



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 PM UTC

PDB ID : 3IBJ / pdb_00003ibj
Title : X-ray structure of PDE2A
Authors : Pandit, J.
Deposited on : 2009-07-16
Resolution : 3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

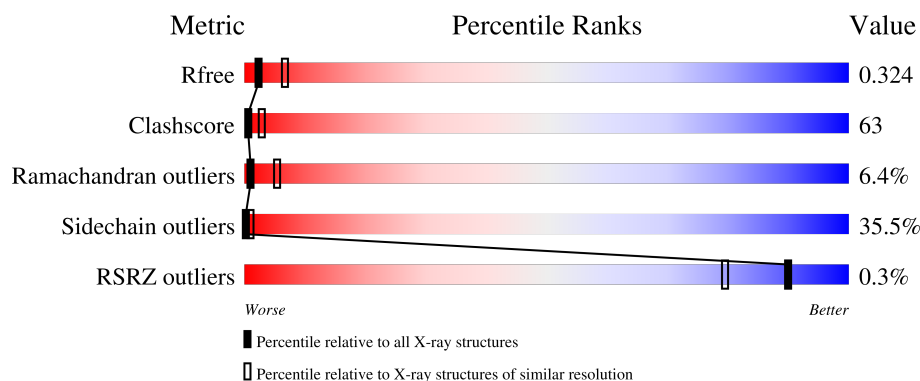
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

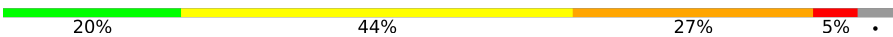
The reported resolution of this entry is 3.02 Å.

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}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	691	
1	B	691	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10650 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

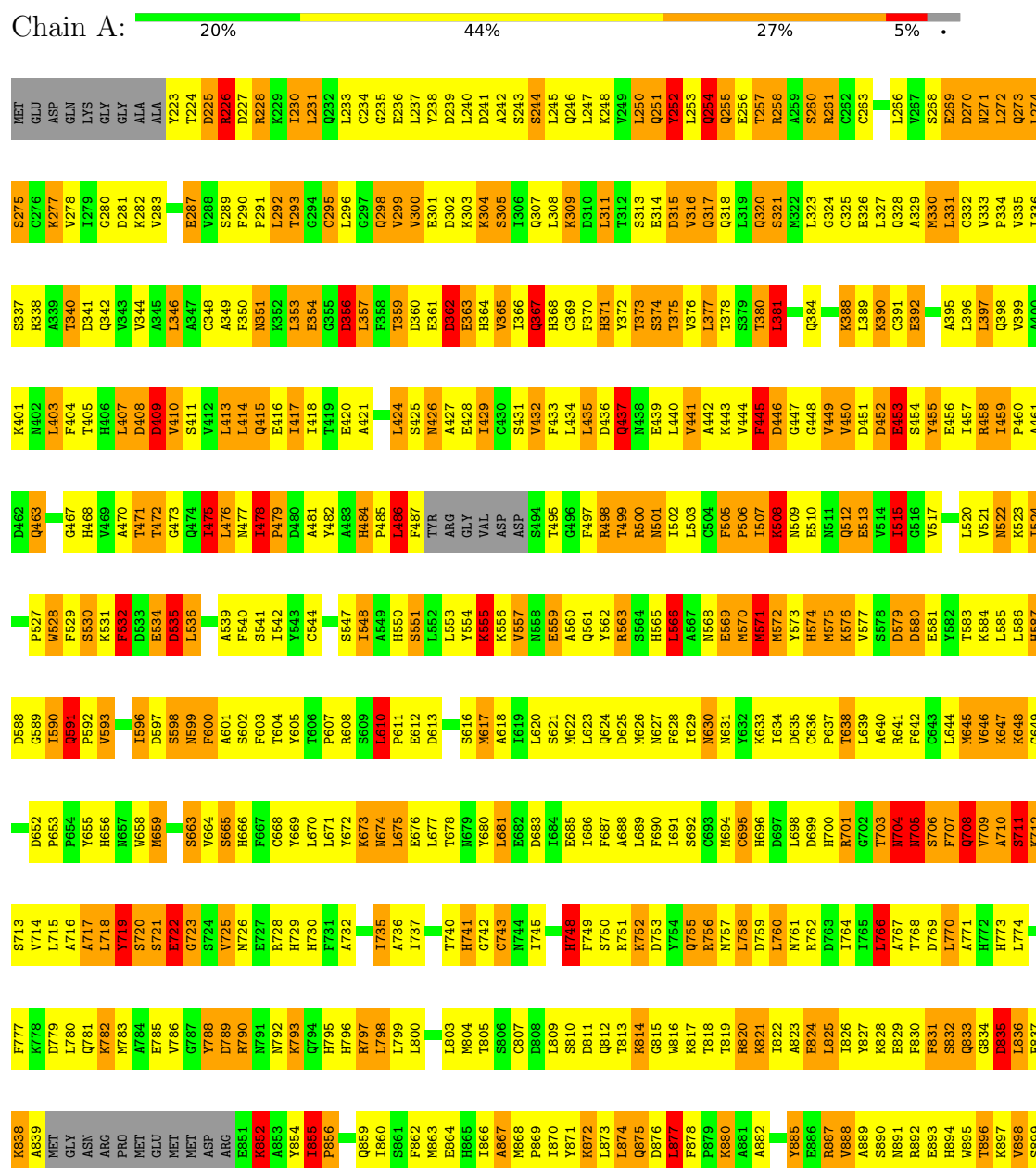
- Molecule 4 is water.

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

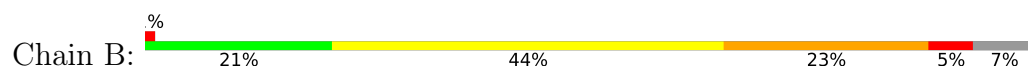
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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



H900
LEU
VAL
PRO
ARG

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



MET	GLU	ASP	GLN	LYS	GLY	GLY	ALA	ALA	Y223	Y224	D225	E226	E227	R228	R229	I230	I231	Q232	L233	C234	G235	E236	L237	Y238	D239	L240	D241	A242	S243	S244	L245	Q246	L247	K248	V249	L250	Q251	Y252	L253	Q254	Q255	E256	T257	R258	A259	R261	L265	L266	Y267	S268	E269	D270	D271	I272	Q273	L274	S275		
	C276	K277	V278	L279	D280	K282	V283	E287	Y288	S289	F290	P291	K292	T293	L296	G297	Q298	V299	V300	E301	D302	K303	K304	S305	L306	K307	L308	C309	D310	L311	T312	S313	E314	D315	V316	Q317	Y252	L318	L319	Q320	S321	K322	L323	G324	C325	L326	L327	Q328	A329	K330	L331	C332	V333	P334	I337	Q338	V339	K340	L401
	A339	T340	D341	Q342	V343	V344	A345	L346	A349	F350	N351	K352	L353	E354	G355	D356	L357	F358	T359	D360	E361	D362	E363	H364	V365	L366	Q367	H368	C369	F370	H371	Y372	T373	S374	T375	V376	L377	T380	L381	A382	F383	E386	Q387	K388	L389	K390	C391	E392	C393	Q394	A395	L396	L397	Q398	V399	A400	K401		
	N402	L403	H406	L407	D408	D409	V410	S411	A421	R422	N423	L424	S425	N426	E428	I429	V432	F433	K434	L435	D436	Q437	N438	T439	L440	V441	A442	K443	V444	PHE	ASP	GLY	GLY	VAL	VAL	ASP	ASP	GLU	S454	Y455	E456	I457	R458	I459	P460	A461	D462	K463	G464										
	I466	A467	H468	V469	A470	T471	G472	G473	A481	Y482	ALA	HIS	PRO	LEU	PHE	TYR	ARG	GLY	VAL	ASP	ASP	SER	THR	GLY	PHE	R498	T499	R500	L501	I502	L503	C504	F505	P506	I507	K508	N509	E510	N511	Q512	E513	V514	I515	G516	V517	A518	L519	L520	V521	N522	K523	I524							
	P527	V528	H529	K530	S531	F532	D533	E534	A537	F540	S541	I542	I546	S547	I548	A549	H550	L553	Y554	K555	R556	V557	N558	E559	A560	Q561	Y562	H565	L566	A567	M570	M571	M572	Y573	H574	M575	K576	V577	S578	D579	D580	R581	Y582	T583	K584	L585	L586	L587	D588	G589	Q591								
	P592	V593	I596	D597	S598	R599	F600	A601	T604	T606	P607	R608	S609	L610	P611	E612	D613	D614	T615	S616	M617	A618	L619	L620	S621	M622	L623	Q624	D625	M626	N627	F628	I629	M630	M631	Y632	K633	I634	D635	C636	P637	T638	A640	R641	F642	M645	V646	K647	K648	R651	D652	P653	P654						
	Y655	H656	M657	W658	S663	H666	P667	H668	C669	L670	L671	Y672	K673	N674	L675	E676	L677	T678	N679	Y680	L681	E682	D683	I684	E685	L686	F687	G688	A689	L689	M694	C695	H696	D697	L698	D699	H700	R701	G702	T703	N704	ASN	SER	PHE	GLN	VAL	ALA	SER	K712	S713	V714	L715	L716	A717	L718	Y719	M783	S721	
	R722	G723	W724	M725	M726	E727	H728	H729	H730	F731	L735	A736	I737	L738	T740	H741	G742	C743	L744	I745	F746	L747	H748	F749	S750	R751	K752	D753	Y754	Q755	R756	M757	D758	L759	L760	M761	R762	D763	I764	I765	L766	A767	T768	D769	L770	A771	H772	H773	L774	R775	L776	F777	L780	Q781	K782	S783	A784		
	E785	V786	G787	Y788	D789	R790	H791	H792	K793	G794	H795	H796	R797	L798	L799	L800	C801	L802	L803	M804	T805	S806	C807	L808	L809	S810	D811	K812	L813	L814	K817	L818	R819	K820	D821	R822	A823	E824	L825	I826	Y827	K828	E829	F830	F831	S832	Q833	G834	D835	L836	E837	K838	A839	MET	GLY	ASN	ARG	PRO	MET
	M848	D849	Y788	R850	E851	R852	A853	H854	R855	P856	E857	Q859	I860	S861	F862	K863	E864	H865	I866	M867	M868	P869	I870	Y871	K872	L873	L874	Q875	D876	L877	F878	A882	Y885	E886	R887	V888	A889	S890	N891	R892	E893	W895	T896	K897	V898	S899	H900	L901	V902	P903	R904								

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 18.26 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.5 (18.26-3.02) 99.0 (18.26-3.02)	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 0.217 , 0.324	Depositor DCC
R_{free} test set	1598 reflections (5.07%)	wwPDB-VP
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 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.79	1/5394 (0.0%)	1.32	72/7292 (1.0%)
1	B	0.84	4/5260 (0.1%)	1.35	68/7105 (1.0%)
All	All	0.82	5/10654 (0.0%)	1.34	140/14397 (1.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	MET	SD-CE	7.39	1.98	1.79
1	A	617	MET	SD-CE	6.51	1.95	1.79
1	B	717	ALA	CA-CB	-5.62	1.46	1.54
1	B	761	MET	SD-CE	5.61	1.93	1.79
1	B	393	CYS	CA-C	-5.31	1.47	1.52

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	902	VAL	CA-C-N	18.28	142.69	119.84
1	B	902	VAL	C-N-CA	18.28	142.69	119.84
1	A	610	LEU	CA-C-N	15.16	134.92	119.76
1	A	610	LEU	C-N-CA	15.16	134.92	119.76
1	A	505	PHE	CA-C-N	13.40	133.08	120.21
1	A	505	PHE	C-N-CA	13.40	133.08	120.21
1	A	478	ILE	CA-C-N	12.76	135.78	119.84
1	A	478	ILE	C-N-CA	12.76	135.78	119.84
1	B	652	ASP	CA-C-N	-12.25	107.77	120.38
1	B	652	ASP	C-N-CA	-12.25	107.77	120.38
1	B	312	THR	N-CA-C	-11.28	93.76	110.46
1	A	652	ASP	CA-C-N	-11.28	108.76	120.38
1	A	652	ASP	C-N-CA	-11.28	108.76	120.38
1	B	325	CYS	N-CA-C	10.13	121.31	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	573	TYR	N-CA-C	-9.87	99.30	112.72
1	B	478	ILE	CA-C-N	9.83	132.12	119.84
1	B	478	ILE	C-N-CA	9.83	132.12	119.84
1	B	836	LEU	N-CA-C	-9.44	100.88	111.82
1	B	832	SER	N-CA-C	9.04	122.34	108.42
1	A	832	SER	N-CA-C	8.82	122.09	108.07
1	A	711	SER	N-CA-C	-8.77	103.16	114.04
1	B	852	LYS	N-CA-C	-8.66	100.63	113.61
1	A	748	HIS	N-CA-C	8.53	122.49	112.93
1	B	867	ALA	N-CA-C	8.52	120.57	111.28
1	A	451	ASP	N-CA-C	-8.49	100.29	111.24
1	B	835	ASP	N-CA-C	-8.10	101.47	113.61
1	B	228	ARG	N-CA-C	-7.98	102.51	112.72
1	A	359	THR	N-CA-C	7.94	120.77	110.53
1	B	505	PHE	CA-C-N	7.94	127.83	120.21
1	B	505	PHE	C-N-CA	7.94	127.83	120.21
1	B	532	PHE	N-CA-C	-7.82	103.87	113.41
1	B	338	ARG	N-CA-C	-7.70	103.89	113.28
1	A	852	LYS	N-CA-C	-7.58	104.18	113.50
1	A	835	ASP	N-CA-C	-7.55	101.95	113.89
1	B	397	LEU	N-CA-C	-7.47	103.08	111.07
1	A	228	ARG	N-CA-C	-7.34	102.28	112.12
1	B	626	MET	N-CA-C	-7.29	103.95	112.92
1	A	535	ASP	N-CA-C	-7.26	103.08	112.23
1	B	362	ASP	N-CA-C	-7.25	103.41	111.82
1	B	393	CYS	N-CA-C	-7.15	103.56	112.72
1	B	723	GLY	N-CA-C	-7.06	96.44	113.18
1	B	850	ARG	N-CA-C	-7.05	104.56	113.02
1	B	344	VAL	N-CA-C	-7.02	105.94	112.96
1	A	486	LEU	N-CA-C	7.01	122.00	113.38
1	B	566	LEU	N-CA-C	-6.93	102.94	111.33
1	A	888	VAL	N-CA-C	-6.87	105.06	111.45
1	A	836	LEU	N-CA-C	-6.77	103.97	111.82
1	A	790	ARG	N-CA-C	-6.76	104.78	113.16
1	B	374	SER	N-CA-C	6.73	118.61	111.28
1	A	562	TYR	N-CA-C	-6.67	104.09	111.36
1	A	226	ARG	N-CA-C	-6.66	104.11	111.36
1	B	748	HIS	N-CA-C	6.62	121.36	113.16
1	A	252	TYR	N-CA-C	-6.55	103.35	112.45
1	A	759	ASP	N-CA-C	-6.54	104.08	111.14
1	B	333	VAL	CA-C-N	6.53	126.29	119.76
1	B	333	VAL	C-N-CA	6.53	126.29	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ASP	N-CA-C	-6.51	104.26	111.82
1	B	610	LEU	CA-C-N	6.37	126.33	120.03
1	B	610	LEU	C-N-CA	6.37	126.33	120.03
1	B	591	GLN	CA-C-N	-6.28	111.99	119.84
1	B	591	GLN	C-N-CA	-6.28	111.99	119.84
1	A	395	ALA	N-CA-C	-6.26	104.14	110.97
1	A	532	PHE	N-CA-C	-6.25	106.20	113.88
1	A	445	PHE	N-CA-C	6.21	124.02	110.80
1	B	226	ARG	N-CA-C	-6.13	104.15	111.69
1	B	738	LEU	N-CA-C	-6.12	104.67	111.71
1	B	245	LEU	N-CA-C	-6.12	104.16	111.69
1	A	723	GLY	N-CA-C	-6.12	98.68	113.18
1	B	542	ILE	N-CA-C	-6.10	104.35	111.00
1	A	484	HIS	N-CA-C	6.07	118.42	109.62
1	B	429	ILE	N-CA-C	6.07	115.83	108.06
1	A	254	GLN	N-CA-C	-6.07	104.73	111.71
1	B	717	ALA	N-CA-C	-6.05	105.71	114.12
1	B	766	LEU	N-CA-C	-6.01	105.80	113.01
1	B	359	THR	N-CA-C	6.01	118.28	110.53
1	A	652	ASP	N-CA-C	5.99	120.02	110.73
1	B	790	ARG	N-CA-C	-5.96	105.27	112.54
1	B	296	LEU	N-CA-C	-5.92	106.09	113.38
1	B	573	TYR	CB-CA-C	5.92	118.50	111.22
1	A	591	GLN	CA-C-N	-5.91	112.45	119.84
1	A	591	GLN	C-N-CA	-5.91	112.45	119.84
1	A	392	GLU	N-CA-C	-5.90	106.08	113.28
1	B	322	MET	N-CA-C	-5.87	104.88	111.28
1	A	705	ASN	N-CA-C	5.87	123.30	110.80
1	A	708	GLN	N-CA-C	-5.85	105.99	113.01
1	B	635	ASP	N-CA-C	-5.82	101.43	110.10
1	B	833	GLN	N-CA-C	5.80	123.15	110.80
1	B	457	ILE	N-CA-C	5.76	115.88	106.72
1	A	623	LEU	N-CA-C	-5.73	105.17	111.82
1	B	408	ASP	CB-CA-C	-5.67	101.05	110.68
1	A	381	LEU	N-CA-C	-5.63	104.78	111.03
1	B	224	THR	N-CA-C	-5.60	106.15	112.87
1	A	515	ILE	CB-CA-C	5.60	116.98	110.88
1	B	801	CYS	N-CA-C	-5.56	104.91	110.97
1	A	867	ALA	N-CA-C	5.55	117.78	111.11
1	B	668	CYS	N-CA-C	-5.55	104.25	111.02
1	A	544	CYS	N-CA-C	-5.54	105.15	111.14
1	A	877	LEU	N-CA-C	-5.53	105.83	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	MET	N-CA-C	5.52	117.29	111.28
1	A	506	PRO	CA-C-N	-5.51	117.52	123.08
1	A	506	PRO	C-N-CA	-5.51	117.52	123.08
1	A	855	ILE	C-N-CD	-5.46	102.61	125.00
1	A	574	HIS	N-CA-C	5.43	118.89	111.39
1	B	695	CYS	N-CA-C	5.43	120.92	113.97
1	B	407	LEU	CA-C-N	5.43	127.82	120.38
1	B	407	LEU	C-N-CA	5.43	127.82	120.38
1	A	374	SER	N-CA-C	5.42	117.19	111.28
1	B	623	LEU	N-CA-C	-5.38	105.86	112.90
1	A	429	ILE	N-CA-C	5.37	116.10	108.42
1	A	880	LYS	N-CA-C	-5.37	105.98	112.54
1	A	301	GLU	N-CA-C	5.37	116.99	111.03
1	A	478	ILE	C-N-CD	-5.36	103.03	125.00
1	A	793	LYS	N-CA-C	-5.36	105.60	111.82
1	A	566	LEU	N-CA-C	-5.34	105.45	111.28
1	A	766	LEU	N-CA-C	-5.34	106.26	112.89
1	B	611	PRO	N-CA-C	-5.34	103.40	111.41
1	A	299	VAL	N-CA-C	-5.32	105.53	110.53
1	A	357	LEU	N-CA-C	5.30	116.22	107.20
1	B	849	ASP	N-CA-C	-5.30	105.56	112.23
1	A	235	GLY	N-CA-C	-5.29	106.39	112.73
1	A	783	MET	N-CA-C	-5.27	105.18	111.03
1	A	655	TYR	N-CA-C	5.26	119.76	112.45
1	A	717	ALA	N-CA-C	-5.26	106.81	114.12
1	B	360	ASP	N-CA-C	-5.22	106.88	113.20
1	A	827	TYR	N-CA-C	5.18	117.83	111.82
1	A	571	MET	N-CA-C	-5.18	107.26	113.21
1	A	893	GLU	N-CA-C	5.17	116.92	111.28
1	A	665	SER	N-CA-C	-5.15	105.57	111.14
1	B	807	CYS	CA-C-N	5.13	127.15	120.28
1	B	807	CYS	C-N-CA	5.13	127.15	120.28
1	B	313	SER	N-CA-C	-5.12	107.03	113.28
1	B	443	LYS	N-CA-C	-5.09	105.74	111.28
1	A	743	CYS	N-CA-C	-5.07	107.77	114.31
1	B	428	GLU	N-CA-C	-5.06	105.84	111.36
1	B	394	GLN	N-CA-C	-5.06	105.28	111.75
1	A	779	ASP	N-CA-C	-5.04	106.97	113.23
1	B	311	LEU	N-CA-C	5.04	117.46	109.50
1	A	831	PHE	N-CA-C	5.03	116.43	109.54
1	A	555	LYS	N-CA-C	-5.02	105.50	110.97
1	A	409	ASP	N-CA-CB	5.01	118.59	110.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5291	0	5225	694	0
1	B	5164	0	5128	677	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	1309	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 63.

All (1309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ASN:ND2	1:A:705:ASN:H	1.41	1.17
1:B:330:MET:HE1	1:B:332:CYS:HB2	1.28	1.16
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:A:572:MET:HE1	1:A:737:ILE:HG12	1.35	1.08
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:B:622:MET:HE1	1:B:666:HIS:HA	1.38	1.05
1:A:440:LEU:HD12	1:A:459:ILE:HD11	1.29	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:TYR:HD2	1:B:225:ASP:HB2	1.19	1.04
1:A:330:MET:HE1	1:A:332:CYS:HB2	1.39	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:H	1:A:309:LYS:HD2	1.20	1.02
1:A:789:ASP:HB3	1:A:792:ASN:HB2	1.42	1.01
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:688:ALA:HA	1:A:757:MET:HE1	1.45	0.96
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:570:MET:HE3	1:B:762:ARG:NH1	1.83	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:571:MET:HE2	1:A:571:MET:HA	1.52	0.91
1:A:732:ALA:HB2	1:B:571:MET:HE1	1.53	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:A:445:PHE:HZ	1:A:450:VAL:HG22	1.37	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:A:487:PHE:HZ	1:A:499:THR:HB	1.40	0.87
1:B:370:PHE:HA	1:B:373:THR:HG22	1.56	0.87
1:B:622:MET:HE1	1:B:666:HIS:CA	2.05	0.87
1:A:304:LYS:HE3	1:A:304:LYS:HA	1.56	0.86
1:B:312:THR:HG22	1:B:314:GLU:N	1.89	0.86
1:A:835:ASP:HA	1:A:838:LYS:CD	2.05	0.86
1:B:572:MET:HE3	1:B:645:MET:HE3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:231:LEU:HD21	1:B:230:ILE:HG22	1.56	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: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:HG3	1:B:887:ARG:HH11	1.43	0.84
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:570:MET:HE3	1:B:762:ARG:HH11	1.43	0.82
1:A:811:ASP:HB2	1:A:822:ILE:HD13	1.60	0.82
1:B:304:LYS:HE3	1:B:304:LYS:HA	1.60	0.82
1:B:323:LEU:HD13	1:B:327:LEU:HD11	1.58	0.82
1:A:647:LYS:HD2	1:A:658:TRP:CD1	2.14	0.82
1:B:579:ASP:O	1:B:583:THR:HG23	1.78	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:B:572:MET:CE	1:B:645:MET:HE3	2.09	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:290:PHE:HB2	1:A:291:PRO:HD2	1.61	0.81
1:A:311:LEU:HD23	1:A:315:ASP:CB	2.11	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:A:875:GLN:HE21	1:A:882:ALA:HA	1.45	0.80
1:B:499:THR:HG22	1:B:500:ARG:N	1.93	0.80
1:A:314:GLU:HB2	4:A:93:HOH:O	1.81	0.79
1:B:623:LEU:HA	1:B:626:MET:HE2	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:PRO:HB2	1:A:829:GLU:OE1	1.83	0.79
1:B:320:GLN:NE2	1:B:327:LEU:HB2	1.96	0.79
1:A:292:LEU:HD11	1:A:300:VAL:HG21	1.65	0.79
1:A:838:LYS:H	1:A:838:LYS:HD2	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:A:251:GLN:NE2	1:A:281:ASP:HA	1.98	0.78
1:B:576:LYS:O	1:B:648:LYS:HE2	1.81	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:B:837:GLU:HB2	1:B:838:LYS:HZ3	1.49	0.78
1:A:238:TYR:HA	1:B:375:THR:OG1	1.84	0.78
1:A:630:ASN:ND2	1:A:631:ASN:H	1.82	0.77
1:A:835:ASP:HA	1:A:838:LYS:HD2	1.64	0.77
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:307:GLN:HG2	1:A:330:MET:O	1.85	0.77
1:A:819:THR:HG21	1:A:891:ASN:ND2	1.99	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:B:572:MET:HE2	1:B:740:THR:OG1	1.85	0.76
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:572:MET:C	1:B:574:HIS:H	1.93	0.76
1:B:299:VAL:HG12	1:B:334:PRO:HG3	1.68	0.76
1:B:479:PRO:HG3	1:B:528:TRP:CZ3	2.19	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:530:SER:C	1:A:532:PHE:H	1.93	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:250:LEU:HD21	1:A:263:CYS:HA	1.68	0.76
1:A:748:HIS:CD2	1:A:748:HIS:H	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:GLU:OE2	1:A:892:ARG:HD3	1.85	0.75
1:B:508:LYS:HA	1:B:513:GLU:O	1.86	0.75
1:B:789:ASP:HB3	1:B:792:ASN:CB	2.04	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:A:508:LYS:HA	1:A:513:GLU:O	1.86	0.75
1:B:561:GLN:HE21	1:B:561:GLN:HA	1.51	0.75
1:B:902:VAL:HG22	1:B:903:PRO:HD2	1.68	0.75
1:A:576:LYS:O	1:A:576:LYS:HD3	1.85	0.75
1:A:410:VAL:O	1:A:414:LEU:HB2	1.87	0.75
1:B:340:THR:OG1	1:B:342:GLN:HG3	1.86	0.75
1:B:799:LEU:O	1:B:803:LEU:HD12	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:303:LYS:HD3	1:A:336:ILE:CD1	2.16	0.74
1:A:671:LEU:HD13	1:A:803:LEU:HD23	1.69	0.74
1:A:468:HIS:O	1:A:472:THR:HG23	1.88	0.74
1:B:330:MET:CE	1:B:332:CYS:HB2	2.14	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:242:ALA:O	1:B:246:GLN:HG3	1.89	0.73
1:B:313:SER:C	1:B:316:VAL:HG12	2.14	0.73
1:B:440:LEU:HG	1:B:461:ALA:HA	1.71	0.73
1:B:764:ILE:O	1:B:767:ALA:HB3	1.88	0.73
1:A:458:ARG:HG2	1:A:458:ARG:NH1	1.93	0.73
1:B:443:LYS:HD2	1:B:456:GLU:CB	2.19	0.73
1:A:700:HIS:HD2	1:A:701:ARG:H	1.36	0.72
1:A:705:ASN:O	1:A:707:PHE:N	2.22	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:410:VAL:CG1	1:A:551:SER:HB3	2.19	0.72
1:A:704:ASN:HD22	1:A:705:ASN:H	0.74	0.72
1:A:333:VAL:HB	1:A:366:ILE:HG21	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:LEU:HD13	1:B:803:LEU:HD23	1.71	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:A:688:ALA:CA	1:A:757:MET:HE1	2.19	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: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:HD2	1:B:309:LYS:N	2.04	0.70
1:B:681:LEU:HD13	1:B:800:LEU:HD21	1.72	0.70
1:B:864:GLU:OE2	1:B:892:ARG:HD3	1.92	0.70
1:B:688:ALA:HA	1:B:757:MET:HE1	1.73	0.70
1:A:895:TRP:HA	1:A:898:VAL:CG2	2.21	0.70
1:B:320:GLN:HA	1:B:323:LEU:HB2	1.73	0.70
1:B:622:MET:O	1:B:626:MET:HE2	1.92	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:605:TYR:OH	1:B:610:LEU:HD11	1.91	0.70
1:B:799:LEU:O	1:B:799:LEU:HD12	1.90	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:223:TYR:CE2	1:A:226:ARG:HG3	2.27	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:669:TYR:CD2	1:A:670:LEU:HD23	2.27	0.69
1:A:226:ARG:C	1:A:228:ARG:H	1.99	0.69
1:A:311:LEU:HB3	1:A:316:VAL:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:MET:HE3	1:B:761:MET:HG3	1.74	0.69
1:A:231:LEU:HD12	1:B:372:TYR:CE1	2.27	0.69
1:A:444:VAL:HG21	1:A:455:TYR:CD2	2.23	0.69
1:A:484:HIS:CD2	1:A:485:PRO:HG2	2.28	0.69
1:A:732:ALA:CB	1:B:571:MET:HE1	2.23	0.69
1:B:261:ARG:HD3	1:B:280:GLY:HA3	1.75	0.69
1:B:479:PRO:HG3	1:B:528:TRP:HZ3	1.58	0.69
1:B:675:LEU:HD13	1:B:878:PHE:CB	2.23	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:B:829:GLU:O	1:B:831:PHE:N	2.25	0.69
1:A:720:SER:CB	1:A:770:LEU:HB2	2.23	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:A:721:SER:HA	1:A:769:ASP:OD2	1.93	0.68
1:B:313:SER:O	1:B:316:VAL:HG12	1.92	0.68
1:A:223:TYR:OH	1:A:364:HIS:NE2	2.25	0.68
1:A:704:ASN:ND2	1:A:705:ASN:N	2.27	0.68
1:B:500:ARG:HG2	1:B:522:ASN:CG	2.18	0.68
1:A:698:LEU:O	1:A:730:HIS:HD2	1.76	0.68
1:B:315:ASP:O	1:B:319:LEU:HB2	1.93	0.68
1:A:481:ALA:O	1:A:487:PHE:HB2	1.94	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: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:B:859:GLN:HA	1:B:859:GLN:NE2	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:A:587:HIS:O	1:A:589:GLY:N	2.27	0.68
1:B:507:ILE:CG2	1:B:515:ILE:HG22	2.24	0.68
1:A:456:GLU:HG2	1:A:458:ARG:HE	1.58	0.67
1:A:872:LYS:HD2	1:A:885:TYR:HE1	1.59	0.67
1:B:623:LEU:HA	1:B:626:MET:CE	2.24	0.67
1:B:443:LYS:HD2	1:B:456:GLU:CG	2.24	0.67
1:A:797:ARG:HD3	4:A:59:HOH:O	1.95	0.67
1:B:354:GLU:OE1	1:B:354:GLU:HA	1.93	0.67
1:A:875:GLN:HA	1:A:878:PHE:O	1.95	0.67
1:B:667:PHE:CD2	1:B:807:CYS:HA	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ASN:ND2	1:B:602:SER:HB3	2.10	0.67
1:A:428:GLU:OE2	1:A:500:ARG:NH2	2.28	0.67
1:A:837:GLU:HB2	1:A:838:LYS:CE	2.24	0.67
1:B:313:SER:CA	1:B:316:VAL:HG12	2.25	0.67
1:B:591:GLN:HG3	1:B:592:PRO:N	2.09	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:A:605:TYR:HE2	1:A:610:LEU:HD11	1.58	0.67
1:B:399:VAL:HG21	1:B:540:PHE:CE1	2.29	0.67
1:A:895:TRP:O	1:A:898:VAL:HG23	1.94	0.67
1:A:528:TRP:CD1	1:A:528:TRP:N	2.61	0.66
1:B:292:LEU:HD11	1:B:300:VAL:HG21	1.75	0.66
1:B:774:LEU:HD21	1:B:866:ILE:CD1	2.24	0.66
1:A:331:LEU:HD22	1:A:333:VAL:HG23	1.77	0.66
1:A:542:ILE:HG21	1:B:401:LYS:NZ	2.10	0.66
1:B:695:CYS:HB3	1:B:698:LEU:HD12	1.77	0.66
1:A:397:LEU:HD13	1:B:397:LEU:CD1	2.25	0.66
1:A:828:LYS:HE2	4:A:122:HOH:O	1.95	0.66
1:A:231:LEU:HD12	1:B:372:TYR:CZ	2.29	0.66
1:A:487:PHE:CZ	1:A:499:THR:HB	2.27	0.66
1:B:530:SER:O	1:B:533:ASP:N	2.28	0.66
1:B:838:LYS:HB2	4:B:4:HOH:O	1.95	0.66
1:A:709:VAL:HB	1:A:712:LYS:H	1.59	0.66
1:A:576:LYS:CD	1:A:576:LYS:H	2.08	0.66
1:A:330:MET:HG3	1:A:350:PHE:CE1	2.31	0.66
1:A:337:SER:O	1:A:341:ASP:HA	1.96	0.66
1:A:829:GLU:O	1:A:831:PHE:N	2.29	0.66
1:B:308:LEU:O	1:B:311:LEU:HB3	1.96	0.66
1:B:320:GLN:CG	1:B:327:LEU:HD13	2.09	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:B:807:CYS:O	1:B:810:SER:HB3	1.95	0.66
1:B:837:GLU:HB2	1:B:838:LYS:NZ	2.10	0.66
1:B:899:SER:O	1:B:902:VAL:HG12	1.95	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:535:ASP:OD1	1:A:535:ASP:N	2.28	0.66
1:A:821:LYS:O	1:A:824:GLU:HG3	1.96	0.66
1:A:444:VAL:CG2	1:A:455:TYR:HD2	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PRO:HB3	1:A:528:TRP:CE3	2.30	0.65
1:B:381:LEU:HD12	1:B:381:LEU:C	2.21	0.65
1:B:622:MET:HE1	1:B:666:HIS:CB	2.26	0.65
1:A:602:SER:O	1:A:604:THR:N	2.29	0.65
1:A:897:LYS:HA	1:A:900:HIS:CD2	2.31	0.65
1:B:630:ASN:ND2	1:B:631:ASN:H	1.93	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:A:405:THR:CG2	1:B:546:ILE:HD12	2.25	0.65
1:B:528:TRP:N	1:B:528:TRP:CD1	2.64	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:A:225:ASP:O	1:A:228:ARG:HB2	1.96	0.65
1:B:780:LEU:CD2	1:B:798:LEU:HB3	2.27	0.65
1:B:498:ARG:O	1:B:522:ASN:ND2	2.29	0.65
1:A:278:VAL:HG22	1:A:283:VAL:HG22	1.78	0.65
1:B:530:SER:C	1:B:532:PHE:H	2.04	0.65
1:A:436:ASP:HB3	1:A:441:VAL:HG21	1.79	0.64
1:B:527:PRO:HG2	1:B:528:TRP:CD1	2.32	0.64
1:B:580:ASP:O	1:B:584:LYS:HG3	1.96	0.64
1:B:653:PRO:HB2	1:B:829:GLU:OE1	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:B:270:ASP:O	1:B:272:LEU:HD23	1.96	0.64
1:A:255:GLN:O	1:A:257:THR:N	2.30	0.64
1:A:450:VAL:HG12	1:A:453:GLU:HA	1.79	0.64
1:B:786:VAL:HG23	1:B:786:VAL:O	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:A:436:ASP:HB3	1:A:441:VAL:CG2	2.27	0.64
1:A:645:MET:HG2	1:A:737:ILE:HG23	1.80	0.64
1:B:827:TYR:CG	1:B:855:ILE:HD13	2.32	0.64
1:A:307:GLN:HB3	1:A:309:LYS:CD	2.27	0.64
1:A:370:PHE:O	1:A:372:TYR:N	2.31	0.64
1:A:476:LEU:HD23	1:A:478:ILE:HD12	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG11	1:A:540:PHE:CE1	2.33	0.64
1:A:260:SER:OG	1:A:351:ASN:HB2	1.98	0.63
1:B:460:PRO:CG	1:B:463:GLN:HB3	2.20	0.63
1:B:648:LYS:HB2	1:B:648:LYS:NZ	2.12	0.63
1:A:269:GLU:O	1:A:271:ASN:ND2	2.30	0.63
1:A:813:THR:O	1:A:887:ARG:HD2	1.97	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:768:THR:HG22	1:B:804:MET:CG	2.28	0.63
1:B:822:ILE:HA	1:B:825:LEU:CD1	2.29	0.63
1:A:863:MET:HA	1:A:867:ALA:HB3	1.80	0.63
1:A:436:ASP:CB	1:A:441:VAL:HG21	2.28	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:630:ASN:HD22	1:B:631:ASN:N	1.96	0.63
1:B:837:GLU:CB	1:B:838:LYS:HZ3	2.12	0.63
1:B:887:ARG:HG3	1:B:887:ARG:NH1	2.08	0.63
1:B:265:LEU:HD13	1:B:274:LEU:HD12	1.80	0.63
1:B:330:MET:HG3	1:B:350:PHE:CD1	2.33	0.63
1:A:768:THR:HG22	1:A:804:MET:HG3	1.80	0.63
1:B:433:PHE:CG	1:B:442:ALA:HB2	2.33	0.63
1:B:875:GLN:O	1:B:875:GLN:HG2	1.98	0.62
1:A:708:GLN:O	1:A:709:VAL:HG23	1.98	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
1:B:458:ARG:HH11	1:B:458:ARG:CG	2.13	0.62
1:B:510:GLU:HA	1:B:510:GLU:OE1	1.99	0.62
1:B:561:GLN:HE21	1:B:561:GLN:CA	2.10	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:630:ASN:HD22	1:B:630:ASN:N	1.97	0.62
1:B:680:TYR:N	1:B:680:TYR:CD1	2.67	0.62
1:B:762:ARG:O	1:B:766:LEU:HD22	2.00	0.62
1:A:634:ILE:CG2	1:A:639:LEU:HB2	2.30	0.62
1:B:230:ILE:HG22	1:B:231:LEU:N	2.14	0.62
1:A:252:TYR:O	1:A:255:GLN:HB2	1.99	0.62
1:B:527:PRO:HB2	1:B:528:TRP:CD1	2.35	0.62
1:A:572:MET:HE3	1:A:736:ALA:HB3	1.80	0.62
1:A:814:LYS:HB3	1:A:818:THR:HG21	1.81	0.62
1:B:328:GLN:HG3	4:B:9:HOH:O	2.00	0.62
1:B:333:VAL:HB	1:B:366:ILE:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:408:ASP:N	1:A:408:ASP:OD1	2.28	0.61
1:B:596:ILE:HG21	1:B:600:PHE:CD1	2.35	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:A:885:TYR:CD2	1:A:885:TYR:C	2.78	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:A:579:ASP:O	1:A:583:THR:HG23	2.01	0.61
1:B:435:LEU:HD11	1:B:437:GLN:O	2.01	0.61
1:A:397:LEU:HD13	1:B:397:LEU:HD12	1.82	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:B:353:LEU:O	1:B:354:GLU:HB2	2.00	0.61
1:B:440:LEU:HD13	1:B:466:ALA:HB1	1.83	0.61
1:A:755:GLN:HG2	1:B:566:LEU:CD1	2.31	0.61
1:A:648:LYS:HB2	1:A:648:LYS:NZ	2.15	0.60
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:B:677:LEU:HD21	1:B:803:LEU:HD21	1.82	0.60
1:B:611:PRO:HG2	1:B:614:ASP:OD2	2.01	0.60
1:B:855:ILE:HB	1:B:856:PRO:HD3	1.83	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:622:MET:HE1	1:B:666:HIS:HB2	1.84	0.60
1:B:355:GLY:O	1:B:357:LEU:N	2.34	0.60
1:B:458:ARG:HH11	1:B:458:ARG:HG2	1.65	0.60
1:B:527:PRO:HG2	1:B:528:TRP:HD1	1.65	0.60
1:A:270:ASP:HB2	1:A:272:LEU:HD23	1.82	0.60
1:A:470:ALA:HB2	1:A:517:VAL:HG21	1.83	0.60
1:A:630:ASN:ND2	1:A:631:ASN:N	2.48	0.60
1:A:715:LEU:C	1:A:717:ALA:H	2.08	0.60
1:B:303:LYS:CD	1:B:336:ILE:HD13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:THR:CG2	1:B:870:ILE:HD13	2.32	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:B:234:CYS:HA	1:B:237:LEU:HD12	1.83	0.60
1:B:356:ASP:OD1	4:B:9:HOH:O	2.17	0.59
1:B:443:LYS:HD2	1:B:456:GLU:HB3	1.83	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:298:GLN:NE2	1:A:302:ASP:OD2	2.35	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:B:257:THR:O	1:B:352:LYS:HE3	2.03	0.59
1:B:330:MET:HE1	1:B:332:CYS:CB	2.19	0.59
1:A:237:LEU:O	1:B:375:THR:HG21	2.01	0.59
1:A:566:LEU:CD1	1:B:755:GLN:HG2	2.21	0.59
1:B:459:ILE:HG13	1:B:463:GLN:OE1	2.02	0.59
1:A:431:SER:HG	1:A:433:PHE:HE1	1.51	0.59
1:A:475:ILE:HG23	1:A:505:PHE:HB3	1.83	0.59
1:A:507:ILE:CG2	1:A:515:ILE:HG22	2.32	0.59
1:A:587:HIS:C	1:A:589:GLY:H	2.10	0.59
1:A:770:LEU:HD12	1:A:770:LEU:O	2.02	0.59
1:B:241:ASP:OD2	1:B:243:SER:HB2	2.02	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
1:B:700:HIS:CD2	1:B:702:GLY:H	2.09	0.59
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:418:ILE:HG12	1:A:432:VAL:HG22	1.84	0.59
1:A:576:LYS:CD	1:A:576:LYS:N	2.65	0.59
1:A:720:SER:HB2	1:A:770:LEU:CB	2.33	0.59
1:A:363:GLU:HG3	1:A:367:GLN:HE22	1.68	0.58
1:A:435:LEU:HD11	1:A:437:GLN:O	2.03	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:575:MET:HG2	1:A:648:LYS:CD	2.33	0.58
1:A:774:LEU:HB2	1:B:838:LYS:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:SER:C	1:B:532:PHE:N	2.62	0.58
1:A:364:HIS:HA	1:A:367:GLN:HE21	1.68	0.58
1:B:535:ASP:OD1	1:B:535:ASP:N	2.27	0.58
1:B:637:PRO:O	1:B:641:ARG:NE	2.29	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: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:B:723:GLY:C	1:B:725:VAL:H	2.11	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: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:860:ILE:HD11	1:A:895:TRP:C	2.29	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:241:ASP:HB3	1:B:244:SER:OG	2.04	0.58
1:B:721:SER:HB2	1:B:769:ASP:OD2	2.02	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:A:570:MET:C	1:A:572:MET:H	2.12	0.57
1:B:475:ILE:HG23	1:B:505:PHE:HB3	1.85	0.57
1:B:837:GLU:C	1:B:838:LYS:HZ3	2.12	0.57
1:B:309:LYS:H	1:B:309:LYS:CD	2.10	0.57
1:B:398:GLN:HE22	1:B:401:LYS:HD3	1.69	0.57
1:A:875:GLN:O	1:A:875:GLN:HG2	2.03	0.57
1:B:304:LYS:HE3	1:B:304:LYS:CA	2.23	0.57
1:B:872:LYS:HE2	1:B:876:ASP:OD1	2.03	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:A:757:MET:HE3	1:A:761:MET:HG3	1.86	0.57
1:A:416:GLU:OE1	1:A:416:GLU:HA	2.03	0.57
1:B:279:ILE:HD11	1:B:322:MET:SD	2.44	0.57
1:B:459:ILE:HD12	1:B:460:PRO:CD	2.35	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:715:LEU:C	1:B:717:ALA:H	2.13	0.57
1:B:833:GLN:HG2	1:B:834:GLY:H	1.70	0.57
1:A:415:GLN:O	1:A:418:ILE:HB	2.05	0.56
1:B:895:TRP:HA	1:B:898:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:HD22	1:B:231:LEU:HD22	1.86	0.56
1:A:416:GLU:O	1:A:420:GLU:HB2	2.05	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: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:A:253:LEU:O	1:A:257:THR:OG1	2.23	0.56
1:A:417:ILE:HD13	1:A:548:ILE:HD11	1.87	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:A:868:MET:HG2	1:A:888:VAL:HG12	1.86	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:B:528:TRP:N	1:B:528:TRP:HD1	2.03	0.56
1:B:607:PRO:HG2	1:B:663:SER:HB3	1.87	0.56
1:B:715:LEU:HD23	1:B:862:PHE:CD2	2.40	0.56
1:B:875:GLN:HE21	1:B:882:ALA:HB1	1.71	0.56
1:B:895:TRP:HA	1:B:898:VAL:CG2	2.35	0.56
1:A:421:ALA:HB2	1:A:540:PHE:HE2	1.64	0.56
1:A:573:TYR:HE1	1:A:699:ASP:OD1	1.89	0.56
1:A:590:ILE:HG21	1:A:624:GLN:OE1	2.05	0.56
1:B:326:GLU:HB3	1:B:328:GLN:HE22	1.70	0.56
1:A:780:LEU:HD23	1:A:798:LEU:HB3	1.88	0.56
1:A:810:SER:HA	1:A:871:TYR:OH	2.05	0.56
1:A:885:TYR:C	1:A:885:TYR:HD2	2.13	0.56
1:B:312:THR:HG21	1:B:314:GLU:HB3	1.88	0.56
1:A:812:GLN:HB3	1:A:888:VAL:HG22	1.87	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:312:THR:CG2	1:B:314:GLU:HB3	2.36	0.56
1:B:822:ILE:HA	1:B:825:LEU:HD12	1.87	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
1:B:273:GLN:HE22	1:B:289:SER:HB2	1.71	0.56
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:894:HIS:O	1:A:898:VAL:HG22	2.05	0.55
1:A:479:PRO:HB3	1:A:528:TRP:CZ3	2.42	0.55
1:A:501:ASN:C	1:A:502:ILE:HG13	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:LEU:HD22	1:A:859:GLN:HE22	1.70	0.55
1:A:550:HIS:CD2	1:B:550:HIS:NE2	2.75	0.55
1:A:610:LEU:HD12	1:A:610:LEU:N	2.21	0.55
1:A:748:HIS:CD2	1:A:748:HIS:N	2.73	0.55
1:A:764:ILE:O	1:A:767:ALA:HB3	2.07	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:A:261:ARG:HD3	1:A:280:GLY:HA3	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:239:ASP:HB2	1:A:245:LEU:HD23	1.89	0.55
1:A:758:LEU:HB3	1:B:570:MET:HE1	1.87	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: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:295:CYS:HB3	1:A:315:ASP:OD2	2.07	0.55
1:B:593:VAL:HG22	1:B:621:SER:O	2.06	0.55
1:B:666:HIS:CE1	1:B:670:LEU:HD21	2.42	0.55
1:A:709:VAL:HB	1:A:712:LYS:HB2	1.87	0.55
1:B:252:TYR:C	1:B:252:TYR:CD2	2.85	0.55
1:B:311:LEU:O	1:B:311:LEU:HG	2.07	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:506:PRO:O	1:B:507:ILE:HD12	2.06	0.55
1:B:530:SER:O	1:B:533:ASP:HB2	2.07	0.55
1:A:224:THR:HG22	1:A:228:ARG:CZ	2.36	0.54
1:A:476:LEU:HD23	1:A:478:ILE:CD1	2.37	0.54
1:A:607:PRO:O	1:A:610:LEU:HD13	2.07	0.54
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:223:TYR:HE2	1:A:226:ARG:CG	2.19	0.54
1:A:530:SER:C	1:A:532:PHE:N	2.61	0.54
1:B:500:ARG:NH2	1:B:523:LYS:O	2.39	0.54
1:B:587:HIS:C	1:B:589:GLY:H	2.14	0.54
1:A:278:VAL:CG2	1:A:283:VAL:HG22	2.36	0.54
1:A:452:ASP:O	1:A:453:GLU:O	2.25	0.54
1:B:648:LYS:HB2	1:B:648:LYS:HZ2	1.71	0.54
1:B:721:SER:O	1:B:722:GLU:CD	2.51	0.54
1:A:275:SER:HB2	1:A:287:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:HIS:CE1	1:A:472:THR:HG21	2.42	0.54
1:A:477:ASN:HD21	1:A:529:PHE:HB2	1.72	0.54
1:A:659:MET:O	1:A:663:SER:OG	2.24	0.54
1:A:665:SER:O	1:A:668:CYS:HB3	2.07	0.54
1:B:403:LEU:HD22	1:B:417:ILE:HG13	1.87	0.54
1:B:418:ILE:CD1	1:B:444:VAL:HG21	2.37	0.54
1:B:630:ASN:ND2	1:B:630:ASN:N	2.53	0.54
1:B:721:SER:HA	1:B:769:ASP:OD2	2.07	0.54
1:B:805:THR:HG22	1:B:870:ILE:HD13	1.90	0.54
1:A:363:GLU:O	1:A:367:GLN:NE2	2.41	0.54
1:A:409:ASP:C	1:A:411:SER:H	2.14	0.54
1:B:361:GLU:O	1:B:365:VAL:HG12	2.08	0.54
1:B:593:VAL:HG12	1:B:600:PHE:CD2	2.42	0.54
1:A:309:LYS:H	1:A:309:LYS:CD	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:A:757:MET:HG3	1:A:757:MET:O	2.06	0.54
1:B:283:VAL:HG12	1:B:283:VAL:O	2.07	0.54
1:B:687:PHE:CE1	1:B:746:PHE:HE1	2.25	0.54
1:B:872:LYS:HE2	1:B:876:ASP:CG	2.33	0.54
1:A:231:LEU:CD2	1:B:231:LEU:HD22	2.38	0.54
1:A:376:VAL:HG21	1:B:375:THR:HG22	1.90	0.54
1:A:542:ILE:HG21	1:B:401:LYS:HZ1	1.73	0.54
1:A:569:GLU:O	1:A:572:MET:HB2	2.07	0.54
1:B:444:VAL:O	1:B:444:VAL:HG13	2.08	0.54
1:B:821:LYS:HD3	1:B:824:GLU:OE1	2.07	0.54
1:A:458:ARG:NH1	1:A:458:ARG:CG	2.66	0.54
1:A:575:MET:HG2	1:A:648:LYS:HD2	1.88	0.54
1:A:767:ALA:C	1:A:769:ASP:H	2.15	0.54
1:B:398:GLN:OE1	1:B:398:GLN:HA	2.06	0.54
1:B:499:THR:O	1:B:500:ARG:HD3	2.08	0.54
1:B:789:ASP:N	1:B:795:HIS:ND1	2.53	0.54
1:A:788:TYR:OH	1:A:799:LEU:HD23	2.08	0.54
1:A:812:GLN:OE1	1:A:863:MET:HE3	2.08	0.54
1:A:815:GLY:O	1:A:818:THR:N	2.39	0.54
1:B:572:MET:HE2	1:B:740:THR:HG1	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:835:ASP:CA	1:A:838:LYS:HD2	2.38	0.53
1:B:859:GLN:HA	1:B:859:GLN:HE21	1.71	0.53
1:B:877:LEU:HB2	1:B:878:PHE:CD2	2.43	0.53
1:A:453:GLU:HA	1:A:453:GLU:OE1	2.07	0.53
1:A:590:ILE:HG21	1:A:624:GLN:CD	2.33	0.53
1:A:642:PHE:O	1:A:646:VAL:HG12	2.08	0.53
1:B:885:TYR:C	1:B:885:TYR:CD2	2.86	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:366:ILE:HG22	1:B:367:GLN:N	2.23	0.53
1:B:443:LYS:CD	1:B:456:GLU:HB3	2.38	0.53
1:B:457:ILE:O	1:B:457:ILE:HG22	2.07	0.53
1:B:596:ILE:HG21	1:B:600:PHE:CE1	2.43	0.53
1:A:335:VAL:HG22	1:A:370:PHE:CD2	2.44	0.53
1:A:495:THR:HG22	1:A:495:THR:O	2.09	0.53
1:A:550:HIS:NE2	1:B:550:HIS:CD2	2.77	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:230:ILE:HG22	1:B:231:LEU:HD21	1.91	0.53
1:A:420:GLU:HA	1:A:420:GLU:OE2	2.09	0.53
1:A:875:GLN:HE21	1:A:882:ALA:CA	2.20	0.53
1:B:521:VAL:HG12	1:B:522:ASN:OD1	2.08	0.53
1:A:341:ASP:C	1:A:342:GLN:HG2	2.34	0.53
1:A:675:LEU:HD13	1:A:878:PHE:CG	2.44	0.53
1:A:829:GLU:C	1:A:831:PHE:H	2.16	0.53
1:B:255:GLN:O	1:B:257:THR:N	2.41	0.53
1:A:501:ASN:ND2	1:A:527:PRO:O	2.42	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:239:ASP:OD1	1:B:248:LYS:NZ	2.34	0.53
1:B:586:LEU:HD21	1:B:636:CYS:HB3	1.91	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:A:838:LYS:HB3	1:B:774:LEU:HB2	1.90	0.52
1:B:226:ARG:C	1:B:228:ARG:H	2.18	0.52
1:B:501:ASN:C	1:B:502:ILE:HG13	2.35	0.52
1:B:702:GLY:HA2	1:B:829:GLU:OE2	2.09	0.52
1:B:252:TYR:O	1:B:256:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLN:O	1:B:344:VAL:HG23	2.10	0.52
1:A:566:LEU:HD22	1:B:755:GLN:HE21	1.75	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:755:GLN:OE1	1:B:759:ASP:OD2	2.28	0.52
1:A:433:PHE:CD2	1:A:442:ALA:HB2	2.44	0.52
1:B:619:ILE:O	1:B:623:LEU:HD12	2.09	0.52
1:B:799:LEU:HD12	1:B:799:LEU:C	2.28	0.52
1:A:270:ASP:OD2	1:A:270:ASP:N	2.39	0.52
1:A:688:ALA:HB2	1:A:760:LEU:HD12	1.92	0.52
1:B:231:LEU:HD12	1:B:231:LEU:O	2.10	0.52
1:B:435:LEU:HD13	1:B:436:ASP:N	2.24	0.52
1:B:606:THR:O	1:B:609:SER:HB3	2.10	0.52
1:B:762:ARG:HG2	1:B:766:LEU:HD22	1.90	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:458:ARG:O	1:B:459:ILE:HB	2.09	0.52
1:B:861:SER:O	1:B:865:HIS:HB2	2.10	0.52
1:A:602:SER:C	1:A:604:THR:H	2.18	0.52
1:A:721:SER:HB2	1:A:769:ASP:OD2	2.09	0.52
1:A:721:SER:O	1:A:722:GLU:OE1	2.27	0.52
1:A:721:SER:OG	1:A:722:GLU:N	2.39	0.52
1:A:770:LEU:O	1:A:774:LEU:HG	2.10	0.52
1:B:369:CYS:O	1:B:373:THR:HB	2.10	0.52
1:B:455:TYR:N	1:B:455:TYR:CD2	2.76	0.52
1:B:467:GLY:O	1:B:471:THR:HB	2.10	0.52
1:A:258:ARG:O	1:A:353:LEU:N	2.40	0.52
1:A:376:VAL:HG13	1:A:377:LEU:N	2.25	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:571:MET:HE2	1:A:571:MET:CA	2.33	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:698:LEU:O	1:A:730:HIS:CD2	2.62	0.51
1:B:479:PRO:HB3	1:B:528:TRP:CE3	2.45	0.51
1:A:348:CYS:HB3	1:A:350:PHE:CZ	2.45	0.51
1:A:854:TYR:CD1	1:A:854:TYR:N	2.77	0.51
1:A:439:GLU:N	1:A:461:ALA:HB2	2.25	0.51
1:A:715:LEU:CD2	1:A:859:GLN:HE22	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:GLN:O	1:B:310:ASP:HB2	2.10	0.51
1:A:591:GLN:HG3	1:A:592:PRO:N	2.25	0.51
1:A:597:ASP:HB3	1:A:600:PHE:HB2	1.91	0.51
1:A:833:GLN:HG2	1:A:837:GLU:OE2	2.11	0.51
1:B:273:GLN:HG2	1:B:291:PRO:HA	1.92	0.51
1:B:627:ASN:ND2	1:B:631:ASN:OD1	2.43	0.51
1:B:634:ILE:CG2	1:B:639:LEU:HB2	2.39	0.51
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:B:799:LEU:HG	1:B:803:LEU:CD1	2.40	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: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:532:PHE:CD1	1:B:532:PHE:C	2.89	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: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:816:TRP:CG	1:A:894:HIS:CD2	2.99	0.50
1:B:421:ALA:HB2	1:B:540:PHE:CE2	2.45	0.50
1:B:508:LYS:HA	1:B:513:GLU:C	2.37	0.50
1:A:418:ILE:CG1	1:A:432:VAL:HG22	2.41	0.50
1:A:484:HIS:CD2	1:A:486:LEU:H	2.28	0.50
1:A:700:HIS:CD2	1:A:701:ARG:N	2.79	0.50
1:A:728:ARG:NE	1:B:701:ARG:NH2	2.59	0.50
1:A:838:LYS:O	1:A:839:ALA:O	2.29	0.50
1:B:782:LYS:O	1:B:786:VAL:HG22	2.11	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:307:GLN:HB3	1:B:309:LYS:HD3	1.93	0.50
1:A:317:GLN:O	1:A:321:SER:HB3	2.12	0.50
1:B:608:ARG:HH22	1:B:655:TYR:HE1	1.60	0.50
1:B:299:VAL:HG13	1:B:304:LYS:O	2.10	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:507:ILE:O	1:B:508:LYS:O	2.30	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:735:ILE:HD13	1:B:735:ILE:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:ILE:HG13	1:B:780:LEU:HG	1.93	0.50
1:A:239:ASP:OD1	1:A:248:LYS:HE3	2.12	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:B:441:VAL:HG22	1:B:458:ARG:HG3	1.94	0.50
1:A:435:LEU:HD22	1:A:440:LEU:HD23	1.94	0.50
1:A:666:HIS:CE1	1:A:670:LEU:HD11	2.43	0.50
1:A:743:CYS:O	1:A:745:ILE:HG23	2.12	0.50
1:B:318:GLN:OE1	1:B:318:GLN:O	2.29	0.50
1:B:320:GLN:HE21	1:B:327:LEU:N	2.10	0.50
1:B:719:TYR:OH	1:B:811:ASP:OD1	2.29	0.50
1:A:399:VAL:HG22	1:A:420:GLU:OE2	2.12	0.50
1:A:571:MET:HA	1:A:571:MET:CE	2.36	0.50
1:A:580:ASP:O	1:A:584:LYS:HG3	2.12	0.50
1:B:536:LEU:HD22	1:B:536:LEU:O	2.12	0.50
1:B:607:PRO:CG	1:B:663:SER:HB3	2.41	0.50
1:B:695:CYS:HB3	1:B:698:LEU:CD1	2.42	0.50
1:A:561:GLN:HE22	1:B:561:GLN:HA	1.77	0.50
1:A:707:PHE:C	1:A:709:VAL:N	2.69	0.50
1:B:441:VAL:HG11	1:B:443:LYS:HE3	1.93	0.50
1:A:528:TRP:N	1:A:528:TRP:HD1	2.09	0.49
1:B:270:ASP:OD1	1:B:272:LEU:HG	2.12	0.49
1:A:666:HIS:CE1	1:A:670:LEU:CD2	2.93	0.49
1:A:475:ILE:HD13	1:A:506:PRO:HD2	1.93	0.49
1:A:628:PHE:O	1:A:634:ILE:HD12	2.13	0.49
1:B:265:LEU:HB3	1:B:274:LEU:HD13	1.94	0.49
1:B:305:SER:HB3	1:B:333:VAL:HA	1.93	0.49
1:B:416:GLU:HA	1:B:416:GLU:OE1	2.12	0.49
1:B:622:MET:CE	1:B:666:HIS:HA	2.25	0.49
1:A:370:PHE:HD1	1:A:373:THR:HG22	1.75	0.49
1:A:500:ARG:NH2	1:A:522:ASN:HB3	2.27	0.49
1:B:376:VAL:CG1	1:B:377:LEU:N	2.75	0.49
1:B:852:LYS:NZ	1:B:852:LYS:CB	2.76	0.49
1:A:453:GLU:CD	1:A:453:GLU:H	2.21	0.49
1:A:668:CYS:O	1:A:671:LEU:HB2	2.13	0.49
1:A:723:GLY:C	1:A:725:VAL:H	2.21	0.49
1:A:811:ASP:HB2	1:A:822:ILE:CD1	2.37	0.49
1:B:277:LYS:HB3	1:B:287:GLU:HG3	1.95	0.49
1:B:417:ILE:HD13	1:B:548:ILE:CD1	2.43	0.49
1:B:417:ILE:CD1	1:B:548:ILE:HD11	2.42	0.49
1:B:428:GLU:O	1:B:429:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:HIS:HA	1:B:798:LEU:HD12	1.94	0.49
1:A:822:ILE:O	1:A:825:LEU:N	2.45	0.49
1:B:265:LEU:CB	1:B:274:LEU:HD13	2.41	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
1:A:390:LYS:HE2	1:B:386:GLU:OE1	2.12	0.49
1:A:675:LEU:N	1:A:675:LEU:HD23	2.28	0.49
1:A:715:LEU:HD22	1:A:859:GLN:NE2	2.27	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:709:VAL:HG12	1:A:710:ALA:N	2.28	0.49
1:A:872:LYS:HB2	1:A:885:TYR:CE1	2.48	0.49
1:B:606:THR:HG1	1:B:609:SER:HB3	1.77	0.49
1:B:848:MET:HA	1:B:851:GLU:HB2	1.94	0.49
1:A:337:SER:HB3	1:A:340:THR:HG23	1.92	0.49
1:A:460:PRO:HG2	1:A:463:GLN:NE2	2.28	0.49
1:B:439:GLU:HA	1:B:461:ALA:N	2.27	0.49
1:A:226:ARG:O	1:A:228:ARG:N	2.46	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:569:GLU:HG3	1:A:574:HIS:CD2	2.48	0.48
1:A:709:VAL:HG21	1:A:712:LYS:HG3	1.95	0.48
1:B:714:VAL:HG12	1:B:716:ALA:N	2.25	0.48
1:B:788:TYR:HA	1:B:795:HIS:ND1	2.28	0.48
1:A:441:VAL:HA	1:A:457:ILE:O	2.13	0.48
1:A:873:LEU:O	1:A:877:LEU:HD12	2.12	0.48
1:B:473:GLY:HA2	1:B:514:VAL:HG21	1.93	0.48
1:B:777:PHE:CE2	1:B:781:GLN:NE2	2.81	0.48
1:A:223:TYR:CD2	1:A:226:ARG:HB2	2.48	0.48
1:A:440:LEU:HB2	1:A:459:ILE:HG13	1.93	0.48
1:A:810:SER:O	1:A:813:THR:OG1	2.28	0.48
1:B:402:ASN:O	1:B:406:HIS:HD2	1.95	0.48
1:B:590:ILE:O	1:B:591:GLN:HB3	2.13	0.48
1:B:799:LEU:HG	1:B:803:LEU:HD11	1.95	0.48
1:B:821:LYS:O	1:B:825:LEU:HD12	2.12	0.48
1:B:852:LYS:O	1:B:852:LYS:HG3	2.13	0.48
1:A:510:GLU:OE1	1:A:510:GLU:HA	2.14	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:353:LEU:O	1:A:354:GLU:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:PRO:HB2	1:A:528:TRP:CD1	2.49	0.48
1:B:648:LYS:HE3	4:B:168:HOH:O	2.13	0.48
1:A:231:LEU:CD1	1:B:372:TYR:CE1	2.97	0.48
1:A:721:SER:O	1:A:722:GLU:CD	2.56	0.48
1:A:247:LEU:CD2	1:A:251:GLN:HE22	2.22	0.48
1:A:305:SER:HB3	1:A:333:VAL:HA	1.94	0.48
1:A:476:LEU:CD2	1:A:478:ILE:HD11	2.44	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: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:330:MET:CG	1:B:350:PHE:CD1	2.97	0.48
1:B:559:GLU:O	1:B:562:TYR:HB3	2.14	0.48
1:B:579:ASP:HA	1:B:582:TYR:CD2	2.49	0.48
1:B:667:PHE:O	1:B:670:LEU:HB2	2.14	0.48
1:B:720:SER:HB2	1:B:770:LEU:CB	2.43	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:A:770:LEU:CD1	1:A:773:HIS:HB3	2.44	0.48
1:B:261:ARG:HD3	1:B:280:GLY:CA	2.44	0.48
1:B:341:ASP:O	1:B:342:GLN:HG2	2.14	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:A:591:GLN:HG3	1:A:592:PRO:CD	2.43	0.47
1:A:648:LYS:HZ2	1:A:648:LYS:CB	2.27	0.47
1:B:393:CYS:O	1:B:397:LEU:N	2.34	0.47
1:A:688:ALA:CB	1:A:757:MET:HE1	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:312:THR:HB	1:B:315:ASP:CG	2.38	0.47
1:A:360:ASP:HB3	4:A:110:HOH:O	2.14	0.47
1:B:433:PHE:CE2	1:B:442:ALA:HB3	2.49	0.47
1:B:479:PRO:CB	1:B:528:TRP:CE3	2.97	0.47
1:B:596:ILE:CG2	1:B:600:PHE:CD1	2.97	0.47
1:B:860:ILE:HD11	1:B:895:TRP:C	2.39	0.47
1:A:527:PRO:CG	1:A:528:TRP:CD1	2.96	0.47
1:A:590:ILE:HG22	1:A:624:GLN:HE22	1.78	0.47
1:A:593:VAL:CG1	1:A:600:PHE:CE2	2.98	0.47
1:A:668:CYS:SG	1:A:689:LEU:CD2	3.03	0.47
1:B:698:LEU:O	1:B:730:HIS:CD2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLN:HG2	1:A:291:PRO:HA	1.94	0.47
1:A:563:ARG:HD3	4:A:57:HOH:O	2.14	0.47
1:B:318:GLN:HA	1:B:321:SER:OG	2.15	0.47
1:B:330:MET:CG	1:B:350:PHE:CE1	2.97	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:A:565:HIS:HA	1:A:568:ASN:HB3	1.96	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:B:627:ASN:ND2	1:B:631:ASN:CG	2.73	0.47
1:B:868:MET:HG2	1:B:888:VAL:HG12	1.95	0.47
1:A:425:SER:OG	1:A:520:LEU:HD22	2.14	0.47
1:A:559:GLU:C	1:A:561:GLN:N	2.72	0.47
1:A:575:MET:HG2	1:A:648:LYS:HG2	1.96	0.47
1:A:605:TYR:CZ	1:A:610:LEU:HD11	2.50	0.47
1:A:605:TYR:O	1:A:814:LYS:HE3	2.14	0.47
1:A:610:LEU:HB3	1:A:611:PRO:CD	2.44	0.47
1:A:630:ASN:HD22	1:A:630:ASN:N	2.11	0.47
1:A:648:LYS:NZ	1:A:648:LYS:CB	2.78	0.47
1:A:814:LYS:HB3	1:A:818:THR:CG2	2.45	0.47
1:A:874:LEU:HA	1:A:874:LEU:HD23	1.74	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: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:440:LEU:HG	1:A:461:ALA:HA	1.97	0.47
1:B:441:VAL:HG21	1:B:458:ARG:NH2	2.29	0.47
1:A:224:THR:CG2	1:A:228:ARG:NH2	2.74	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: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:636:CYS:N	1:B:637:PRO:HD2	2.30	0.47
1:B:672:TYR:N	1:B:677:LEU:HD12	2.29	0.47
1:A:230:ILE:HD13	1:A:230:ILE:HA	1.48	0.47
1:A:641:ARG:NH1	1:A:742:GLY:HA3	2.30	0.47
1:A:656:HIS:HD2	1:A:829:GLU:OE2	1.98	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:B:597:ASP:HB3	1:B:600:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:HD2	1:A:223:TYR:O	1.98	0.46
1:A:566:LEU:HD13	1:B:755:GLN:HE21	1.80	0.46
1:A:602:SER:C	1:A:604:THR:N	2.74	0.46
1:A:681:LEU:HB3	1:A:685:GLU:OE1	2.15	0.46
1:A:252:TYR:C	1:A:252:TYR:CD2	2.93	0.46
1:A:331:LEU:HD13	1:A:366:ILE:HD12	1.96	0.46
1:A:403:LEU:CD1	1:A:417:ILE:HG13	2.45	0.46
1:A:575:MET:CE	1:A:649:GLY:HA2	2.45	0.46
1:A:860:ILE:HD11	1:A:895:TRP:HB3	1.96	0.46
1:B:253:LEU:C	1:B:255:GLN:N	2.68	0.46
1:B:458:ARG:CG	1:B:458:ARG:NH1	2.73	0.46
1:B:508:LYS:N	1:B:514:VAL:HA	2.31	0.46
1:A:311:LEU:HD23	1:A:315:ASP:HB2	1.97	0.46
1:A:572:MET:HE3	1:A:736:ALA:CB	2.46	0.46
1:A:852:LYS:NZ	1:A:852:LYS:HB2	2.30	0.46
1:B:460:PRO:CG	1:B:463:GLN:NE2	2.78	0.46
1:B:820:ARG:O	1:B:824:GLU:HG2	2.16	0.46
1:A:593:VAL:HG12	1:A:600:PHE:CE2	2.49	0.46
1:B:258:ARG:HD3	1:B:352:LYS:HZ3	1.79	0.46
1:B:268:SER:HB3	1:B:273:GLN:O	2.15	0.46
1:B:270:ASP:OD2	1:B:270:ASP:N	2.48	0.46
1:B:503:LEU:HD12	1:B:504:CYS:N	2.30	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: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:A:816:TRP:O	1:A:820:ARG:HB2	2.14	0.46
1:B:748:HIS:CD2	1:B:748:HIS:H	2.33	0.46
1:B:630:ASN:ND2	1:B:631:ASN:N	2.59	0.46
1:B:637:PRO:C	1:B:641:ARG:HH21	2.23	0.46
1:B:320:GLN:HE21	1:B:327:LEU:CB	2.23	0.46
1:A:484:HIS:CD2	1:A:485:PRO:CG	2.99	0.46
1:A:521:VAL:O	1:A:522:ASN:HB2	2.16	0.46
1:A:715:LEU:C	1:A:717:ALA:N	2.74	0.46
1:A:718:LEU:C	1:A:720:SER:N	2.74	0.46
1:B:333:VAL:CB	1:B:366:ILE:HG21	2.46	0.46
1:B:465:ILE:CD1	1:B:502:ILE:HD13	2.46	0.46
1:B:576:LYS:C	1:B:648:LYS:HE2	2.40	0.46
1:A:274:LEU:HD23	1:A:274:LEU:N	2.31	0.46
1:A:370:PHE:CD1	1:A:373:THR:HG22	2.50	0.46
1:A:388:LYS:HB3	1:A:388:LYS:HE3	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:MET:HE1	1:A:690:PHE:CD1	2.50	0.46
1:B:671:LEU:HB3	1:B:677:LEU:HD11	1.96	0.46
1:B:818:THR:O	1:B:822:ILE:HD12	2.16	0.46
1:B:837:GLU:CB	1:B:838:LYS:NZ	2.77	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:854:TYR:HE1	4:A:75:HOH:O	1.98	0.46
1:A:669:TYR:CD2	1:A:669:TYR:C	2.93	0.45
1:A:707:PHE:C	1:A:709:VAL:H	2.23	0.45
1:A:821:LYS:C	1:A:824:GLU:HG3	2.41	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:366:ILE:O	1:B:369:CYS:HB3	2.15	0.45
1:B:471:THR:CG2	1:B:472:THR:N	2.79	0.45
1:B:720:SER:HA	1:B:770:LEU:HB2	1.97	0.45
1:B:727:GLU:OE2	1:B:727:GLU:N	2.50	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: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:B:718:LEU:CG	1:B:719:TYR:N	2.76	0.45
1:A:330:MET:CG	1:A:350:PHE:CD1	2.98	0.45
1:A:528:TRP:HD1	1:A:528:TRP:H	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:A:777:PHE:CE2	1:A:781:GLN:NE2	2.85	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: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:366:ILE:HG22	1:A:367:GLN:N	2.30	0.45
1:A:479:PRO:CB	1:A:528:TRP:CE3	2.97	0.45
1:A:536:LEU:O	1:A:536:LEU:HD22	2.17	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: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:617:MET:O	1:A:620:LEU:HB2	2.16	0.45
1:A:855:ILE:N	1:A:856:PRO:CD	2.79	0.45
1:B:225:ASP:HA	1:B:228:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:LEU:CD2	1:B:617:MET:HE2	2.47	0.45
1:A:273:GLN:HE21	1:A:273:GLN:HB3	1.51	0.45
1:A:602:SER:HB3	4:A:184:HOH:O	2.16	0.45
1:A:862:PHE:HE1	1:A:866:ILE:HG21	1.82	0.45
1:B:829:GLU:C	1:B:831:PHE:H	2.24	0.45
1:A:326:GLU:C	1:A:327:LEU:HD12	2.42	0.45
1:A:610:LEU:HA	1:A:611:PRO:HD3	1.60	0.45
1:A:721:SER:CA	1:A:769:ASP:OD2	2.63	0.45
1:A:838:LYS:CD	1:A:838:LYS:N	2.78	0.45
1:A:873:LEU:HA	1:A:876:ASP:HB2	1.99	0.45
1:B:254:GLN:OE1	1:B:280:GLY:HA2	2.16	0.45
1:B:428:GLU:HB2	1:B:522:ASN:HB2	1.97	0.45
1:B:674:ASN:H	1:B:674:ASN:ND2	2.13	0.45
1:A:445:PHE:HB3	1:A:446:ASP:H	1.42	0.45
1:A:593:VAL:CG2	1:A:625:ASP:HB2	2.46	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:B:755:GLN:O	1:B:758:LEU:HB2	2.16	0.45
1:A:231:LEU:CD1	1:B:372:TYR:CZ	2.98	0.45
1:B:290:PHE:CB	1:B:291:PRO:HD2	2.21	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:313:SER:O	1:B:317:GLN:HB2	2.17	0.45
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.61	0.45
1:B:395:ALA:O	1:B:399:VAL:HG12	2.17	0.45
1:B:602:SER:C	1:B:604:THR:H	2.25	0.45
1:A:240:LEU:HD11	1:B:340:THR:HG22	1.99	0.44
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.84	0.44
1:A:497:PHE:O	1:A:498:ARG:HB2	2.16	0.44
1:A:756:ARG:HE	1:A:756:ARG:HB2	1.71	0.44
1:B:258:ARG:NH1	1:B:258:ARG:HG2	2.31	0.44
1:B:719:TYR:O	1:B:720:SER:HB3	2.16	0.44
1:B:735:ILE:HD12	1:B:738:LEU:HD12	1.98	0.44
1:B:754:TYR:O	1:B:758:LEU:HD13	2.18	0.44
1:A:376:VAL:O	1:A:380:THR:OG1	2.34	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: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:B:433:PHE:CE2	1:B:442:ALA:CB	2.99	0.44
1:B:887:ARG:NH1	1:B:887:ARG:CG	2.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:LEU:HD21	1:A:636:CYS:HB3	2.00	0.44
1:A:789:ASP:HB3	1:A:792:ASN:H	1.81	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:251:GLN:NE2	1:B:281:ASP:HA	2.31	0.44
1:B:645:MET:HE2	1:B:740:THR:HG21	1.99	0.44
1:B:851:GLU:HA	1:B:854:TYR:CE1	2.52	0.44
1:A:275:SER:CB	1:A:287:GLU:OE2	2.65	0.44
1:B:425:SER:O	1:B:426:ASN:HB2	2.17	0.44
1:B:837:GLU:C	1:B:838:LYS:NZ	2.74	0.44
1:B:854:TYR:CD1	1:B:854:TYR:N	2.86	0.44
1:A:251:GLN:NE2	1:A:281:ASP:CA	2.78	0.44
1:A:681:LEU:HD13	1:A:800:LEU:HD21	2.00	0.44
1:A:889:ALA:O	1:A:892:ARG:HB3	2.17	0.44
1:B:323:LEU:HD12	1:B:327:LEU:HD11	1.94	0.44
1:B:330:MET:CE	1:B:332:CYS:N	2.81	0.44
1:B:409:ASP:HB3	1:B:412:VAL:HB	1.99	0.44
1:B:459:ILE:HG13	1:B:460:PRO:HD2	2.00	0.44
1:B:459:ILE:CG1	1:B:460:PRO:HD2	2.47	0.44
1:B:508:LYS:CA	1:B:514:VAL:HA	2.48	0.44
1:A:239:ASP:HB2	1:A:245:LEU:CD2	2.48	0.44
1:A:542:ILE:HG21	1:B:401:LYS:HZ3	1.83	0.44
1:A:715:LEU:HD23	1:A:862:PHE:CD2	2.53	0.44
1:B:421:ALA:HB2	1:B:540:PHE:HE2	1.83	0.44
1:B:618:ALA:O	1:B:622:MET:HG3	2.18	0.44
1:B:675:LEU:HD13	1:B:878:PHE:CG	2.53	0.44
1:B:809:LEU:O	1:B:811:ASP:N	2.50	0.44
1:B:872:LYS:HA	1:B:872:LYS:HD2	1.60	0.44
1:A:413:LEU:O	1:A:416:GLU:HB2	2.17	0.44
1:A:868:MET:HB2	1:A:869:PRO:HD3	2.00	0.44
1:B:439:GLU:HA	1:B:461:ALA:H	1.83	0.44
1:B:718:LEU:C	1:B:720:SER:N	2.75	0.44
1:B:770:LEU:HA	1:B:770:LEU:HD13	1.36	0.44
1:B:859:GLN:HE21	1:B:859:GLN:CA	2.29	0.44
1:A:299:VAL:HG12	1:A:334:PRO:HG3	1.99	0.44
1:A:805:THR:CG2	1:A:870:ILE:HD13	2.48	0.44
1:B:258:ARG:HH11	1:B:258:ARG:HG2	1.83	0.44
1:B:586:LEU:HD12	1:B:640:ALA:HB3	2.00	0.44
1:A:381:LEU:C	1:A:381:LEU:HD12	2.42	0.43
1:A:508:LYS:H	1:A:515:ILE:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:726:MET:O	1:B:729:HIS:HB3	2.18	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:902:VAL:HA	1:B:903:PRO:HD3	1.34	0.43
1:A:600:PHE:CD2	1:A:600:PHE:C	2.96	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:682:GLU:HG3	1:B:685:GLU:OE1	2.19	0.43
1:B:855:ILE:N	1:B:856:PRO:CD	2.80	0.43
1:A:561:GLN:HE22	1:B:561:GLN:HE21	1.66	0.43
1:A:672:TYR:HD1	1:A:686:ILE:HG21	1.82	0.43
1:A:673:LYS:HB2	1:A:674:ASN:H	1.60	0.43
1:A:689:LEU:HA	1:A:764:ILE:HD13	2.01	0.43
1:A:726:MET:O	1:A:729:HIS:HB3	2.19	0.43
1:B:255:GLN:C	1:B:257:THR:H	2.26	0.43
1:B:600:PHE:CD2	1:B:600:PHE:O	2.71	0.43
1:B:721:SER:OG	1:B:722:GLU:N	2.51	0.43
1:B:746:PHE:CZ	1:B:757:MET:HE2	2.53	0.43
1:B:809:LEU:C	1:B:811:ASP:H	2.26	0.43
1:B:418:ILE:CG1	1:B:432:VAL:CG2	2.96	0.43
1:B:903:PRO:O	1:B:904:ARG:HG3	2.17	0.43
1:A:226:ARG:C	1:A:228:ARG:N	2.69	0.43
1:A:304:LYS:HE3	1:A:304:LYS:CA	2.31	0.43
1:A:337:SER:HB2	1:A:344:VAL:HG21	2.00	0.43
1:A:376:VAL:CG1	1:A:377:LEU:N	2.81	0.43
1:A:670:LEU:O	1:A:674:ASN:ND2	2.46	0.43
1:B:223:TYR:C	1:B:225:ASP:N	2.76	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:356:ASP:O	1:B:357:LEU:HG	2.19	0.43
1:A:376:VAL:CG2	1:B:375:THR:HG22	2.48	0.43
1:A:448:GLY:O	1:A:449:VAL:HG23	2.18	0.43
1:A:796:HIS:O	1:A:800:LEU:HD12	2.19	0.43
1:A:860:ILE:HD13	1:A:895:TRP:HB3	2.00	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: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:417:ILE:CD1	1:B:548:ILE:CD1	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:PHE:N	1:B:749:PHE:HD1	2.16	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: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:372:TYR:CE2	1:B:231:LEU:HD11	2.53	0.43
1:A:478:ILE:HA	1:A:479:PRO:HD2	1.48	0.43
1:A:482:TYR:C	1:A:484:HIS:H	2.26	0.43
1:A:812:GLN:O	1:A:888:VAL:HG22	2.19	0.43
1:A:855:ILE:HB	1:A:856:PRO:HD3	2.01	0.43
1:B:354:GLU:HB3	1:B:355:GLY:H	1.25	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:231:LEU:HD11	1:B:372:TYR:CD2	2.54	0.42
1:A:540:PHE:C	1:A:542:ILE:N	2.75	0.42
1:A:656:HIS:CG	1:A:700:HIS:CE1	3.07	0.42
1:A:672:TYR:O	1:A:676:GLU:HA	2.19	0.42
1:A:788:TYR:CZ	1:A:799:LEU:HD23	2.54	0.42
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.88	0.42
1:B:270:ASP:HB2	1:B:272:LEU:CG	2.46	0.42
1:B:527:PRO:CG	1:B:528:TRP:CD1	3.01	0.42
1:B:829:GLU:C	1:B:831:PHE:N	2.77	0.42
1:A:231:LEU:HD21	1:B:230:ILE:CG2	2.39	0.42
1:A:590:ILE:CG2	1:A:624:GLN:CD	2.91	0.42
1:A:671:LEU:HD13	1:A:803:LEU:CD2	2.42	0.42
1:B:274:LEU:HD22	1:B:274:LEU:HA	1.87	0.42
1:B:602:SER:C	1:B:604:THR:N	2.77	0.42
1:B:680:TYR:HB3	1:B:788:TYR:CE2	2.54	0.42
1:B:712:LYS:N	4:B:52:HOH:O	2.51	0.42
1:A:225:ASP:HA	1:A:228:ARG:HE	1.84	0.42
1:A:233:LEU:O	1:A:236:GLU:HB2	2.19	0.42
1:A:444:VAL:HB	1:A:454:SER:O	2.19	0.42
1:A:507:ILE:C	1:A:508:LYS:CG	2.92	0.42
1:A:600:PHE:HA	1:A:605:TYR:CD1	2.54	0.42
1:A:834:GLY:O	1:A:838:LYS:NZ	2.49	0.42
1:B:233:LEU:C	1:B:233:LEU:HD12	2.44	0.42
1:B:504:CYS:SG	1:B:519:GLU:HB3	2.59	0.42
1:B:688:ALA:CA	1:B:757:MET:HE1	2.46	0.42
1:B:895:TRP:O	1:B:898:VAL:HG23	2.19	0.42
1:A:399:VAL:HG22	1:A:420:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HB	1:B:345:ALA:HB3	2.01	0.42
1:B:357:LEU:HD23	1:B:357:LEU:HA	1.88	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:A:688:ALA:CB	1:A:760:LEU:CD1	2.98	0.42
1:B:437:GLN:NE2	1:B:437:GLN:C	2.77	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:540:PHE:O	1:A:542:ILE:N	2.53	0.42
1:A:599:ASN:C	1:A:601:ALA:N	2.76	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:381:LEU:HD12	1:A:381:LEU:O	2.20	0.42
1:A:735:ILE:HD13	1:A:735:ILE:HA	1.73	0.42
1:A:799:LEU:CD1	1:A:803:LEU:HD11	2.48	0.42
1:A:852:LYS:NZ	1:A:852:LYS:CB	2.83	0.42
1:B:422:ARG:HD3	1:B:429:ILE:HA	2.01	0.42
1:B:236:GLU:O	1:B:248:LYS:NZ	2.39	0.42
1:B:253:LEU:O	1:B:254:GLN:C	2.62	0.42
1:B:398:GLN:NE2	1:B:401:LYS:HD3	2.34	0.42
1:A:418:ILE:CG1	1:A:432:VAL:CG2	2.98	0.42
1:A:542:ILE:HD13	1:B:401:LYS:HZ1	1.85	0.42
1:A:703:THR:HB	1:A:718:LEU:HD12	2.00	0.42
1:A:726:MET:HG2	1:A:730:HIS:CE1	2.54	0.42
1:A:821:LYS:HD3	1:A:824:GLU:OE1	2.20	0.42
1:B:251:GLN:HE22	1:B:281:ASP:HA	1.84	0.42
1:A:529:PHE:O	1:A:530:SER:C	2.62	0.41
1:A:635:ASP:OD2	1:A:638:THR:N	2.53	0.41
1:B:226:ARG:HB3	1:B:368:HIS:CE1	2.55	0.41
1:B:237:LEU:HD21	1:B:249:VAL:CG2	2.49	0.41
1:B:258:ARG:CG	1:B:258:ARG:NH1	2.83	0.41
1:B:508:LYS:H	1:B:515:ILE:H	1.68	0.41
1:B:582:TYR:O	1:B:586:LEU:HB2	2.19	0.41
1:B:697:ASP:O	1:B:700:HIS:HB2	2.20	0.41
1:A:389:LEU:HA	1:A:389:LEU:HD23	1.59	0.41
1:A:636:CYS:HB2	1:A:637:PRO:HD3	2.02	0.41
1:A:647:LYS:C	1:A:649:GLY:N	2.76	0.41
1:A:671:LEU:HD23	1:A:671:LEU:HA	1.80	0.41
1:B:289:SER:C	1:B:290:PHE:CD2	2.98	0.41
1:B:608:ARG:NH2	1:B:655:TYR:HE1	2.17	0.41
1:B:694:MET:HE2	1:B:694:MET:HB3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:O	1:A:293:THR:O	2.39	0.41
1:A:555:LYS:O	1:A:556:LYS:C	2.63	0.41
1:A:575:MET:HG2	1:A:648:LYS:CG	2.51	0.41
1:B:301:GLU:HA	1:B:301:GLU:OE1	2.19	0.41
1:B:781:GLN:O	1:B:784:ALA:N	2.53	0.41
1:A:428:GLU:HB2	1:A:522:ASN:HB2	2.02	0.41
1:A:509:ASN:OD1	1:A:513:GLU:HG3	2.19	0.41
1:A:571:MET:CE	1:B:731:PHE:HE2	2.33	0.41
1:A:576:LYS:HD3	1:A:576:LYS:C	2.45	0.41
1:A:596:ILE:HG21	1:A:600:PHE:CD1	2.55	0.41
1:A:620:LEU:CD2	1:A:639:LEU:HD21	2.51	0.41
1:A:821:LYS:HD3	1:A:821:LYS:HA	1.80	0.41
1:A:255:GLN:C	1:A:257:THR:H	2.26	0.41
1:A:329:ALA:O	1:A:330:MET:HB2	2.19	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:481:ALA:HB1	1:A:487:PHE:CD1	2.55	0.41
1:A:819:THR:HA	1:A:822:ILE:HD12	2.02	0.41
1:B:279:ILE:CD1	1:B:322:MET:SD	3.08	0.41
1:B:428:GLU:C	1:B:429:ILE:HG23	2.45	0.41
1:B:629:ILE:HA	1:B:634:ILE:HD12	2.01	0.41
1:A:362:ASP:O	1:A:365:VAL:HG13	2.20	0.41
1:A:366:ILE:O	1:A:369:CYS:HB3	2.20	0.41
1:A:380:THR:O	1:A:384:GLN:HG3	2.21	0.41
1:A:399:VAL:HG13	1:A:420:GLU:HG3	2.03	0.41
1:A:427:ALA:CB	1:A:520:LEU:CD2	2.99	0.41
1:A:618:ALA:O	1:A:622:MET:N	2.53	0.41
1:B:655:TYR:OH	1:B:719:TYR:OH	2.20	0.41
1:B:671:LEU:HD23	1:B:671:LEU:HA	1.81	0.41
1:B:715:LEU:C	1:B:717:ALA:N	2.78	0.41
1:A:277:LYS:HB3	1:A:287:GLU:HG3	2.03	0.41
1:A:409:ASP:C	1:A:411:SER:N	2.76	0.41
1:A:837:GLU:CB	1:A:838:LYS:HE3	2.41	0.41
1:B:256:GLU:HG2	1:B:256:GLU:H	1.54	0.41
1:B:572:MET:CE	1:B:645:MET:CE	2.91	0.41
1:B:586:LEU:CD1	1:B:640:ALA:CB	2.98	0.41
1:B:901:LEU:N	1:B:901:LEU:CD2	2.75	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:A:532:PHE:CD1	1:A:532:PHE:C	2.98	0.41
1:A:570:MET:C	1:A:572:MET:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LEU:CD2	1:A:826:ILE:HG23	2.51	0.41
1:A:750:SER:C	1:A:752:LYS:N	2.76	0.41
1:A:822:ILE:C	1:A:824:GLU:N	2.77	0.41
1:B:275:SER:HB3	1:B:287:GLU:OE2	2.20	0.41
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.79	0.41
1:B:656:HIS:CD2	1:B:829:GLU:OE2	2.54	0.41
1:B:812:GLN:HA	1:B:812:GLN:NE2	2.36	0.41
1:A:254:GLN:OE1	1:A:280:GLY:HA2	2.21	0.41
1:A:370:PHE:C	1:A:372:TYR:N	2.79	0.41
1:A:539:ALA:O	1:A:542:ILE:HB	2.21	0.41
1:A:638:THR:CG2	1:A:745:ILE:HG22	2.42	0.41
1:A:688:ALA:CB	1:A:760:LEU:HD12	2.50	0.41
1:A:774:LEU:HD21	1:A:866:ILE:CD1	2.51	0.41
1:A:868:MET:N	1:A:869:PRO:HD2	2.35	0.41
1:B:320:GLN:HG3	1:B:327:LEU:HD22	2.03	0.41
1:B:338:ARG:HD2	1:B:338:ARG:HA	1.75	0.41
1:B:441:VAL:CG1	1:B:443:LYS:HD3	2.51	0.41
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.71	0.41
1:B:677:LEU:HD21	1:B:803:LEU:CD2	2.50	0.41
1:B:740:THR:CG2	1:B:743:CYS:SG	3.05	0.41
1:B:859:GLN:HG2	1:B:895:TRP:CE2	2.56	0.41
1:B:868:MET:HB2	1:B:869:PRO:CD	2.50	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:B:578:SER:O	1:B:581:GLU:HB2	2.21	0.41
1:B:838:LYS:O	1:B:839:ALA:HB3	2.21	0.41
1:A:550:HIS:CD2	1:B:407:LEU:HD23	2.56	0.40
1:A:636:CYS:N	1:A:637:PRO:CD	2.83	0.40
1:A:687:PHE:O	1:A:691:ILE:HG12	2.21	0.40
1:A:709:VAL:CG2	1:A:712:LYS:HB2	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:319:LEU:HD22	1:B:322:MET:CE	2.51	0.40
1:B:647:LYS:HD2	1:B:658:TRP:CD1	2.56	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:819:THR:CG2	1:A:891:ASN:ND2	2.79	0.40
1:A:833:GLN:O	1:A:836:LEU:HD12	2.21	0.40
1:B:393:CYS:C	1:B:395:ALA:N	2.77	0.40
1:B:620:LEU:O	1:B:624:GLN:HB3	2.21	0.40
1:B:897:LYS:C	1:B:899:SER:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:CE2	1:A:226:ARG:CB	2.96	0.40
1:A:404:PHE:HA	1:A:407:LEU:HD21	2.02	0.40
1:A:575:MET:CE	1:A:649:GLY:CA	2.99	0.40
1:A:647:LYS:HD2	1:A:658:TRP:CG	2.56	0.40
1:A:694:MET:HE2	1:A:694:MET:HB3	1.89	0.40
1:A:788:TYR:O	1:A:788:TYR:CG	2.74	0.40
1:A:459:ILE:O	1:A:460:PRO:C	2.61	0.40
1:A:540:PHE:C	1:A:542:ILE:H	2.29	0.40
1:A:566:LEU:CD1	1:B:755:GLN:HE21	2.34	0.40
1:A:648:LYS:HB2	1:A:648:LYS:HZ2	1.83	0.40
1:B:629:ILE:HA	1:B:634:ILE:HB	2.04	0.40
1:B:814:LYS:HD2	1:B:814:LYS:HA	1.90	0.40
1:A:364:HIS:HA	1:A:367:GLN:NE2	2.36	0.40
1:A:370:PHE:O	1:A:371:HIS:C	2.64	0.40
1:A:685:GLU:C	1:A:687:PHE:N	2.78	0.40
1:A:770:LEU:HD13	1:A:770:LEU:HA	1.39	0.40
1:A:896:THR:O	1:A:899:SER:OG	2.33	0.40
1:B:237:LEU:HD21	1:B:249:VAL:HG22	2.04	0.40
1:B:376:VAL:O	1:B:377:LEU:C	2.64	0.40
1:B:536:LEU:HD22	1:B:536:LEU:C	2.47	0.40
1:B:624:GLN:CG	1:B:625:ASP:N	2.84	0.40
1:B:687:PHE:CE1	1:B:746:PHE:CE1	3.08	0.40
1:B:809:LEU:C	1:B:811:ASP:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	655/691 (95%)	512 (78%)	95 (14%)	48 (7%)	1 4
1	B	633/691 (92%)	514 (81%)	84 (13%)	35 (6%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1288/1382 (93%)	1026 (80%)	179 (14%)	83 (6%)	1	5

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%)	372 (63%)	218 (37%)	0	1
1	B	577/614 (94%)	381 (66%)	196 (34%)	0	1
All	All	1167/1228 (95%)	753 (64%)	414 (36%)	0	1

All (414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	ASP
1	A	226	ARG
1	A	230	ILE
1	A	231	LEU
1	A	234	CYS
1	A	244	SER
1	A	250	LEU
1	A	251	GLN
1	A	252	TYR
1	A	254	GLN
1	A	257	THR
1	A	258	ARG
1	A	260	SER
1	A	261	ARG
1	A	266	LEU
1	A	269	GLU
1	A	270	ASP
1	A	271	ASN
1	A	272	LEU

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Mol	Chain	Res	Type
1	A	273	GLN
1	A	274	LEU
1	A	275	SER
1	A	277	LYS
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	308	LEU
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	346	LEU
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

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Mol	Chain	Res	Type
1	A	390	LYS
1	A	391	CYS
1	A	396	LEU
1	A	397	LEU
1	A	398	GLN
1	A	403	LEU
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	452	ASP
1	A	453	GLU
1	A	458	ARG
1	A	459	ILE
1	A	463	GLN
1	A	471	THR
1	A	472	THR
1	A	475	ILE
1	A	476	LEU
1	A	478	ILE
1	A	486	LEU
1	A	498	ARG
1	A	499	THR
1	A	500	ARG
1	A	501	ASN
1	A	503	LEU
1	A	507	ILE

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Mol	Chain	Res	Type
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	531	LYS
1	A	532	PHE
1	A	534	GLU
1	A	535	ASP
1	A	536	LEU
1	A	548	ILE
1	A	551	SER
1	A	553	LEU
1	A	555	LYS
1	A	557	VAL
1	A	559	GLU
1	A	563	ARG
1	A	566	LEU
1	A	569	GLU
1	A	571	MET
1	A	572	MET
1	A	575	MET
1	A	576	LYS
1	A	577	VAL
1	A	579	ASP
1	A	580	ASP
1	A	581	GLU
1	A	585	LEU
1	A	587	HIS
1	A	590	ILE
1	A	591	GLN
1	A	593	VAL
1	A	596	ILE
1	A	598	SER
1	A	599	ASN
1	A	600	PHE
1	A	608	ARG
1	A	610	LEU
1	A	612	GLU
1	A	613	ASP

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Mol	Chain	Res	Type
1	A	616	SER
1	A	621	SER
1	A	629	ILE
1	A	630	ASN
1	A	633	LYS
1	A	638	THR
1	A	644	LEU
1	A	645	MET
1	A	646	VAL
1	A	647	LYS
1	A	648	LYS
1	A	659	MET
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	692	SER
1	A	695	CYS
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	718	LEU
1	A	719	TYR
1	A	721	SER
1	A	722	GLU
1	A	725	VAL
1	A	735	ILE
1	A	741	HIS
1	A	748	HIS
1	A	751	ARG
1	A	752	LYS
1	A	755	GLN
1	A	756	ARG
1	A	758	LEU
1	A	760	LEU

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Mol	Chain	Res	Type
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	809	LEU
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	855	ILE
1	A	872	LYS
1	A	874	LEU
1	A	875	GLN
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	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

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Mol	Chain	Res	Type
1	B	257	THR
1	B	258	ARG
1	B	266	LEU
1	B	269	GLU
1	B	270	ASP
1	B	271	ASN
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	289	SER
1	B	292	LEU
1	B	293	THR
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
1	B	311	LEU
1	B	312	THR
1	B	314	GLU
1	B	315	ASP
1	B	317	GLN
1	B	319	LEU
1	B	325	CYS
1	B	326	GLU
1	B	328	GLN
1	B	330	MET
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

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Mol	Chain	Res	Type
1	B	361	GLU
1	B	363	GLU
1	B	365	VAL
1	B	367	GLN
1	B	373	THR
1	B	375	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	428	GLU
1	B	429	ILE
1	B	432	VAL
1	B	435	LEU
1	B	437	GLN
1	B	455	TYR
1	B	457	ILE
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	501	ASN
1	B	507	ILE
1	B	512	GLN
1	B	515	ILE
1	B	521	VAL

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Mol	Chain	Res	Type
1	B	524	ILE
1	B	528	TRP
1	B	531	LYS
1	B	532	PHE
1	B	534	GLU
1	B	535	ASP
1	B	536	LEU
1	B	541	SER
1	B	546	ILE
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	579	ASP
1	B	580	ASP
1	B	581	GLU
1	B	585	LEU
1	B	587	HIS
1	B	590	ILE
1	B	591	GLN
1	B	593	VAL
1	B	596	ILE
1	B	598	SER
1	B	599	ASN
1	B	608	ARG
1	B	609	SER
1	B	613	ASP
1	B	616	SER
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	634	ILE
1	B	638	THR
1	B	646	VAL
1	B	647	LYS

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Mol	Chain	Res	Type
1	B	648	LYS
1	B	663	SER
1	B	675	LEU
1	B	678	THR
1	B	680	TYR
1	B	681	LEU
1	B	683	ASP
1	B	684	ILE
1	B	695	CYS
1	B	701	ARG
1	B	703	THR
1	B	704	ASN
1	B	712	LYS
1	B	713	SER
1	B	718	LEU
1	B	719	TYR
1	B	721	SER
1	B	722	GLU
1	B	725	VAL
1	B	735	ILE
1	B	740	THR
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	760	LEU
1	B	766	LEU
1	B	770	LEU
1	B	776	ILE
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
1	B	809	LEU
1	B	817	LYS
1	B	820	ARG
1	B	824	GLU

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Mol	Chain	Res	Type
1	B	833	GLN
1	B	835	ASP
1	B	838	LYS
1	B	848	MET
1	B	850	ARG
1	B	852	LYS
1	B	855	ILE
1	B	857	GLU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	255	GLN
1	A	271	ASN
1	A	273	GLN
1	A	317	GLN
1	A	367	GLN
1	A	371	HIS
1	A	387	GLN
1	A	402	ASN
1	A	426	ASN
1	A	463	GLN
1	A	484	HIS
1	A	511	ASN
1	A	574	HIS
1	A	591	GLN
1	A	630	ASN
1	A	656	HIS
1	A	666	HIS
1	A	674	ASN
1	A	700	HIS
1	A	704	ASN

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Mol	Chain	Res	Type
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	255	GLN
1	B	271	ASN
1	B	273	GLN
1	B	298	GLN
1	B	317	GLN
1	B	318	GLN
1	B	320	GLN
1	B	328	GLN
1	B	364	HIS
1	B	368	HIS
1	B	371	HIS
1	B	398	GLN
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	796	HIS
1	B	812	GLN
1	B	833	GLN
1	B	859	GLN
1	B	875	GLN
1	B	900	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.30	0 100 100	43, 79, 109, 128	0
1	B	643/691 (93%)	-0.33	4 (0%) 85 69	46, 74, 107, 125	0
All	All	1304/1382 (94%)	-0.31	4 (0%) 90 79	43, 76, 108, 128	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	SER	2.9
1	B	849	ASP	2.5
1	B	315	ASP	2.4
1	B	529	PHE	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	905	1/1	0.90	0.26	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	905	1/1	0.92	0.42	58,58,58,58	0
2	ZN	A	1	1/1	0.98	0.06	73,73,73,73	0
2	ZN	B	2	1/1	0.98	0.07	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.