69	0.46
1:A:707:PHE:C	1:A:709:VAL:N	2.69	0.45
1:B:471:THR:CG2	1:B:472:THR:N	2.79	0.45
1:B:626:MET:HB2	1:B:626:MET:HE2	1.78	0.45
1:B:366:ILE:O	1:B:369:CYS:HB3	2.15	0.45
1:A:838:LYS:CB	1:B:774:LEU:HD12	2.46	0.45
1:B:326:GLU:HB3	1:B:328:GLN:NE2	2.31	0.45
1:B:720:SER:HA	1:B:770:LEU:HB2	1.97	0.45
1:B:727:GLU:N	1:B:727:GLU:OE2	2.50	0.45
1:B:505:PHE:HE1	1:B:541:SER:HG	1.62	0.45
1:B:715:LEU:HD22	1:B:859:GLN:HE22	1.81	0.45
1:A:620:LEU:HD23	1:A:639:LEU:HD21	1.98	0.45
1:A:805:THR:HG22	1:A:870:ILE:HD13	1.96	0.45
1:A:788:TYR:CZ	1:A:799:LEU:CD2	2.99	0.45
1:B:392:GLU:OE2	1:B:532:PHE:CE1	2.70	0.45
1:A:330:MET:CG	1:A:350:PHE:CD1	2.98	0.45
1:A:528:TRP:H	1:A:528:TRP:HD1	1.65	0.45
1:A:622:MET:SD	1:A:669:TYR:CG	3.09	0.45
1:A:675:LEU:CD1	1:A:878:PHE:CG	2.99	0.45
1:B:399:VAL:CG2	1:B:540:PHE:HE1	2.24	0.45
1:B:689:LEU:HA	1:B:764:ILE:HD13	1.97	0.45
1:B:738:LEU:HD22	1:B:744:ASN:OD1	2.17	0.45
1:A:777:PHE:CE2	1:A:781:GLN:NE2	2.85	0.45
1:A:536:LEU:O	1:A:536:LEU:HD22	2.17	0.45
1:A:479:PRO:CB	1:A:528:TRP:CE3	2.97	0.45
1:A:366:ILE:HG22	1:A:367:GLN:N	2.30	0.45
1:B:648:LYS:HB2	1:B:648:LYS:HZ2	1.80	0.45
1:A:755:GLN:HE21	1:B:566:LEU:HD13	1.82	0.45
1:B:852:LYS:HE3	1:B:852:LYS:HB2	1.74	0.45
1:B:225:ASP:HA	1:B:228:ARG:HE	1.81	0.45
1:A:484:HIS:CD2	1:A:485:PRO:CD	2.99	0.45
1:A:507:ILE:O	1:A:508:LYS:HG3	2.17	0.45
1:A:855:ILE:N	1:A:856:PRO:CD	2.79	0.45
1:A:617:MET:O	1:A:620:LEU:HB2	2.16	0.45
1:B:606:THR:HG1	1:B:609:SER:HB3	1.81	0.45
1:A:862:PHE:HE1	1:A:866:ILE:HG21	1.82	0.45
1:A:273:GLN:HB3	1:A:273:GLN:HE21	1.51	0.45
1:A:602:SER:HB3	4:A:184:HOH:O	2.16	0.45
1:A:721:SER:CA	1:A:769:ASP:OD2	2.63	0.45
1:B:428:GLU:HB2	1:B:522:ASN:HB2	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:838:LYS:N	1:A:838:LYS:CD	2.78	0.45
1:A:610:LEU:HA	1:A:611:PRO:HD3	1.60	0.45
1:B:254:GLN:OE1	1:B:280:GLY:HA2	2.16	0.45
1:A:873:LEU:HA	1:A:876:ASP:HB2	1.99	0.45
1:B:755:GLN:O	1:B:758:LEU:HB2	2.16	0.45
1:A:445:PHE:HB3	1:A:446:ASP:H	1.42	0.45
1:B:230:ILE:HD13	1:B:230:ILE:HA	1.64	0.45
1:B:576:LYS:H	1:B:648:LYS:HD3	1.82	0.45
1:A:593:VAL:CG2	1:A:625:ASP:HB2	2.46	0.45
1:B:290:PHE:CB	1:B:291:PRO:HD2	2.21	0.45
1:A:231:LEU:CD1	1:B:372:TYR:CZ	2.98	0.45
1:B:572:MET:CE	1:B:645:MET:HE3	2.47	0.45
1:A:623:LEU:HA	1:A:626:MET:HE3	1.98	0.45
1:B:313:SER:O	1:B:317:GLN:HB2	2.17	0.45
1:B:395:ALA:O	1:B:399:VAL:HG12	2.17	0.45
1:A:277:LYS:HB3	1:A:287:GLU:CG	2.46	0.45
1:A:338:ARG:NH2	1:B:238:TYR:CD2	2.84	0.45
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.61	0.45
1:B:754:TYR:O	1:B:758:LEU:HD13	2.18	0.44
1:A:240:LEU:HD11	1:B:340:THR:HG22	1.99	0.44
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.84	0.44
1:B:258:ARG:HG2	1:B:258:ARG:NH1	2.31	0.44
1:B:719:TYR:O	1:B:720:SER:HB3	2.16	0.44
1:A:723:GLY:C	1:A:725:VAL:H	2.21	0.44
1:B:735:ILE:HD12	1:B:738:LEU:HD12	1.98	0.44
1:A:497:PHE:O	1:A:498:ARG:HB2	2.16	0.44
1:A:756:ARG:HB2	1:A:756:ARG:HE	1.71	0.44
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.76	0.44
1:B:290:PHE:CB	1:B:291:PRO:CD	2.94	0.44
1:A:453:GLU:CD	1:A:453:GLU:H	2.21	0.44
1:B:887:ARG:NH1	1:B:887:ARG:CG	2.78	0.44
1:A:376:VAL:O	1:A:380:THR:OG1	2.34	0.44
1:B:433:PHE:CE2	1:B:442:ALA:CB	2.99	0.44
1:A:436:ASP:HB2	1:A:441:VAL:HG21	1.96	0.44
1:A:505:PHE:HA	1:A:506:PRO:HD3	1.76	0.44
1:A:789:ASP:HB3	1:A:792:ASN:H	1.81	0.44
1:A:586:LEU:HD21	1:A:636:CYS:HB3	2.00	0.44
1:A:709:VAL:O	1:A:710:ALA:HB2	2.16	0.44
1:A:799:LEU:CD1	1:A:803:LEU:CD1	2.95	0.44
1:A:812:GLN:CB	1:A:888:VAL:HG22	2.47	0.44
1:B:851:GLU:HA	1:B:854:TYR:CE1	2.52	0.44
1:B:251:GLN:NE2	1:B:281:ASP:HA	2.31	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:275:SER:CB	1:A:287:GLU:OE2	2.65	0.44
1:B:854:TYR:CD1	1:B:854:TYR:N	2.86	0.44
1:B:425:SER:O	1:B:426:ASN:HB2	2.17	0.44
1:B:323:LEU:HD12	1:B:327:LEU:HD11	1.94	0.44
1:B:459:ILE:CG1	1:B:460:PRO:HD2	2.47	0.44
1:B:459:ILE:HG13	1:B:460:PRO:HD2	2.00	0.44
1:B:330:MET:CE	1:B:332:CYS:N	2.81	0.44
1:B:508:LYS:CA	1:B:514:VAL:HA	2.48	0.44
1:A:251:GLN:NE2	1:A:281:ASP:CA	2.78	0.44
1:A:889:ALA:O	1:A:892:ARG:HB3	2.17	0.44
1:A:681:LEU:HD13	1:A:800:LEU:HD21	2.00	0.44
1:B:409:ASP:HB3	1:B:412:VAL:HB	1.99	0.44
1:A:715:LEU:HD23	1:A:862:PHE:CD2	2.53	0.44
1:A:542:ILE:HG21	1:B:401:LYS:HZ3	1.83	0.44
1:B:618:ALA:O	1:B:622:MET:HG3	2.18	0.44
1:B:421:ALA:HB2	1:B:540:PHE:HE2	1.83	0.44
1:B:809:LEU:O	1:B:811:ASP:N	2.50	0.44
1:B:675:LEU:HD13	1:B:878:PHE:CG	2.53	0.44
1:B:872:LYS:HD2	1:B:872:LYS:HA	1.60	0.44
1:A:239:ASP:HB2	1:A:245:LEU:CD2	2.48	0.44
1:B:439:GLU:HA	1:B:461:ALA:H	1.83	0.44
1:A:413:LEU:O	1:A:416:GLU:HB2	2.17	0.44
1:B:770:LEU:HD13	1:B:770:LEU:HA	1.36	0.44
1:B:859:GLN:CA	1:B:859:GLN:HE21	2.29	0.44
1:A:868:MET:HB2	1:A:869:PRO:HD3	2.00	0.44
1:A:299:VAL:HG12	1:A:334:PRO:HG3	1.99	0.44
1:B:586:LEU:HD12	1:B:640:ALA:HB3	2.00	0.44
1:B:258:ARG:HG2	1:B:258:ARG:HH11	1.83	0.44
1:A:805:THR:CG2	1:A:870:ILE:HD13	2.48	0.44
1:B:478:ILE:HA	1:B:479:PRO:HD2	1.61	0.43
1:B:501:ASN:OD1	1:B:522:ASN:HA	2.18	0.43
1:B:902:VAL:HA	1:B:903:PRO:HD3	1.34	0.43
1:A:508:LYS:H	1:A:515:ILE:H	1.66	0.43
1:B:749:PHE:N	1:B:749:PHE:CD1	2.85	0.43
1:B:848:MET:O	1:B:852:LYS:HB3	2.18	0.43
1:B:726:MET:O	1:B:729:HIS:HB3	2.18	0.43
1:A:719:TYR:OH	1:A:811:ASP:OD1	2.29	0.43
1:B:472:THR:O	1:B:474:GLN:HG3	2.17	0.43
1:B:855:ILE:N	1:B:856:PRO:CD	2.80	0.43
1:B:682:GLU:HG3	1:B:685:GLU:OE1	2.19	0.43
1:A:689:LEU:HA	1:A:764:ILE:HD13	2.01	0.43
1:A:672:TYR:HD1	1:A:686:ILE:HG21	1.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:726:MET:O	1:A:729:HIS:HB3	2.19	0.43
1:A:673:LYS:HB2	1:A:674:ASN:H	1.60	0.43
1:B:721:SER:OG	1:B:722:GLU:N	2.51	0.43
1:A:561:GLN:HE22	1:B:561:GLN:HE21	1.66	0.43
1:B:600:PHE:O	1:B:600:PHE:CD2	2.71	0.43
1:A:721:SER:O	1:A:722:GLU:CD	2.56	0.43
1:A:226:ARG:C	1:A:228:ARG:N	2.69	0.43
1:B:903:PRO:O	1:B:904:ARG:HG3	2.17	0.43
1:B:418:ILE:CG1	1:B:432:VAL:CG2	2.96	0.43
1:A:304:LYS:CA	1:A:304:LYS:HE3	2.31	0.43
1:A:670:LEU:O	1:A:674:ASN:ND2	2.46	0.43
1:A:376:VAL:CG1	1:A:377:LEU:N	2.81	0.43
1:B:356:ASP:O	1:B:357:LEU:HG	2.19	0.43
1:A:337:SER:HB2	1:A:344:VAL:HG21	2.00	0.43
1:B:266:LEU:CD1	1:B:277:LYS:HE2	2.47	0.43
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.71	0.43
1:B:443:LYS:O	1:B:455:TYR:O	2.36	0.43
1:B:501:ASN:HB2	1:B:529:PHE:CE1	2.54	0.43
1:A:376:VAL:CG2	1:B:375:THR:HG22	2.48	0.43
1:A:860:ILE:HD13	1:A:895:TRP:HB3	2.00	0.43
1:A:796:HIS:O	1:A:800:LEU:HD12	2.19	0.43
1:A:448:GLY:O	1:A:449:VAL:HG23	2.18	0.43
1:A:372:TYR:CE1	1:B:231:LEU:HD12	2.54	0.43
1:A:814:LYS:N	1:A:814:LYS:CD	2.81	0.43
1:B:749:PHE:N	1:B:749:PHE:HD1	2.16	0.43
1:A:572:MET:HE3	1:A:737:ILE:N	2.34	0.43
1:B:417:ILE:CD1	1:B:548:ILE:CD1	2.97	0.43
1:B:443:LYS:HA	1:B:457:ILE:H	1.84	0.43
1:B:499:THR:CG2	1:B:500:ARG:N	2.63	0.43
1:B:769:ASP:O	1:B:772:HIS:N	2.51	0.43
1:A:559:GLU:C	1:A:561:GLN:N	2.72	0.43
1:B:224:THR:HG22	1:B:228:ARG:HH21	1.80	0.43
1:B:537:ALA:O	1:B:541:SER:HB2	2.18	0.43
1:A:478:ILE:HA	1:A:479:PRO:HD2	1.48	0.43
1:A:372:TYR:CE2	1:B:231:LEU:HD11	2.53	0.43
1:B:354:GLU:HB3	1:B:355:GLY:H	1.25	0.43
1:A:855:ILE:HB	1:A:856:PRO:HD3	2.01	0.43
1:B:860:ILE:HD11	1:B:895:TRP:C	2.39	0.43
1:A:812:GLN:O	1:A:888:VAL:HG22	2.19	0.43
1:A:711:SER:CB	1:A:854:TYR:CE2	2.96	0.42
1:B:258:ARG:HD3	1:B:352:LYS:CE	2.47	0.42
1:A:788:TYR:CZ	1:A:799:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:527:PRO:CG	1:B:528:TRP:CD1	3.01	0.42
1:A:672:TYR:O	1:A:676:GLU:HA	2.19	0.42
1:B:270:ASP:HB2	1:B:272:LEU:CG	2.46	0.42
1:A:231:LEU:HD11	1:B:372:TYR:CD2	2.54	0.42
1:A:656:HIS:CG	1:A:700:HIS:CE1	3.07	0.42
1:B:250:LEU:HA	1:B:250:LEU:HD12	1.88	0.42
1:A:671:LEU:HD13	1:A:803:LEU:CD2	2.42	0.42
1:B:680:TYR:HB3	1:B:788:TYR:CE2	2.54	0.42
1:A:231:LEU:HD21	1:B:230:ILE:CG2	2.39	0.42
1:B:627:ASN:ND2	1:B:631:ASN:CG	2.73	0.42
1:B:274:LEU:HD22	1:B:274:LEU:HA	1.87	0.42
1:B:712:LYS:N	4:B:52:HOH:O	2.51	0.42
1:B:504:CYS:SG	1:B:519:GLU:HB3	2.59	0.42
1:A:444:VAL:HB	1:A:454:SER:O	2.19	0.42
1:A:834:GLY:O	1:A:838:LYS:NZ	2.49	0.42
1:A:225:ASP:HA	1:A:228:ARG:HE	1.84	0.42
1:B:258:ARG:HD3	1:B:352:LYS:HZ3	1.83	0.42
1:A:600:PHE:HA	1:A:605:TYR:CD1	2.54	0.42
1:B:895:TRP:O	1:B:898:VAL:HG23	2.19	0.42
1:B:301:GLU:HA	1:B:301:GLU:OE1	2.19	0.42
1:A:233:LEU:O	1:A:236:GLU:HB2	2.19	0.42
1:B:476:LEU:CD2	1:B:478:ILE:CD1	2.98	0.42
1:B:528:TRP:HB2	1:B:529:PHE:H	1.49	0.42
1:B:357:LEU:HA	1:B:357:LEU:HD23	1.88	0.42
1:B:852:LYS:HZ1	1:B:852:LYS:CB	2.33	0.42
1:B:335:VAL:HB	1:B:345:ALA:HB3	2.01	0.42
1:B:439:GLU:N	1:B:461:ALA:HB2	2.35	0.42
1:B:476:LEU:HD23	1:B:478:ILE:CD1	2.48	0.42
1:A:688:ALA:CB	1:A:760:LEU:CD1	2.98	0.42
1:A:540:PHE:O	1:A:542:ILE:N	2.53	0.42
1:B:821:LYS:HA	1:B:824:GLU:HG3	2.01	0.42
1:B:848:MET:O	1:B:852:LYS:N	2.52	0.42
1:A:799:LEU:CD1	1:A:803:LEU:HD11	2.48	0.42
1:B:422:ARG:HD3	1:B:429:ILE:HA	2.01	0.42
1:A:852:LYS:CB	1:A:852:LYS:NZ	2.83	0.42
1:A:735:ILE:HD13	1:A:735:ILE:HA	1.73	0.42
1:A:381:LEU:O	1:A:381:LEU:HD12	2.20	0.42
1:B:398:GLN:NE2	1:B:401:LYS:HD3	2.34	0.42
1:A:602:SER:C	1:A:604:THR:N	2.74	0.42
1:A:703:THR:HB	1:A:718:LEU:HD12	2.00	0.42
1:A:542:ILE:HD13	1:B:401:LYS:HZ1	1.85	0.42
1:A:726:MET:HG2	1:A:730:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:821:LYS:HD3	1:A:824:GLU:OE1	2.20	0.42
1:A:252:TYR:CD2	1:A:252:TYR:C	2.93	0.42
1:A:418:ILE:CG1	1:A:432:VAL:CG2	2.98	0.42
1:B:251:GLN:HE22	1:B:281:ASP:HA	1.84	0.42
1:B:226:ARG:HB3	1:B:368:HIS:CE1	2.55	0.41
1:B:697:ASP:O	1:B:700:HIS:HB2	2.20	0.41
1:B:582:TYR:O	1:B:586:LEU:HB2	2.19	0.41
1:A:635:ASP:OD2	1:A:638:THR:N	2.53	0.41
1:B:508:LYS:H	1:B:515:ILE:H	1.68	0.41
1:B:258:ARG:NH1	1:B:258:ARG:CG	2.83	0.41
1:B:237:LEU:HD21	1:B:249:VAL:CG2	2.49	0.41
1:A:671:LEU:HD23	1:A:671:LEU:HA	1.80	0.41
1:B:608:ARG:NH2	1:B:655:TYR:HE1	2.17	0.41
1:A:636:CYS:HB2	1:A:637:PRO:HD3	2.02	0.41
1:A:389:LEU:HA	1:A:389:LEU:HD23	1.59	0.41
1:A:292:LEU:O	1:A:293:THR:O	2.39	0.41
1:A:575:MET:HG2	1:A:648:LYS:CG	2.51	0.41
1:B:781:GLN:O	1:B:784:ALA:N	2.53	0.41
1:A:571:MET:CE	1:B:731:PHE:HE2	2.33	0.41
1:B:637:PRO:C	1:B:641:ARG:HH21	2.23	0.41
1:A:596:ILE:HG21	1:A:600:PHE:CD1	2.55	0.41
1:A:509:ASN:OD1	1:A:513:GLU:HG3	2.19	0.41
1:A:821:LYS:HD3	1:A:821:LYS:HA	1.80	0.41
1:A:428:GLU:HB2	1:A:522:ASN:HB2	2.02	0.41
1:A:620:LEU:CD2	1:A:639:LEU:HD21	2.51	0.41
1:B:279:ILE:CD1	1:B:322:MET:SD	3.08	0.41
1:A:819:THR:HA	1:A:822:ILE:HD12	2.02	0.41
1:A:439:GLU:HA	1:A:461:ALA:H	1.85	0.41
1:A:467:GLY:O	1:A:471:THR:HB	2.19	0.41
1:A:329:ALA:O	1:A:330:MET:HB2	2.19	0.41
1:A:481:ALA:HB1	1:A:487:PHE:CD1	2.55	0.41
1:B:629:ILE:HA	1:B:634:ILE:HD12	2.01	0.41
1:A:718:LEU:C	1:A:720:SER:N	2.74	0.41
1:A:399:VAL:HG13	1:A:420:GLU:HG3	2.03	0.41
1:B:671:LEU:HD23	1:B:671:LEU:HA	1.81	0.41
1:A:366:ILE:O	1:A:369:CYS:HB3	2.20	0.41
1:A:618:ALA:O	1:A:622:MET:N	2.53	0.41
1:A:380:THR:O	1:A:384:GLN:HG3	2.21	0.41
1:B:655:TYR:OH	1:B:719:TYR:OH	2.20	0.41
1:B:572:MET:HE3	1:B:645:MET:CE	2.51	0.41
1:A:427:ALA:CB	1:A:520:LEU:CD2	2.99	0.41
1:A:362:ASP:O	1:A:365:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:837:GLU:CB	1:A:838:LYS:HE3	2.41	0.41
1:B:586:LEU:CD1	1:B:640:ALA:CB	2.98	0.41
1:B:576:LYS:C	1:B:648:LYS:HE2	2.40	0.41
1:B:901:LEU:N	1:B:901:LEU:CD2	2.75	0.41
1:A:277:LYS:HB3	1:A:287:GLU:HG3	2.03	0.41
1:B:256:GLU:H	1:B:256:GLU:HG2	1.54	0.41
1:A:718:LEU:CD2	1:A:826:ILE:HG23	2.51	0.41
1:B:656:HIS:CD2	1:B:829:GLU:OE2	2.54	0.41
1:A:320:GLN:O	1:A:324:GLY:N	2.41	0.41
1:A:468:HIS:NE2	1:A:472:THR:HG21	2.34	0.41
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.79	0.41
1:B:275:SER:HB3	1:B:287:GLU:OE2	2.20	0.41
1:B:812:GLN:NE2	1:B:812:GLN:HA	2.36	0.41
1:B:320:GLN:HG3	1:B:327:LEU:HD22	2.03	0.41
1:A:774:LEU:HD21	1:A:866:ILE:CD1	2.51	0.41
1:B:441:VAL:CG1	1:B:443:LYS:HD3	2.51	0.41
1:A:539:ALA:O	1:A:542:ILE:HB	2.21	0.41
1:B:677:LEU:HD21	1:B:803:LEU:CD2	2.50	0.41
1:A:638:THR:CG2	1:A:745:ILE:HG22	2.42	0.41
1:A:669:TYR:C	1:A:669:TYR:CD2	2.93	0.41
1:B:740:THR:CG2	1:B:743:CYS:SG	3.05	0.41
1:A:821:LYS:C	1:A:824:GLU:HG3	2.41	0.41
1:B:859:GLN:HG2	1:B:895:TRP:CE2	2.56	0.41
1:A:575:MET:HE1	1:A:649:GLY:CA	2.51	0.41
1:A:688:ALA:CB	1:A:760:LEU:HD12	2.50	0.41
1:A:868:MET:N	1:A:869:PRO:HD2	2.35	0.41
1:A:254:GLN:OE1	1:A:280:GLY:HA2	2.21	0.41
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.71	0.41
1:B:868:MET:HB2	1:B:869:PRO:CD	2.50	0.41
1:B:338:ARG:HA	1:B:338:ARG:HD2	1.75	0.41
1:B:837:GLU:C	1:B:838:LYS:NZ	2.74	0.41
1:B:838:LYS:O	1:B:839:ALA:HB3	2.21	0.41
1:B:578:SER:O	1:B:581:GLU:HB2	2.21	0.41
1:A:740:THR:CG2	1:A:741:HIS:N	2.84	0.41
1:B:511:ASN:N	1:B:511:ASN:ND2	2.69	0.41
1:A:707:PHE:C	1:A:709:VAL:H	2.23	0.40
1:A:709:VAL:CG2	1:A:712:LYS:HB2	2.51	0.40
1:B:319:LEU:HD22	1:B:322:MET:CE	2.51	0.40
1:A:720:SER:OG	1:A:721:SER:N	2.48	0.40
1:A:774:LEU:HD12	1:B:838:LYS:CB	2.51	0.40
1:B:622:MET:O	1:B:626:MET:HE2	2.22	0.40
1:A:550:HIS:CD2	1:B:407:LEU:HD23	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:572:MET:CE	1:B:645:MET:HE2	2.51	0.40
1:A:636:CYS:N	1:A:637:PRO:CD	2.83	0.40
1:B:647:LYS:HD2	1:B:658:TRP:CD1	2.56	0.40
1:A:687:PHE:O	1:A:691:ILE:HG12	2.21	0.40
1:A:819:THR:CG2	1:A:891:ASN:ND2	2.79	0.40
1:A:461:ALA:O	1:A:467:GLY:HA2	2.21	0.40
1:A:566:LEU:CD2	1:B:755:GLN:HE21	2.33	0.40
1:A:833:GLN:O	1:A:836:LEU:HD12	2.21	0.40
1:B:620:LEU:O	1:B:624:GLN:HB3	2.21	0.40
1:B:312:THR:HB	1:B:315:ASP:CG	2.38	0.40
1:A:788:TYR:CG	1:A:788:TYR:O	2.74	0.40
1:B:829:GLU:C	1:B:831:PHE:H	2.24	0.40
1:A:223:TYR:CE2	1:A:226:ARG:CB	2.96	0.40
1:A:647:LYS:HD2	1:A:658:TRP:CG	2.56	0.40
1:A:575:MET:CE	1:A:649:GLY:CA	2.99	0.40
1:A:404:PHE:HA	1:A:407:LEU:HD21	2.02	0.40
1:A:566:LEU:CD1	1:B:755:GLN:HE21	2.34	0.40
1:A:326:GLU:C	1:A:327:LEU:HD12	2.42	0.40
1:B:814:LYS:HD2	1:B:814:LYS:HA	1.90	0.40
1:B:629:ILE:HA	1:B:634:ILE:HB	2.04	0.40
1:A:770:LEU:HA	1:A:770:LEU:HD13	1.39	0.40
1:A:364:HIS:HA	1:A:367:GLN:NE2	2.36	0.40
1:B:237:LEU:HD21	1:B:249:VAL:HG22	2.04	0.40
1:B:687:PHE:CE1	1:B:746:PHE:CE1	3.08	0.40
1:B:624:GLN:CG	1:B:625:ASP:N	2.84	0.40
1:A:896:THR:O	1:A:899:SER:OG	2.33	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	655/691 (95%)	512 (78%)	95 (14%)	48 (7%)	2 8
1	B	633/691 (92%)	514 (81%)	84 (13%)	35 (6%)	3 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1288/1382 (93%)	1026 (80%)	179 (14%)	83 (6%)	2	11

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLU
1	A	293	THR
1	A	354	GLU
1	A	356	ASP
1	A	371	HIS
1	A	449	VAL
1	A	453	GLU
1	A	508	LYS
1	A	512	GLN
1	A	588	ASP
1	A	598	SER
1	A	603	PHE
1	A	705	ASN
1	A	706	SER
1	A	709	VAL
1	A	710	ALA
1	A	719	TYR
1	A	720	SER
1	A	788	TYR
1	A	830	PHE
1	B	256	GLU
1	B	293	THR
1	B	355	GLY
1	B	356	ASP
1	B	475	ILE
1	B	499	THR
1	B	500	ARG
1	B	508	LYS
1	B	512	GLN
1	B	588	ASP
1	B	719	TYR
1	B	720	SER
1	B	788	TYR
1	B	830	PHE
1	A	351	ASN
1	A	367	GLN
1	A	445	PHE

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Mol	Chain	Res	Type
1	A	534	GLU
1	A	541	SER
1	A	673	LYS
1	A	704	ASN
1	A	823	ALA
1	B	323	LEU
1	B	354	GLU
1	B	522	ASN
1	B	534	GLU
1	B	598	SER
1	B	599	ASN
1	B	603	PHE
1	A	227	ASP
1	A	353	LEU
1	A	426	ASN
1	A	437	GLN
1	A	560	ALA
1	A	696	HIS
1	A	856	PRO
1	B	437	GLN
1	B	575	MET
1	B	673	LYS
1	B	696	HIS
1	B	810	SER
1	A	255	GLN
1	A	368	HIS
1	A	479	PRO
1	A	707	PHE
1	A	722	GLU
1	B	254	GLN
1	A	315	ASP
1	A	330	MET
1	A	455	TYR
1	A	522	ASN
1	B	351	ASN
1	B	479	PRO
1	B	722	GLU
1	B	856	PRO
1	A	316	VAL
1	B	426	ASN
1	B	528	TRP
1	A	475	ILE

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Mol	Chain	Res	Type
1	B	592	PRO
1	B	903	PRO
1	A	557	VAL
1	A	591	GLN

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	590/614 (96%)	393 (67%)	197 (33%)	0	1
1	B	577/614 (94%)	397 (69%)	180 (31%)	0	2
All	All	1167/1228 (95%)	790 (68%)	377 (32%)	0	2

All (377) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	TYR
1	A	225	ASP
1	A	226	ARG
1	A	228	ARG
1	A	230	ILE
1	A	231	LEU
1	A	244	SER
1	A	250	LEU
1	A	252	TYR
1	A	254	GLN
1	A	257	THR
1	A	258	ARG
1	A	261	ARG
1	A	266	LEU
1	A	269	GLU
1	A	270	ASP
1	A	271	ASN
1	A	272	LEU
1	A	273	GLN
1	A	275	SER
1	A	277	LYS

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Mol	Chain	Res	Type
1	A	282	LYS
1	A	287	GLU
1	A	289	SER
1	A	292	LEU
1	A	295	CYS
1	A	296	LEU
1	A	298	GLN
1	A	300	VAL
1	A	304	LYS
1	A	305	SER
1	A	309	LYS
1	A	311	LEU
1	A	313	SER
1	A	317	GLN
1	A	318	GLN
1	A	320	GLN
1	A	321	SER
1	A	323	LEU
1	A	328	GLN
1	A	331	LEU
1	A	340	THR
1	A	356	ASP
1	A	359	THR
1	A	361	GLU
1	A	362	ASP
1	A	363	GLU
1	A	365	VAL
1	A	367	GLN
1	A	373	THR
1	A	374	SER
1	A	375	THR
1	A	377	LEU
1	A	378	THR
1	A	380	THR
1	A	381	LEU
1	A	388	LYS
1	A	390	LYS
1	A	391	CYS
1	A	396	LEU
1	A	397	LEU
1	A	398	GLN
1	A	403	LEU

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Mol	Chain	Res	Type
1	A	407	LEU
1	A	408	ASP
1	A	409	ASP
1	A	410	VAL
1	A	413	LEU
1	A	414	LEU
1	A	415	GLN
1	A	417	ILE
1	A	424	LEU
1	A	426	ASN
1	A	429	ILE
1	A	432	VAL
1	A	435	LEU
1	A	437	GLN
1	A	441	VAL
1	A	443	LYS
1	A	445	PHE
1	A	446	ASP
1	A	450	VAL
1	A	451	ASP
1	A	452	ASP
1	A	453	GLU
1	A	458	ARG
1	A	463	GLN
1	A	471	THR
1	A	472	THR
1	A	476	LEU
1	A	478	ILE
1	A	486	LEU
1	A	498	ARG
1	A	501	ASN
1	A	507	ILE
1	A	508	LYS
1	A	512	GLN
1	A	513	GLU
1	A	515	ILE
1	A	524	ILE
1	A	528	TRP
1	A	530	SER
1	A	532	PHE
1	A	535	ASP
1	A	536	LEU

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Mol	Chain	Res	Type
1	A	551	SER
1	A	553	LEU
1	A	557	VAL
1	A	559	GLU
1	A	563	ARG
1	A	566	LEU
1	A	569	GLU
1	A	572	MET
1	A	575	MET
1	A	576	LYS
1	A	579	ASP
1	A	580	ASP
1	A	582	TYR
1	A	585	LEU
1	A	587	HIS
1	A	590	ILE
1	A	593	VAL
1	A	598	SER
1	A	599	ASN
1	A	600	PHE
1	A	603	PHE
1	A	608	ARG
1	A	610	LEU
1	A	613	ASP
1	A	616	SER
1	A	621	SER
1	A	630	ASN
1	A	631	ASN
1	A	633	LYS
1	A	638	THR
1	A	645	MET
1	A	646	VAL
1	A	647	LYS
1	A	659	MET
1	A	662	PHE
1	A	663	SER
1	A	674	ASN
1	A	675	LEU
1	A	678	THR
1	A	681	LEU
1	A	683	ASP
1	A	695	CYS

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Mol	Chain	Res	Type
1	A	701	ARG
1	A	703	THR
1	A	704	ASN
1	A	706	SER
1	A	708	GLN
1	A	711	SER
1	A	712	LYS
1	A	713	SER
1	A	719	TYR
1	A	721	SER
1	A	722	GLU
1	A	725	VAL
1	A	741	HIS
1	A	748	HIS
1	A	751	ARG
1	A	752	LYS
1	A	756	ARG
1	A	758	LEU
1	A	760	LEU
1	A	766	LEU
1	A	770	LEU
1	A	782	LYS
1	A	785	GLU
1	A	789	ASP
1	A	790	ARG
1	A	793	LYS
1	A	797	ARG
1	A	798	LEU
1	A	810	SER
1	A	814	LYS
1	A	817	LYS
1	A	820	ARG
1	A	821	LYS
1	A	824	GLU
1	A	825	LEU
1	A	832	SER
1	A	833	GLN
1	A	835	ASP
1	A	838	LYS
1	A	852	LYS
1	A	872	LYS
1	A	874	LEU

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Mol	Chain	Res	Type
1	A	875	GLN
1	A	876	ASP
1	A	877	LEU
1	A	885	TYR
1	A	887	ARG
1	A	890	SER
1	A	896	THR
1	A	898	VAL
1	B	224	THR
1	B	225	ASP
1	B	226	ARG
1	B	228	ARG
1	B	230	ILE
1	B	231	LEU
1	B	233	LEU
1	B	243	SER
1	B	244	SER
1	B	250	LEU
1	B	252	TYR
1	B	254	GLN
1	B	257	THR
1	B	258	ARG
1	B	263	CYS
1	B	266	LEU
1	B	268	SER
1	B	269	GLU
1	B	270	ASP
1	B	272	LEU
1	B	273	GLN
1	B	274	LEU
1	B	275	SER
1	B	277	LYS
1	B	282	LYS
1	B	287	GLU
1	B	292	LEU
1	B	296	LEU
1	B	298	GLN
1	B	300	VAL
1	B	304	LYS
1	B	305	SER
1	B	307	GLN
1	B	309	LYS

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Mol	Chain	Res	Type
1	B	311	LEU
1	B	314	GLU
1	B	315	ASP
1	B	317	GLN
1	B	325	CYS
1	B	326	GLU
1	B	328	GLN
1	B	331	LEU
1	B	337	SER
1	B	340	THR
1	B	346	LEU
1	B	352	LYS
1	B	353	LEU
1	B	354	GLU
1	B	356	ASP
1	B	359	THR
1	B	361	GLU
1	B	363	GLU
1	B	365	VAL
1	B	367	GLN
1	B	373	THR
1	B	380	THR
1	B	381	LEU
1	B	383	PHE
1	B	388	LYS
1	B	390	LYS
1	B	394	GLN
1	B	397	LEU
1	B	399	VAL
1	B	401	LYS
1	B	407	LEU
1	B	413	LEU
1	B	414	LEU
1	B	415	GLN
1	B	416	GLU
1	B	424	LEU
1	B	426	ASN
1	B	429	ILE
1	B	432	VAL
1	B	435	LEU
1	B	437	GLN
1	B	455	TYR

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Mol	Chain	Res	Type
1	B	458	ARG
1	B	459	ILE
1	B	463	GLN
1	B	471	THR
1	B	472	THR
1	B	475	ILE
1	B	476	LEU
1	B	478	ILE
1	B	500	ARG
1	B	501	ASN
1	B	512	GLN
1	B	515	ILE
1	B	528	TRP
1	B	532	PHE
1	B	534	GLU
1	B	535	ASP
1	B	536	LEU
1	B	541	SER
1	B	548	ILE
1	B	553	LEU
1	B	555	LYS
1	B	557	VAL
1	B	561	GLN
1	B	565	HIS
1	B	566	LEU
1	B	570	MET
1	B	578	SER
1	B	579	ASP
1	B	580	ASP
1	B	581	GLU
1	B	582	TYR
1	B	585	LEU
1	B	587	HIS
1	B	588	ASP
1	B	590	ILE
1	B	593	VAL
1	B	598	SER
1	B	599	ASN
1	B	608	ARG
1	B	609	SER
1	B	613	ASP
1	B	616	SER

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Mol	Chain	Res	Type
1	B	621	SER
1	B	622	MET
1	B	623	LEU
1	B	624	GLN
1	B	630	ASN
1	B	633	LYS
1	B	638	THR
1	B	645	MET
1	B	646	VAL
1	B	647	LYS
1	B	663	SER
1	B	678	THR
1	B	681	LEU
1	B	683	ASP
1	B	684	ILE
1	B	695	CYS
1	B	703	THR
1	B	704	ASN
1	B	712	LYS
1	B	713	SER
1	B	719	TYR
1	B	721	SER
1	B	722	GLU
1	B	725	VAL
1	B	735	ILE
1	B	741	HIS
1	B	748	HIS
1	B	751	ARG
1	B	752	LYS
1	B	755	GLN
1	B	756	ARG
1	B	766	LEU
1	B	770	LEU
1	B	776	ILE
1	B	778	LYS
1	B	785	GLU
1	B	790	ARG
1	B	793	LYS
1	B	797	ARG
1	B	798	LEU
1	B	799	LEU
1	B	803	LEU

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Mol	Chain	Res	Type
1	B	809	LEU
1	B	817	LYS
1	B	820	ARG
1	B	824	GLU
1	B	833	GLN
1	B	835	ASP
1	B	848	MET
1	B	849	ASP
1	B	850	ARG
1	B	852	LYS
1	B	855	ILE
1	B	872	LYS
1	B	874	LEU
1	B	877	LEU
1	B	887	ARG
1	B	890	SER
1	B	896	THR
1	B	901	LEU
1	B	902	VAL
1	B	904	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	271	ASN
1	A	273	GLN
1	A	298	GLN
1	A	317	GLN
1	A	367	GLN
1	A	371	HIS
1	A	398	GLN
1	A	463	GLN
1	A	484	HIS
1	A	511	ASN
1	A	574	HIS
1	A	591	GLN
1	A	624	GLN
1	A	630	ASN
1	A	656	HIS
1	A	666	HIS
1	A	674	ASN

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Mol	Chain	Res	Type
1	A	700	HIS
1	A	704	ASN
1	A	730	HIS
1	A	748	HIS
1	A	755	GLN
1	A	781	GLN
1	A	859	GLN
1	A	875	GLN
1	A	894	HIS
1	A	900	HIS
1	B	232	GLN
1	B	271	ASN
1	B	273	GLN
1	B	298	GLN
1	B	318	GLN
1	B	320	GLN
1	B	328	GLN
1	B	371	HIS
1	B	398	GLN
1	B	406	HIS
1	B	437	GLN
1	B	463	GLN
1	B	511	ASN
1	B	561	GLN
1	B	565	HIS
1	B	591	GLN
1	B	599	ASN
1	B	630	ASN
1	B	656	HIS
1	B	700	HIS
1	B	730	HIS
1	B	748	HIS
1	B	755	GLN
1	B	781	GLN
1	B	859	GLN
1	B	875	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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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	661/691 (95%)	-0.27	2 (0%) 91 47	43, 79, 109, 128	0
1	B	643/691 (93%)	-0.29	0 100 100	46, 74, 107, 125	0
All	All	1304/1382 (94%)	-0.28	2 (0%) 93 53	43, 76, 108, 128	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	588	ASP	2.5
1	A	452	ASP	2.3

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
3	MG	A	905	1/1	0.88	22.92	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	B	905	1/1	0.72	16.63	44,44,44,44	0
2	ZN	B	2	1/1	0.14	-0.47	67,67,67,67	0
2	ZN	A	1	1/1	0.16	-0.63	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.