



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:37 AM UTC

PDB ID : 1WAF / pdb_00001waf
Title : DNA POLYMERASE FROM BACTERIOPHAGE RB69
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Steitz, T.A.
Deposited on : 1997-04-13
Resolution : 3.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

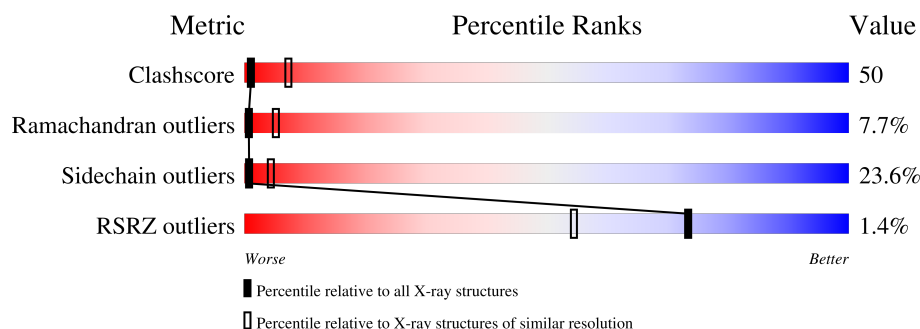
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	903	
1	B	903	

2 Entry composition [i](#)

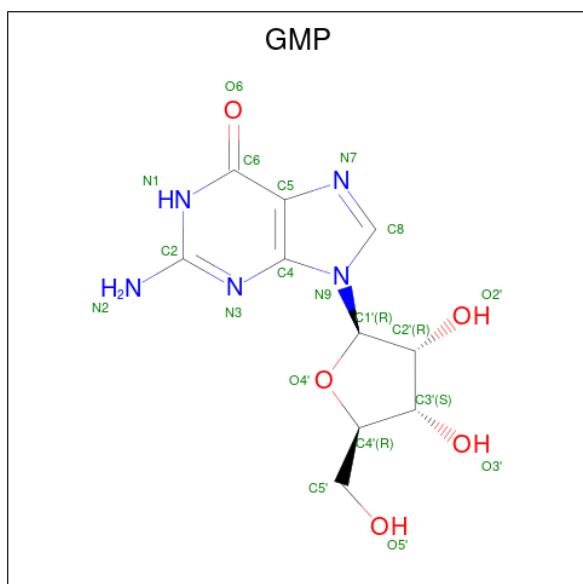
There are 2 unique types of molecules in this entry. The entry contains 14800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7380	4739	1226	1382	33			
1	B	903	Total	C	N	O	S	0	0	0
			7380	4739	1226	1382	33			

- Molecule 2 is GUANOSINE (CCD ID: GMP) (formula: $C_{10}H_{13}N_5O_5$).

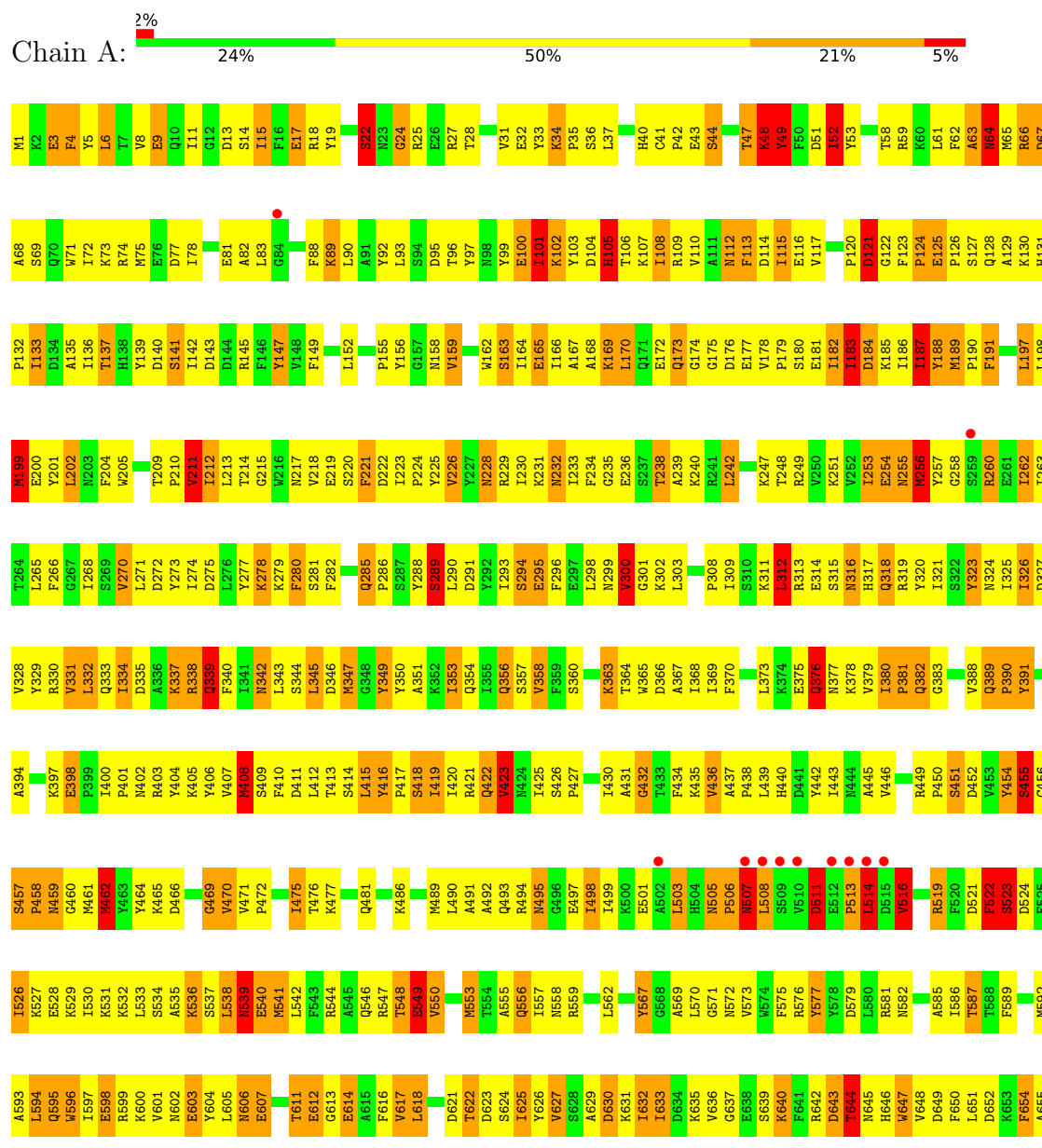


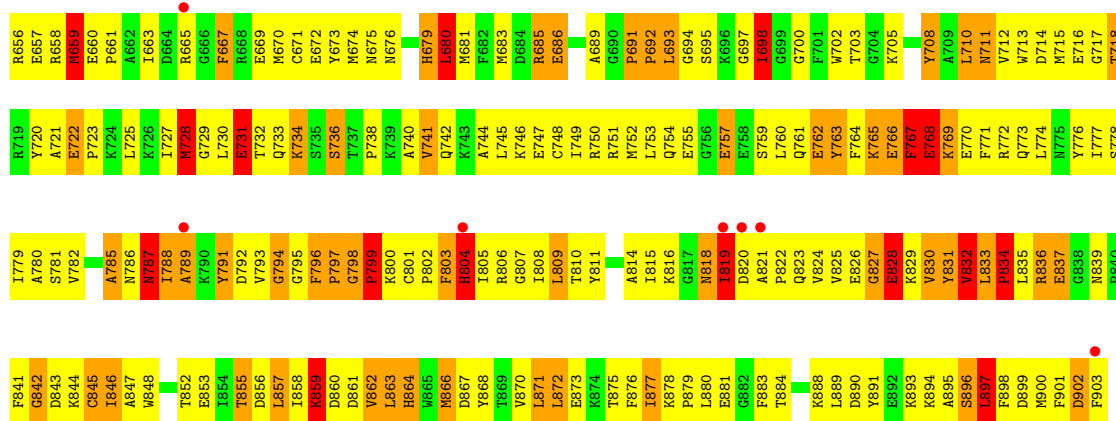
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	10	5	5		
2	B	1	Total	C	N	O	0	0
			20	10	5	5		

3 Residue-property plots

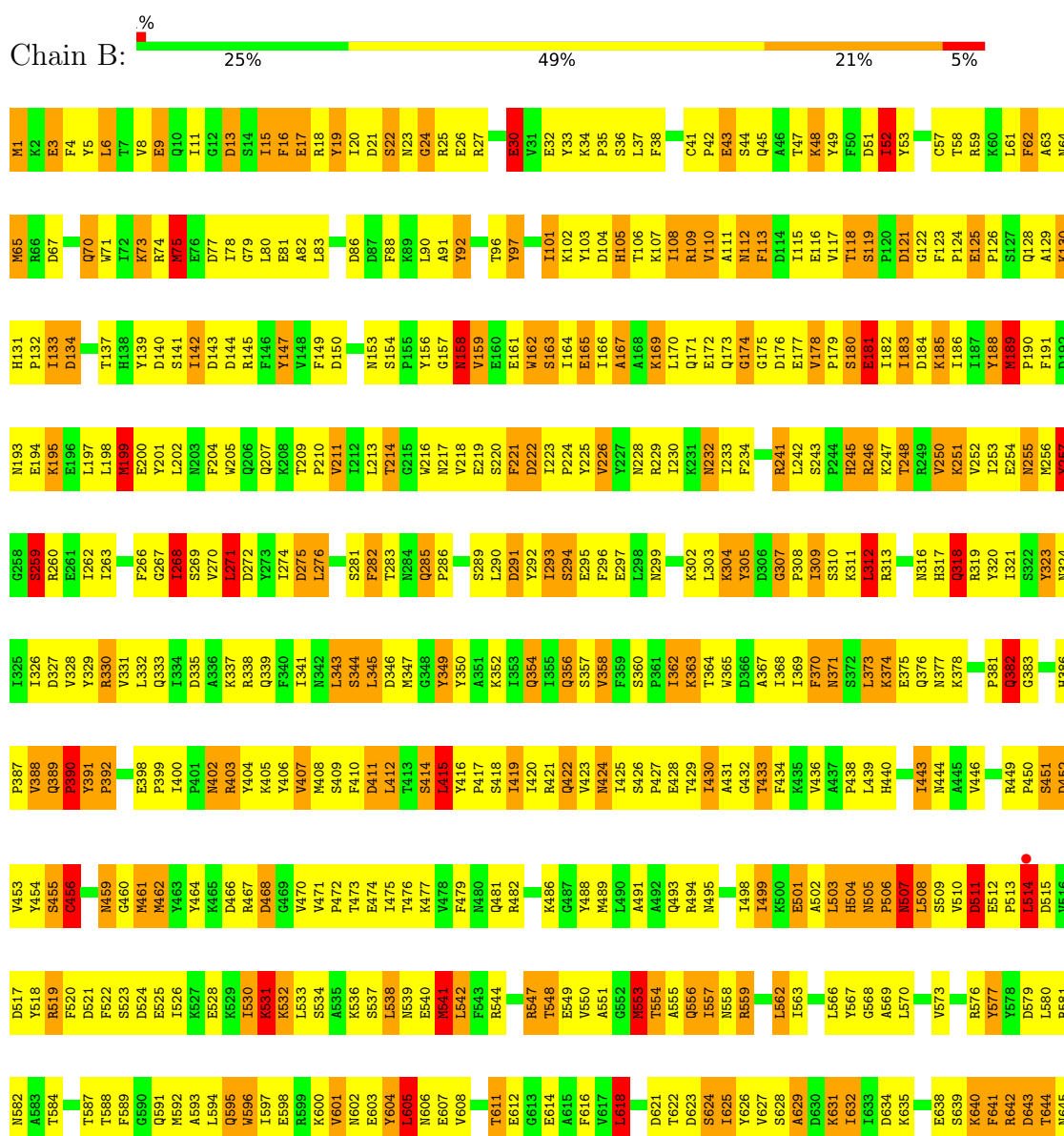
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA POLYMERASE





• Molecule 1: DNA POLYMERASE



H646	W647	V648	D649	F650	L651	D652	K653	F654	A655	R656	E657	R658	E660	P661	A662	I663	D664	R665	G666	F667	R668	E669	M670				M674	N675	N676	K677	Q678	H679	L680	M681	F682	M683	D684	R685	E686	A687	I688	A689	G690	P691	F692	L693	G694	S695	L698	G699	G700	F701	W702	T703				K706	R707	Y708	A709				
L710	N711	W712	W713				E716				R719	Y720	A721	E722	P723	K724	L725	K726	I727	M728	G729	I663	L730	E731	T732	Q733				A744	L745	K746	E747	C748	I749	R750	R751	M752	L753	Q754				E757	E758	S759	L760	Q761	E762	Y763				E766	F767	E768	K769	E770	F771	R772	Q773	L774	N775	Y776	I777
S778	I779	A780	S781				A785	N786	N787	I788	A789	K790	Y791	D792	V793	G794	F796	P797	G798	P799				P802	F803	H804	I805	R806	G807	I808	L809	T810	Y811	R812	R813	A814	I815	K816	G817	R818	I819	D820	A821	P822	G823	V824				G827	E828	K829	Y830	Y831	H832	L833	P834	L835	R836	E837	G838	N839	P840	F841	
G842	D843	K844	C845	I846	A847	S850	E853	I854	T855	D856	L857	I858	K859	D860	D861	V862	L863	H864	W865	W866	D867	Y868	T869	W870	L871	L872	E873				F876	I877	K878	P879	L880	E881	G882	F883	T884	A885	A886	L889	D890	K894	A895	S896	L897	F898	D899	W900	F901	D902	F903												

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.32Å 196.86Å 118.31Å 90.00° 92.57° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 82.2 (40.00-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 3.18Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , 0.274 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14800	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: GMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.04	12/7561 (0.2%)	1.45	126/10217 (1.2%)
1	B	1.02	9/7561 (0.1%)	1.44	125/10217 (1.2%)
All	All	1.03	21/15122 (0.1%)	1.45	251/20434 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	6
All	All	0	10

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	MET	SD-CE	8.22	2.00	1.79
1	B	268	ILE	CA-CB	7.42	1.64	1.54
1	B	1	MET	SD-CE	7.39	1.98	1.79
1	A	199	MET	SD-CE	7.17	1.97	1.79
1	B	553	MET	SD-CE	6.93	1.96	1.79
1	A	728	MET	SD-CE	6.43	1.95	1.79
1	B	199	MET	SD-CE	6.36	1.95	1.79
1	B	75	MET	SD-CE	6.17	1.95	1.79
1	A	75	MET	SD-CE	6.14	1.95	1.79
1	A	498	ILE	CA-CB	6.12	1.61	1.54
1	A	270	VAL	CA-CB	-6.01	1.47	1.54
1	B	461	MET	SD-CE	-5.96	1.64	1.79
1	B	563	ILE	CA-CB	-5.94	1.47	1.54
1	A	432	GLY	C-O	-5.92	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	MET	SD-CE	5.89	1.94	1.79
1	A	715	MET	SD-CE	5.88	1.94	1.79
1	A	819	ILE	CA-CB	5.86	1.62	1.54
1	A	334	ILE	CA-CB	-5.46	1.47	1.54
1	A	256	MET	SD-CE	5.45	1.93	1.79
1	B	629	ALA	CA-CB	-5.26	1.45	1.53
1	B	123	PHE	CA-C	5.03	1.57	1.52

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	VAL	N-CA-C	-16.47	97.40	111.56
1	B	788	ILE	N-CA-C	-16.01	94.29	110.62
1	A	461	MET	N-CA-C	14.43	131.73	113.55
1	B	101	ILE	N-CA-C	13.72	123.60	110.42
1	B	211	VAL	N-CA-C	-13.11	101.26	111.62
1	A	767	PHE	N-CA-C	-12.02	91.92	109.59
1	B	698	ILE	N-CA-C	11.50	124.08	111.88
1	A	732	THR	N-CA-C	-11.30	98.71	111.82
1	A	457	SER	CA-C-N	10.60	133.09	119.84
1	A	457	SER	C-N-CA	10.60	133.09	119.84
1	A	831	TYR	N-CA-C	10.59	127.76	111.56
1	B	769	LYS	N-CA-C	-10.23	100.12	111.07
1	A	221	PHE	N-CA-C	10.11	126.39	111.02
1	B	3	GLU	N-CA-C	9.96	124.79	109.96
1	B	318	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	318	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	A	679	HIS	N-CA-C	9.68	125.09	113.28
1	B	694	GLY	N-CA-C	-9.62	103.63	115.08
1	A	48	LYS	N-CA-C	-9.51	90.54	110.80
1	A	755	GLU	N-CA-C	9.36	125.13	112.68
1	A	710	LEU	N-CA-C	9.33	123.06	108.79
1	A	833	LEU	CA-C-N	9.26	131.42	119.84
1	A	833	LEU	C-N-CA	9.26	131.42	119.84
1	A	691	PRO	CA-C-N	9.20	131.34	119.84
1	A	691	PRO	C-N-CA	9.20	131.34	119.84
1	A	389	GLN	CA-C-N	9.18	131.31	119.84
1	A	389	GLN	C-N-CA	9.18	131.31	119.84
1	B	538	LEU	N-CA-C	-9.07	98.56	110.53
1	A	612	GLU	N-CA-C	9.04	124.69	108.69
1	B	354	GLN	N-CA-C	-8.97	98.14	110.35
1	A	540	GLU	N-CA-C	-8.82	101.59	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	THR	N-CA-C	8.76	120.44	111.07
1	B	119	SER	CA-C-N	8.68	129.22	119.32
1	B	119	SER	C-N-CA	8.68	129.22	119.32
1	A	101	ILE	N-CA-C	8.55	127.12	109.34
1	A	897	LEU	N-CA-C	-8.50	101.96	111.82
1	B	30	GLU	N-CA-C	-8.46	95.11	108.90
1	A	253	ILE	CA-C-O	-8.42	113.08	121.67
1	B	389	GLN	CA-C-N	8.37	130.31	119.84
1	B	389	GLN	C-N-CA	8.37	130.31	119.84
1	B	125	GLU	CA-C-N	8.37	128.02	119.82
1	B	125	GLU	C-N-CA	8.37	128.02	119.82
1	B	732	THR	N-CA-C	-8.34	102.12	111.71
1	A	644	THR	N-CA-C	-8.31	102.22	111.28
1	B	221	PHE	N-CA-C	8.24	123.61	111.34
1	B	285	GLN	CA-C-N	8.15	128.93	119.47
1	B	285	GLN	C-N-CA	8.15	128.93	119.47
1	B	768	GLU	N-CA-C	-8.13	93.49	110.80
1	B	540	GLU	N-CA-C	-8.13	102.25	112.90
1	B	62	PHE	N-CA-C	8.10	123.46	113.50
1	A	516	VAL	N-CA-C	8.09	119.92	108.36
1	B	680	LEU	N-CA-C	8.03	127.90	110.80
1	B	174	GLY	N-CA-C	-8.00	103.48	115.32
1	B	501	GLU	N-CA-C	7.99	119.90	111.03
1	B	289	SER	N-CA-C	-7.82	99.99	110.55
1	B	486	LYS	N-CA-C	-7.71	103.14	112.54
1	A	106	THR	N-CA-C	-7.64	103.06	112.38
1	A	25	ARG	N-CA-C	7.59	122.06	109.46
1	B	398	GLU	N-CA-C	-7.53	98.28	109.42
1	A	680	LEU	N-CA-C	7.52	126.82	110.80
1	B	536	LYS	N-CA-C	-7.46	103.98	113.23
1	B	522	PHE	N-CA-C	7.40	123.51	111.37
1	A	159	VAL	N-CA-C	7.34	119.39	108.96
1	B	511	ASP	N-CA-C	7.32	121.23	110.17
1	B	217	ASN	N-CA-C	-7.32	103.38	113.56
1	A	768	GLU	N-CA-C	-7.32	95.21	110.80
1	B	163	SER	N-CA-C	7.29	120.14	108.41
1	A	411	ASP	N-CA-C	7.26	121.02	108.76
1	A	522	PHE	N-CA-C	7.22	126.17	110.80
1	B	779	ILE	N-CA-C	7.21	119.82	112.90
1	B	833	LEU	CA-C-N	7.20	128.84	119.84
1	B	833	LEU	C-N-CA	7.20	128.84	119.84
1	A	67	ASP	N-CA-C	-7.18	103.38	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	LEU	N-CA-C	7.18	120.62	110.50
1	A	258	GLY	N-CA-C	-7.12	96.32	113.18
1	A	769	LYS	N-CA-C	-7.10	103.15	111.03
1	A	789	ALA	N-CA-C	-7.10	103.55	111.71
1	A	698	ILE	N-CA-C	7.08	120.95	112.80
1	B	38	PHE	N-CA-C	7.07	121.07	109.06
1	A	828	GLU	N-CA-C	7.06	119.99	108.55
1	B	389	GLN	N-CA-C	7.06	119.85	109.62
1	B	514	LEU	N-CA-C	7.05	120.44	110.50
1	B	159	VAL	N-CA-C	7.04	119.08	108.80
1	A	182	ILE	CB-CA-C	-7.00	104.79	111.44
1	B	167	ALA	N-CA-C	-7.00	103.65	111.28
1	B	753	LEU	N-CA-C	6.97	118.96	111.36
1	A	505	ASN	CA-C-N	6.97	128.55	119.84
1	A	505	ASN	C-N-CA	6.97	128.55	119.84
1	B	798	GLY	CA-C-N	6.93	128.50	119.84
1	B	798	GLY	C-N-CA	6.93	128.50	119.84
1	A	388	VAL	N-CA-C	6.87	117.12	107.37
1	B	710	LEU	N-CA-C	6.86	119.65	108.26
1	A	435	LYS	N-CA-C	-6.80	99.59	109.59
1	B	641	PHE	N-CA-C	6.80	119.81	108.73
1	B	436	VAL	N-CA-C	6.76	117.58	108.11
1	A	436	VAL	N-CA-C	6.74	117.83	107.99
1	A	830	VAL	N-CA-C	6.73	117.03	108.82
1	A	507	ASN	N-CA-C	6.71	125.10	110.80
1	A	382	GLN	N-CA-C	-6.71	98.04	109.24
1	B	307	GLY	CA-C-N	6.70	126.66	120.03
1	B	307	GLY	C-N-CA	6.70	126.66	120.03
1	B	318	GLN	CG-CD-NE2	6.67	126.41	116.40
1	B	692	PRO	N-CA-C	6.65	121.60	114.68
1	B	331	VAL	N-CA-C	-6.64	103.84	110.62
1	A	318	GLN	CG-CD-NE2	6.62	126.34	116.40
1	A	864	HIS	N-CA-C	-6.62	104.06	111.28
1	A	827	GLY	N-CA-C	6.62	128.87	113.18
1	A	3	GLU	N-CA-C	6.58	124.83	110.80
1	B	828	GLU	N-CA-C	6.58	116.93	108.24
1	A	24	GLY	N-CA-C	6.58	128.78	113.18
1	B	178	VAL	N-CA-C	6.58	115.14	107.77
1	B	398	GLU	CA-C-N	6.55	128.03	119.84
1	B	398	GLU	C-N-CA	6.55	128.03	119.84
1	A	511	ASP	N-CA-C	6.49	120.06	110.46
1	B	596	TRP	N-CA-C	-6.49	103.90	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLU	N-CA-C	6.48	120.08	109.06
1	A	611	THR	N-CA-C	-6.46	100.00	109.18
1	B	293	ILE	N-CA-C	6.46	116.49	110.42
1	A	725	LEU	N-CA-C	6.46	119.13	109.25
1	B	781	SER	N-CA-C	-6.43	101.87	110.55
1	A	248	THR	N-CA-C	6.42	118.62	108.79
1	B	507	ASN	N-CA-C	6.41	124.45	110.80
1	A	495	ASN	N-CA-C	-6.40	105.23	113.16
1	B	706	LYS	N-CA-C	6.39	120.86	113.38
1	A	455	SER	N-CA-C	-6.38	100.12	110.20
1	B	455	SER	N-CA-C	-6.37	98.89	109.46
1	A	832	VAL	N-CA-C	6.36	122.57	109.34
1	A	100	GLU	N-CA-C	-6.35	101.54	110.50
1	A	794	GLY	N-CA-C	-6.35	98.12	113.18
1	A	163	SER	N-CA-C	6.33	118.61	108.41
1	A	454	TYR	N-CA-C	6.31	119.81	109.72
1	A	853	GLU	N-CA-C	-6.31	100.08	109.86
1	B	371	ASN	N-CA-C	6.30	117.95	111.14
1	B	679	HIS	N-CA-C	6.29	121.08	113.41
1	A	572	ASN	N-CA-C	6.27	118.95	108.73
1	A	694	GLY	N-CA-C	-6.27	105.83	114.67
1	A	88	PHE	N-CA-C	6.24	118.16	111.36
1	A	825	VAL	N-CA-C	6.17	117.35	107.73
1	A	720	TYR	N-CA-C	6.16	119.51	109.59
1	A	548	THR	N-CA-C	-6.15	105.27	112.89
1	B	13	ASP	N-CA-C	-6.12	105.66	112.57
1	B	275	ASP	N-CA-C	-6.11	104.54	111.14
1	B	438	PRO	N-CA-C	-6.09	101.70	111.38
1	A	408	MET	N-CA-C	6.07	119.14	108.75
1	A	836	ARG	N-CA-C	-6.06	101.96	110.50
1	B	113	PHE	N-CA-C	6.06	117.75	108.42
1	A	549	GLU	N-CA-C	-6.05	104.60	112.23
1	A	875	THR	CB-CA-C	-6.04	101.40	110.88
1	A	785	ALA	N-CA-C	-5.98	95.97	107.57
1	B	305	TYR	N-CA-C	5.97	116.45	108.38
1	A	133	ILE	CB-CA-C	-5.97	103.51	110.91
1	A	711	ASN	N-CA-C	5.96	119.19	107.98
1	B	456	CYS	N-CA-C	5.95	118.45	109.23
1	A	613	GLY	N-CA-C	-5.92	105.17	114.10
1	A	34	LYS	CA-C-N	5.92	125.85	119.76
1	A	34	LYS	C-N-CA	5.92	125.85	119.76
1	A	339	GLN	N-CA-C	5.91	121.78	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	837	GLU	N-CA-C	5.91	119.54	110.20
1	B	669	GLU	N-CA-C	-5.91	103.81	111.02
1	A	798	GLY	CA-C-N	5.90	127.21	119.84
1	A	798	GLY	C-N-CA	5.90	127.21	119.84
1	A	486	LYS	N-CA-C	-5.87	104.80	111.14
1	A	712	VAL	N-CA-C	5.87	117.19	109.21
1	B	158	ASN	N-CA-C	-5.83	99.23	108.73
1	B	530	ILE	N-CA-C	5.82	121.45	109.34
1	A	398	GLU	N-CA-C	-5.77	99.00	109.44
1	A	64	ASN	N-CA-C	-5.75	101.11	110.20
1	B	286	PRO	N-CA-C	5.75	122.15	113.81
1	B	382	GLN	N-CA-C	-5.72	102.30	110.59
1	A	418	SER	N-CA-C	-5.69	104.98	111.07
1	B	9	GLU	N-CA-C	-5.69	100.65	109.24
1	A	300	VAL	N-CA-C	5.69	121.17	109.34
1	B	16	PHE	N-CA-C	-5.68	99.15	108.41
1	B	625	ILE	CB-CA-C	-5.66	100.98	111.18
1	B	108	ILE	N-CA-C	5.65	115.71	106.72
1	B	110	VAL	N-CA-C	-5.65	97.58	109.34
1	B	407	VAL	N-CA-C	5.65	116.50	108.42
1	B	282	PHE	N-CA-C	-5.65	105.69	112.58
1	B	48	LYS	N-CA-C	-5.64	98.78	110.80
1	B	73	LYS	N-CA-C	-5.63	104.83	110.97
1	A	814	ALA	N-CA-C	-5.63	106.46	113.55
1	B	531	LYS	N-CA-C	-5.62	105.04	112.34
1	B	134	ASP	N-CA-C	5.61	120.12	112.88
1	A	383	GLY	N-CA-C	-5.58	103.97	112.51
1	A	289	SER	N-CA-C	-5.57	102.06	110.24
1	A	31	VAL	N-CA-C	5.55	116.09	107.99
1	B	842	GLY	N-CA-C	-5.53	100.24	112.17
1	A	852	THR	N-CA-C	5.52	118.69	110.52
1	B	505	ASN	N-CA-C	-5.51	97.62	109.81
1	B	618	LEU	N-CA-C	5.51	117.74	111.02
1	B	312	LEU	N-CA-C	5.47	122.46	110.80
1	B	785	ALA	N-CA-C	-5.47	97.69	107.98
1	B	310	SER	N-CA-C	-5.47	105.42	111.71
1	A	380	ILE	CA-C-N	5.45	126.65	119.84
1	A	380	ILE	C-N-CA	5.45	126.65	119.84
1	A	523	SER	N-CA-C	-5.44	99.21	110.80
1	B	541	MET	N-CA-C	-5.44	105.26	111.14
1	B	899	ASP	N-CA-C	-5.42	101.33	109.79
1	A	801	CYS	N-CA-C	-5.42	102.83	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASP	N-CA-C	-5.42	98.93	108.20
1	B	162	TRP	N-CA-C	5.42	118.29	109.24
1	A	842	GLY	N-CA-C	-5.41	100.35	113.18
1	B	832	VAL	CB-CA-C	-5.41	102.42	111.29
1	B	400	ILE	N-CA-CB	5.40	116.01	110.23
1	A	728	MET	N-CA-C	5.40	117.86	107.44
1	B	407	VAL	CB-CA-C	-5.39	101.47	111.18
1	A	722	GLU	N-CA-C	-5.38	97.91	109.81
1	B	832	VAL	N-CA-C	5.38	120.54	109.34
1	B	133	ILE	N-CA-C	-5.34	101.83	108.89
1	A	834	PRO	N-CA-C	5.34	123.47	112.47
1	B	818	ASN	N-CA-C	5.33	122.15	110.80
1	A	898	PHE	N-CA-C	5.33	122.14	110.80
1	B	508	LEU	N-CA-C	-5.32	99.48	110.80
1	B	720	TYR	N-CA-C	5.31	118.66	110.42
1	A	416	TYR	CA-C-N	5.31	124.94	119.05
1	A	416	TYR	C-N-CA	5.31	124.94	119.05
1	A	423	VAL	N-CA-C	5.30	117.27	112.29
1	A	757	GLU	N-CA-C	5.30	117.06	111.28
1	B	881	GLU	N-CA-C	-5.30	104.92	111.33
1	B	632	ILE	CB-CA-C	-5.28	105.22	111.81
1	B	214	THR	CA-C-O	-5.27	115.46	121.68
1	A	596	TRP	N-CA-C	-5.26	105.23	110.97
1	A	456	CYS	N-CA-C	5.25	117.80	109.50
1	A	708	TYR	N-CA-C	5.25	116.79	108.96
1	A	571	GLY	N-CA-C	-5.23	107.41	115.73
1	B	649	ASP	N-CA-C	-5.21	105.68	111.36
1	B	304	LYS	N-CA-C	5.20	117.56	110.55
1	B	391	TYR	CA-C-N	5.17	126.30	119.84
1	B	391	TYR	C-N-CA	5.17	126.30	119.84
1	A	360	SER	CA-C-N	5.17	124.79	119.05
1	A	360	SER	C-N-CA	5.17	124.79	119.05
1	B	226	VAL	CB-CA-C	-5.17	105.09	111.70
1	A	121	ASP	N-CA-C	-5.16	101.35	109.25
1	B	259	SER	N-CA-C	5.15	121.76	110.80
1	A	539	ASN	N-CA-C	5.14	121.76	110.80
1	B	691	PRO	N-CA-C	-5.14	104.42	110.70
1	B	345	LEU	N-CA-C	-5.14	105.37	110.97
1	B	548	THR	N-CA-C	-5.14	105.37	111.69
1	A	137	THR	N-CA-C	-5.12	101.36	109.59
1	B	271	LEU	N-CA-C	5.11	116.96	107.60
1	B	402	ASN	N-CA-C	5.11	114.58	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	GLY	N-CA-C	-5.09	107.06	114.90
1	A	569	ALA	N-CA-C	5.08	116.90	111.36
1	A	787	ASN	N-CA-C	5.08	121.63	110.80
1	A	183	ILE	N-CA-C	5.08	119.91	109.34
1	A	469	GLY	N-CA-C	5.08	117.30	111.36
1	B	189	MET	CB-CA-C	-5.02	105.05	110.98
1	B	504	HIS	N-CA-C	-5.02	107.10	113.43
1	B	415	LEU	N-CA-C	5.02	121.49	110.80
1	B	803	PHE	N-CA-C	-5.02	105.70	111.07
1	A	260	ARG	N-CA-C	-5.01	97.77	107.44

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	TYR	Sidechain
1	A	349	TYR	Sidechain
1	A	350	TYR	Sidechain
1	A	567	TYR	Sidechain
1	B	188	TYR	Sidechain
1	B	323	TYR	Sidechain
1	B	349	TYR	Sidechain
1	B	350	TYR	Sidechain
1	B	464	TYR	Sidechain
1	B	577	TYR	Sidechain

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	7380	0	7265	754	0
1	B	7380	0	7265	724	0
2	A	20	0	13	2	0
2	B	20	0	13	2	0
All	All	14800	0	14556	1478	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 50.

All (1478) 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:B:253:ILE:CG2	1:B:260:ARG:HB2	1.63	1.26
1:B:246:ARG:HG2	1:B:246:ARG:HH11	1.06	1.13
1:B:253:ILE:HG22	1:B:260:ARG:HB2	1.20	1.12
1:B:253:ILE:HG12	1:B:254:GLU:H	1.18	1.09
1:A:796:PHE:HB3	1:A:797:PRO:HD2	1.33	1.08
1:A:593:ALA:HA	1:A:670:MET:HE1	1.33	1.07
1:B:246:ARG:HH11	1:B:246:ARG:CG	1.71	1.04
1:B:489:MET:SD	1:B:553:MET:HB2	1.97	1.03
1:B:593:ALA:HA	1:B:670:MET:HE1	1.41	1.02
1:B:34:LYS:HD2	1:B:63:ALA:HA	1.44	0.99
1:B:149:PHE:HB3	1:B:197:LEU:HD11	1.42	0.98
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.45	0.97
1:A:857:LEU:HD23	1:A:857:LEU:H	1.27	0.97
1:B:514:LEU:HD21	1:B:530:ILE:HD11	1.47	0.96
1:A:162:TRP:HB3	1:A:188:TYR:HE2	1.29	0.93
1:A:347:MET:HE2	1:A:358:VAL:HG22	1.49	0.93
1:B:41:CYS:HB2	1:B:45:GLN:HG3	1.48	0.93
1:A:103:TYR:HE2	1:A:346:ASP:HA	1.33	0.93
1:B:356:GLN:H	1:B:356:GLN:HE21	1.14	0.92
1:B:489:MET:SD	1:B:553:MET:HE2	2.09	0.92
1:B:171:GLN:HG2	1:B:177:GLU:HG3	1.51	0.92
1:A:605:LEU:HB3	1:A:616:PHE:CE2	2.06	0.91
1:A:508:LEU:HD22	1:A:532:LYS:HA	1.54	0.90
1:A:164:ILE:H	1:A:164:ILE:HD12	1.37	0.89
1:B:246:ARG:HG2	1:B:246:ARG:NH1	1.87	0.88
1:B:644:THR:HB	1:B:692:PRO:O	1.73	0.88
1:B:347:MET:HE2	1:B:358:VAL:HG13	1.57	0.87
1:A:642:ARG:O	1:A:643:ASP:HB2	1.74	0.87
1:A:832:VAL:H	1:A:847:ALA:HA	1.39	0.87
1:A:303:LEU:HD23	1:A:323:TYR:HB2	1.56	0.87
1:A:661:PRO:O	1:A:665:ARG:HG3	1.74	0.87
1:B:164:ILE:HD12	1:B:164:ILE:H	1.39	0.87
1:B:253:ILE:HG22	1:B:260:ARG:CB	2.04	0.87
1:A:27:ARG:HG3	1:A:28:THR:H	1.39	0.86
1:A:752:MET:HG2	1:A:760:LEU:HD12	1.57	0.86
1:B:272:ASP:OD1	1:B:274:ILE:HG22	1.76	0.85
1:B:182:ILE:HA	1:B:185:LYS:HG3	1.55	0.85
1:A:788:ILE:HB	1:A:791:TYR:HD2	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HD13	1:A:52:ILE:H	1.39	0.84
1:A:728:MET:HE2	1:A:728:MET:HA	1.59	0.84
1:B:11:ILE:HD13	1:B:247:LYS:HG3	1.59	0.84
1:B:330:ARG:HA	1:B:333:GLN:NE2	1.91	0.84
1:A:162:TRP:HB3	1:A:188:TYR:CE2	2.12	0.84
1:B:547:ARG:HB3	1:B:547:ARG:NH1	1.93	0.84
1:B:855:THR:HB	1:B:857:LEU:CD2	2.08	0.83
1:B:356:GLN:HE21	1:B:356:GLN:N	1.76	0.83
1:A:163:SER:HB3	1:A:166:ILE:HD12	1.61	0.83
1:A:640:LYS:HD3	1:A:640:LYS:N	1.92	0.83
1:B:854:ILE:HG22	1:B:859:LYS:HB2	1.61	0.82
1:B:256:MET:SD	1:B:788:ILE:HG12	2.20	0.82
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.61	0.82
1:A:656:ARG:HH11	1:A:656:ARG:HB3	1.44	0.82
1:A:356:GLN:NE2	1:A:356:GLN:H	1.78	0.82
1:B:167:ALA:HA	1:B:176:ASP:HB2	1.62	0.81
1:B:291:ASP:HB3	1:B:302:LYS:HB2	1.61	0.81
1:B:727:ILE:O	1:B:728:MET:HE2	1.80	0.81
1:B:253:ILE:HG21	1:B:260:ARG:HB2	1.58	0.81
1:A:713:TRP:CH2	1:A:723:PRO:HG3	2.15	0.81
1:A:356:GLN:H	1:A:356:GLN:HE21	1.26	0.81
1:A:33:TYR:HD2	1:A:65:MET:HE1	1.46	0.81
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.63	0.81
1:A:117:VAL:HG13	1:A:132:PRO:O	1.81	0.80
1:B:303:LEU:HD23	1:B:323:TYR:HA	1.63	0.80
1:B:482:ARG:HG3	1:B:556:GLN:HG2	1.63	0.80
1:A:90:LEU:HD11	1:A:363:LYS:HE3	1.63	0.80
1:A:576:ARG:HD2	1:A:577:TYR:CE1	2.17	0.80
1:A:577:TYR:HD1	1:A:577:TYR:H	1.30	0.80
1:B:233:ILE:HG13	1:B:234:PHE:HD1	1.48	0.79
1:A:605:LEU:HB3	1:A:616:PHE:CD2	2.17	0.79
1:A:899:ASP:C	1:A:900:MET:SD	2.65	0.79
1:B:253:ILE:HG12	1:B:254:GLU:N	1.96	0.79
1:B:642:ARG:O	1:B:643:ASP:HB3	1.80	0.79
1:B:149:PHE:HB3	1:B:197:LEU:CD1	2.12	0.79
1:A:33:TYR:CD2	1:A:65:MET:HE1	2.18	0.79
1:B:233:ILE:HG13	1:B:234:PHE:CD1	2.17	0.79
1:B:880:LEU:HA	1:B:883:PHE:CE2	2.17	0.79
1:B:356:GLN:H	1:B:356:GLN:NE2	1.80	0.79
1:A:101:ILE:HG21	1:A:349:TYR:HB3	1.65	0.78
1:B:581:ARG:HG3	1:B:581:ARG:HH11	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLN:NE2	1:A:342:ASN:HB2	1.98	0.78
1:B:219:GLU:HA	1:B:223:ILE:HD12	1.64	0.78
1:B:434:PHE:CZ	1:B:460:GLY:HA2	2.18	0.78
1:B:195:LYS:H	1:B:195:LYS:HD2	1.48	0.78
1:A:320:TYR:HD1	1:A:321:ILE:HD12	1.49	0.78
1:A:593:ALA:CA	1:A:670:MET:HE1	2.14	0.78
1:B:3:GLU:HB3	1:B:21:ASP:HA	1.63	0.78
1:A:233:ILE:HG13	1:A:234:PHE:HD1	1.49	0.77
1:A:421:ARG:HD2	1:A:475:ILE:HG22	1.66	0.77
1:B:112:ASN:HD22	1:B:113:PHE:N	1.82	0.77
1:A:763:TYR:O	1:A:766:GLU:HB2	1.85	0.77
1:B:4:PHE:HA	1:B:97:TYR:HE2	1.47	0.77
1:A:421:ARG:HD2	1:A:475:ILE:CG2	2.14	0.77
1:B:253:ILE:CG1	1:B:254:GLU:H	1.95	0.77
1:B:481:GLN:HE21	1:B:559:ARG:NH1	1.83	0.77
1:B:414:SER:O	1:B:417:PRO:HD2	1.85	0.77
1:A:830:VAL:HG12	1:A:831:TYR:H	1.48	0.76
1:A:214:THR:HG22	1:A:215:GLY:H	1.48	0.76
1:A:9:GLU:HG2	1:A:266:PHE:HD1	1.48	0.76
1:B:295:GLU:O	1:B:299:ASN:HA	1.86	0.76
1:B:511:ASP:HB2	1:B:534:SER:OG	1.86	0.76
1:A:763:TYR:O	1:A:763:TYR:HD1	1.67	0.76
1:B:748:CYS:O	1:B:752:MET:HG3	1.86	0.76
1:B:832:VAL:HG22	1:B:847:ALA:HB2	1.67	0.76
1:A:818:ASN:HA	1:A:822:PRO:HG3	1.68	0.76
1:B:423:VAL:HB	1:B:425:ILE:HG13	1.67	0.76
1:B:645:ASN:HD21	1:B:719:ARG:HH11	1.31	0.76
1:A:546:GLN:O	1:A:550:VAL:HG23	1.86	0.75
1:A:788:ILE:HB	1:A:791:TYR:CD2	2.21	0.75
1:A:163:SER:OG	1:A:165:GLU:HG2	1.86	0.74
1:A:647:TRP:O	1:A:650:PHE:HB3	1.87	0.74
1:B:65:MET:HE2	1:B:88:PHE:HB3	1.69	0.74
1:B:250:VAL:HG12	1:B:251:LYS:H	1.53	0.74
1:B:880:LEU:HA	1:B:883:PHE:CD2	2.22	0.74
1:B:661:PRO:O	1:B:665:ARG:HG3	1.87	0.74
1:A:315:SER:O	1:A:316:ASN:HB2	1.87	0.74
1:A:577:TYR:N	1:A:577:TYR:CD1	2.54	0.74
1:B:404:TYR:CZ	1:B:618:LEU:HD21	2.22	0.74
1:A:291:ASP:HB3	1:A:302:LYS:HB2	1.68	0.74
1:B:647:TRP:O	1:B:650:PHE:HB3	1.88	0.73
1:B:832:VAL:HA	1:B:846:ILE:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:HD1	1:A:189:MET:N	1.87	0.73
1:A:131:HIS:HB3	1:A:132:PRO:HD2	1.69	0.73
1:B:806:ARG:HH21	1:B:843:ASP:HA	1.53	0.73
1:A:748:CYS:O	1:A:752:MET:HG3	1.89	0.73
1:A:214:THR:HG22	1:A:215:GLY:N	2.03	0.73
1:A:356:GLN:HE21	1:A:356:GLN:N	1.87	0.73
1:B:514:LEU:HD21	1:B:530:ILE:CD1	2.19	0.73
1:A:247:LYS:O	1:A:266:PHE:HB2	1.88	0.72
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.24	0.72
1:A:523:SER:HB3	1:A:526:ILE:HG12	1.72	0.72
1:B:18:ARG:NH2	1:B:211:VAL:HA	2.04	0.72
1:A:123:PHE:CE2	1:A:828:GLU:HB3	2.24	0.72
1:A:796:PHE:HB3	1:A:797:PRO:CD	2.16	0.72
1:B:147:TYR:HD1	1:B:147:TYR:N	1.88	0.72
1:B:281:SER:O	1:B:282:PHE:HB2	1.90	0.72
1:B:504:HIS:O	1:B:506:PRO:HD3	1.90	0.71
1:B:514:LEU:HD12	1:B:541:MET:SD	2.29	0.71
1:A:740:ALA:HB2	1:A:778:SER:HB2	1.72	0.71
1:B:831:TYR:CE2	1:B:850:SER:HA	2.25	0.71
1:A:834:PRO:HB3	1:A:867:ASP:HB3	1.71	0.71
1:A:116:GLU:HB2	1:A:135:ALA:HB3	1.72	0.71
1:B:606:ASN:HB2	1:B:611:THR:O	1.89	0.71
1:B:855:THR:HB	1:B:857:LEU:HD21	1.71	0.71
1:A:773:GLN:HA	1:B:78:ILE:HD11	1.73	0.71
1:A:233:ILE:HG13	1:A:234:PHE:CD1	2.26	0.71
1:A:680:LEU:HD23	1:A:680:LEU:H	1.55	0.71
1:B:246:ARG:CG	1:B:246:ARG:NH1	2.41	0.71
1:B:339:GLN:HE21	1:B:339:GLN:HA	1.56	0.71
1:B:834:PRO:O	1:B:835:LEU:HD23	1.91	0.71
1:A:291:ASP:CB	1:A:302:LYS:HB2	2.21	0.70
1:B:169:LYS:HB2	1:B:175:GLY:HA3	1.71	0.70
1:A:897:LEU:H	1:A:897:LEU:HD12	1.55	0.70
1:B:526:ILE:O	1:B:530:ILE:HG12	1.90	0.70
1:B:544:ARG:O	1:B:548:THR:HG23	1.90	0.70
1:A:873:GLU:HA	1:A:877:ILE:HD12	1.73	0.70
1:A:280:PHE:CD1	1:A:280:PHE:N	2.58	0.70
1:B:222:ASP:O	1:B:226:VAL:HG23	1.92	0.70
1:B:866:MET:HE2	1:B:868:TYR:CE1	2.26	0.70
1:A:547:ARG:HA	1:A:550:VAL:HG23	1.74	0.69
1:A:643:ASP:HB3	1:A:646:HIS:H	1.57	0.69
1:A:47:THR:HB	1:A:48:LYS:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ARG:O	1:A:810:THR:HG22	1.92	0.69
1:B:541:MET:HE3	1:B:541:MET:HA	1.74	0.69
1:A:173:GLN:H	1:A:173:GLN:HE21	1.37	0.69
1:A:162:TRP:HE3	1:A:188:TYR:CD2	2.09	0.69
1:B:213:LEU:HB2	1:B:268:ILE:HD11	1.75	0.69
1:A:188:TYR:C	1:A:189:MET:HG3	2.18	0.69
1:A:414:SER:HB2	1:A:417:PRO:HG3	1.73	0.69
1:B:188:TYR:HE1	1:B:190:PRO:HB3	1.58	0.69
1:B:707:ARG:HH11	1:B:707:ARG:HB2	1.58	0.69
1:B:4:PHE:HA	1:B:97:TYR:CE2	2.27	0.69
1:A:162:TRP:CE3	1:A:188:TYR:CD2	2.81	0.69
1:A:727:ILE:HG22	1:A:733:GLN:HE22	1.58	0.69
1:A:878:LYS:O	1:A:881:GLU:HB3	1.91	0.69
1:B:597:ILE:HB	1:B:667:PHE:CE1	2.28	0.69
1:B:788:ILE:HG22	1:B:791:TYR:CD2	2.27	0.69
1:A:232:ASN:N	1:A:232:ASN:HD22	1.91	0.69
1:B:223:ILE:HB	1:B:224:PRO:CD	2.20	0.69
1:B:402:ASN:CG	1:B:403:ARG:H	2.01	0.68
1:B:449:ARG:NH1	1:B:451:SER:O	2.25	0.68
1:A:145:ARG:HH21	1:A:185:LYS:HD2	1.57	0.68
1:A:381:PRO:HD2	1:A:576:ARG:HD3	1.75	0.68
1:A:167:ALA:HA	1:A:176:ASP:HB2	1.75	0.68
1:A:644:THR:HB	1:A:692:PRO:O	1.93	0.68
1:B:303:LEU:HD23	1:B:323:TYR:CA	2.23	0.68
1:B:767:PHE:HA	1:B:770:GLU:HG2	1.76	0.68
1:B:873:GLU:HA	1:B:877:ILE:HD13	1.75	0.68
1:A:776:TYR:O	1:A:779:ILE:HG12	1.92	0.68
1:A:821:ALA:N	1:A:822:PRO:HD2	2.09	0.68
1:B:877:ILE:HD12	1:B:877:ILE:H	1.58	0.68
1:B:53:TYR:HE1	1:B:428:GLU:HA	1.59	0.68
1:B:147:TYR:N	1:B:147:TYR:CD1	2.58	0.68
1:B:538:LEU:O	1:B:539:ASN:HB2	1.91	0.68
1:A:109:ARG:HA	1:A:142:ILE:HG12	1.76	0.68
1:A:162:TRP:CE3	1:A:188:TYR:HD2	2.12	0.68
1:A:403:ARG:HH11	1:A:888:LYS:HB2	1.58	0.68
1:B:460:GLY:O	1:B:461:MET:HG2	1.94	0.68
1:B:750:ARG:HG2	1:B:754:GLN:OE1	1.94	0.68
1:B:897:LEU:HD12	1:B:897:LEU:H	1.59	0.68
1:B:162:TRP:HB3	1:B:188:TYR:HE2	1.60	0.67
1:A:105:HIS:HA	1:A:108:ILE:HG13	1.76	0.67
1:A:120:PRO:HD3	1:A:156:TYR:HE2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:SER:HG	1:A:165:GLU:HG2	1.57	0.67
1:A:270:VAL:O	1:A:271:LEU:HD23	1.94	0.67
1:A:596:TRP:CG	1:A:670:MET:HE3	2.28	0.67
1:A:820:ASP:C	1:A:822:PRO:HD2	2.19	0.67
1:B:389:GLN:NE2	1:B:390:PRO:HD2	2.09	0.67
1:A:163:SER:OG	1:A:166:ILE:HG13	1.94	0.67
1:B:97:TYR:HB3	1:B:101:ILE:HD11	1.77	0.67
1:B:481:GLN:HE21	1:B:559:ARG:HH11	1.41	0.67
1:B:52:ILE:HD13	1:B:52:ILE:H	1.59	0.67
1:A:353:ILE:HG12	1:A:354:GLN:N	2.07	0.67
1:A:655:ALA:HA	1:A:659:MET:HB2	1.75	0.67
1:B:632:ILE:O	1:B:635:LYS:HB3	1.95	0.67
1:A:280:PHE:N	1:A:280:PHE:HD1	1.90	0.67
1:A:830:VAL:HG12	1:A:831:TYR:N	2.09	0.67
1:A:330:ARG:HA	1:A:333:GLN:HE21	1.59	0.66
1:B:162:TRP:CE3	1:B:188:TYR:CD2	2.84	0.66
1:B:869:THR:O	1:B:873:GLU:HG3	1.96	0.66
1:A:804:HIS:ND1	1:A:804:HIS:N	2.40	0.66
1:B:747:GLU:HG3	1:B:763:TYR:CE2	2.30	0.66
1:A:172:GLU:H	1:A:172:GLU:CD	2.02	0.66
1:B:835:LEU:HD12	1:B:839:ASN:CG	2.20	0.66
1:A:82:ALA:O	1:A:382:GLN:HB3	1.95	0.66
1:B:449:ARG:HH12	1:B:452:ASP:HA	1.60	0.66
1:A:52:ILE:H	1:A:52:ILE:CD1	2.07	0.66
1:A:691:PRO:HB3	1:A:697:GLY:O	1.96	0.66
1:A:741:VAL:O	1:A:744:ALA:HB3	1.96	0.66
1:B:499:ILE:HG21	1:B:542:LEU:HB2	1.78	0.66
1:B:663:ILE:HD13	1:B:683:MET:HE3	1.77	0.66
1:B:191:PHE:CD1	1:B:197:LEU:HD13	2.31	0.66
1:A:833:LEU:O	1:A:845:CYS:HA	1.96	0.65
1:A:727:ILE:HG22	1:A:733:GLN:NE2	2.09	0.65
1:A:321:ILE:O	1:A:325:ILE:HD12	1.97	0.65
1:A:730:LEU:O	1:A:731:GLU:HG2	1.95	0.65
1:B:404:TYR:CE2	1:B:618:LEU:HD21	2.30	0.65
1:B:421:ARG:NH2	1:B:476:THR:HG23	2.12	0.65
1:B:593:ALA:CA	1:B:670:MET:HE1	2.23	0.65
1:A:120:PRO:HD3	1:A:156:TYR:CE2	2.32	0.65
1:A:581:ARG:HG3	1:A:581:ARG:HH11	1.61	0.65
1:A:303:LEU:HD23	1:A:323:TYR:CB	2.27	0.65
1:B:391:TYR:HB2	1:B:392:PRO:HD2	1.78	0.65
1:B:757:GLU:O	1:B:761:GLN:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:LEU:O	1:B:813:ARG:HG3	1.95	0.65
1:A:489:MET:CE	1:A:490:LEU:HG	2.27	0.65
1:B:6:LEU:HB2	1:B:18:ARG:O	1.97	0.65
1:A:513:PRO:HG3	1:A:537:SER:O	1.98	0.64
1:A:640:LYS:HD3	1:A:640:LYS:H	1.62	0.64
1:A:416:TYR:N	1:A:417:PRO:HD2	2.10	0.64
1:A:577:TYR:HD1	1:A:577:TYR:N	1.92	0.64
1:B:163:SER:OG	1:B:166:ILE:HG13	1.96	0.64
1:A:454:TYR:HD2	1:A:462:MET:HG2	1.62	0.64
1:A:489:MET:HE2	1:A:490:LEU:HG	1.79	0.64
1:A:738:PRO:O	1:A:742:GLN:HG3	1.97	0.64
1:A:765:LYS:O	1:A:768:GLU:HB3	1.97	0.64
1:B:205:TRP:HZ3	1:B:242:LEU:O	1.79	0.64
1:A:152:LEU:HD11	1:A:190:PRO:HB2	1.78	0.64
1:B:83:LEU:N	1:B:83:LEU:HD12	2.13	0.64
1:B:647:TRP:HZ3	1:B:693:LEU:HB2	1.60	0.64
1:A:74:ARG:O	1:A:77:ASP:HB2	1.97	0.64
1:A:702:TRP:CE3	1:A:708:TYR:HB3	2.32	0.64
1:A:544:ARG:O	1:A:548:THR:HG23	1.96	0.64
1:A:19:TYR:CD1	1:A:19:TYR:N	2.66	0.64
1:A:128:GLN:N	1:A:128:GLN:OE1	2.31	0.64
1:B:475:ILE:HD11	1:B:566:LEU:HD23	1.78	0.64
1:A:103:TYR:CE2	1:A:346:ASP:HA	2.23	0.63
1:A:170:LEU:HB2	1:A:173:GLN:NE2	2.13	0.63
1:A:679:HIS:O	1:A:681:MET:N	2.28	0.63
1:B:193:ASN:HD22	1:B:195:LYS:HD3	1.62	0.63
1:B:270:VAL:C	1:B:271:LEU:HD23	2.23	0.63
1:A:647:TRP:HZ3	1:A:693:LEU:HB2	1.63	0.63
1:B:75:MET:HG3	1:B:82:ALA:HB2	1.80	0.63
1:B:268:ILE:C	1:B:268:ILE:HD12	2.23	0.63
1:B:647:TRP:HH2	1:B:691:PRO:O	1.80	0.63
1:B:867:ASP:HB3	1:B:870:VAL:HB	1.79	0.63
1:A:133:ILE:HD12	1:A:198:LEU:HD21	1.81	0.63
1:A:618:LEU:O	1:A:618:LEU:HD22	1.98	0.63
1:A:643:ASP:HB3	1:A:646:HIS:HB2	1.80	0.63
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.64	0.63
1:A:835:LEU:HD12	1:A:845:CYS:H	1.64	0.63
1:B:707:ARG:HB2	1:B:707:ARG:NH1	2.13	0.63
1:B:511:ASP:HB3	1:B:537:SER:OG	1.98	0.63
1:A:857:LEU:H	1:A:857:LEU:CD2	2.06	0.63
1:B:228:ASN:O	1:B:232:ASN:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:TYR:HD1	1:A:763:TYR:C	2.07	0.63
1:A:832:VAL:HA	1:A:846:ILE:O	1.99	0.63
1:B:897:LEU:HD12	1:B:897:LEU:N	2.14	0.63
1:B:374:LYS:HA	2:B:999:GMP:N2	2.13	0.62
1:B:663:ILE:HG22	1:B:664:ASP:N	2.14	0.62
1:A:135:ALA:O	1:A:136:ILE:HG13	1.99	0.62
1:A:317:HIS:O	1:A:321:ILE:HD13	1.99	0.62
1:B:42:PRO:O	1:B:45:GLN:HG2	1.98	0.62
1:B:164:ILE:H	1:B:164:ILE:CD1	2.10	0.62
1:B:303:LEU:HD22	1:B:326:ILE:HG13	1.79	0.62
1:B:772:ARG:HA	1:B:868:TYR:CE2	2.34	0.62
1:A:35:PRO:HG2	1:A:62:PHE:HB2	1.79	0.62
1:A:112:ASN:HD22	1:A:113:PHE:N	1.97	0.62
1:A:857:LEU:HD23	1:A:857:LEU:N	2.07	0.62
1:B:105:HIS:C	1:B:107:LYS:H	2.06	0.62
1:B:117:VAL:HG22	1:B:133:ILE:HA	1.80	0.62
1:B:680:LEU:HD23	1:B:680:LEU:H	1.65	0.62
1:B:180:SER:O	1:B:183:ILE:HG12	1.98	0.62
1:B:104:ASP:CG	1:B:107:LYS:HD2	2.24	0.62
1:A:625:ILE:HD11	1:A:683:MET:SD	2.40	0.62
1:B:547:ARG:HB3	1:B:547:ARG:HH11	1.60	0.62
1:A:9:GLU:HG2	1:A:266:PHE:CD1	2.33	0.61
1:B:92:TYR:CD1	1:B:92:TYR:C	2.78	0.61
1:B:125:GLU:HB3	1:B:128:GLN:OE1	2.00	0.61
1:B:139:TYR:CZ	1:B:141:SER:HA	2.34	0.61
1:B:653:LYS:HA	1:B:656:ARG:NH1	2.15	0.61
1:A:279:LYS:HB2	1:A:280:PHE:CD1	2.35	0.61
1:A:728:MET:HA	1:A:728:MET:CE	2.30	0.61
1:A:178:VAL:HG12	1:A:183:ILE:HD11	1.81	0.61
1:B:140:ASP:OD1	1:B:142:ILE:HB	2.00	0.61
1:B:584:THR:O	1:B:588:THR:HG23	2.00	0.61
1:B:426:SER:HB3	1:B:429:THR:HG23	1.83	0.61
1:A:846:ILE:HG22	1:A:847:ALA:N	2.16	0.61
1:A:37:LEU:CD1	1:A:72:ILE:HD11	2.31	0.61
1:B:434:PHE:CE2	1:B:460:GLY:HA2	2.35	0.61
1:B:592:MET:SD	1:B:670:MET:HE2	2.41	0.61
1:A:654:PHE:C	1:A:654:PHE:HD1	2.09	0.61
1:B:51:ASP:C	1:B:53:TYR:H	2.08	0.61
1:B:645:ASN:HD21	1:B:719:ARG:NH1	1.97	0.61
1:A:186:ILE:HG22	1:A:187:ILE:N	2.15	0.60
1:A:834:PRO:CB	1:A:867:ASP:HB3	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ILE:HD13	1:B:52:ILE:N	2.16	0.60
1:B:116:GLU:HB3	1:B:320:TYR:OH	2.01	0.60
1:B:303:LEU:HD11	1:B:319:ARG:HE	1.65	0.60
1:B:653:LYS:HD2	1:B:656:ARG:NH1	2.16	0.60
1:A:767:PHE:CD1	1:A:767:PHE:C	2.79	0.60
1:A:855:THR:CG2	1:A:857:LEU:HD21	2.31	0.60
1:A:27:ARG:HG3	1:A:28:THR:N	2.15	0.60
1:A:654:PHE:C	1:A:654:PHE:CD1	2.77	0.60
1:A:803:PHE:O	1:A:806:ARG:HB3	2.00	0.60
1:B:20:ILE:HG23	1:B:24:GLY:HA2	1.83	0.60
1:B:730:LEU:O	1:B:731:GLU:HG2	2.01	0.60
1:A:164:ILE:H	1:A:164:ILE:CD1	2.09	0.60
1:A:205:TRP:CH2	1:A:210:PRO:HD2	2.37	0.60
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.83	0.60
1:B:247:LYS:O	1:B:266:PHE:HB2	2.01	0.60
1:B:647:TRP:CZ3	1:B:693:LEU:HB2	2.37	0.60
1:A:231:LYS:O	1:A:235:GLY:N	2.34	0.60
1:A:576:ARG:HD2	1:A:577:TYR:HE1	1.64	0.60
1:A:859:LYS:O	1:A:863:LEU:HD12	2.01	0.60
1:B:110:VAL:HG12	1:B:111:ALA:N	2.16	0.60
1:B:806:ARG:NH2	1:B:843:ASP:HA	2.15	0.60
1:A:173:GLN:NE2	1:A:173:GLN:N	2.49	0.60
1:A:265:LEU:HB3	1:A:268:ILE:HD11	1.82	0.60
1:A:281:SER:O	1:A:282:PHE:HB2	2.01	0.60
1:A:656:ARG:HB3	1:A:656:ARG:NH1	2.15	0.60
1:B:406:TYR:HE1	1:B:647:TRP:CZ2	2.19	0.60
1:B:518:TYR:CE2	1:B:544:ARG:HB3	2.36	0.60
1:A:406:TYR:CB	1:A:629:ALA:HB3	2.32	0.60
1:B:621:ASP:O	1:B:623:ASP:N	2.35	0.60
1:A:173:GLN:HE21	1:A:173:GLN:N	2.00	0.60
1:B:647:TRP:CH2	1:B:691:PRO:O	2.55	0.60
1:A:657:GLU:O	1:A:661:PRO:HG2	2.01	0.60
1:A:410:PHE:O	1:A:624:SER:HA	2.02	0.59
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.37	0.59
1:A:366:ASP:OD1	1:A:576:ARG:NH1	2.35	0.59
1:A:763:TYR:C	1:A:763:TYR:CD1	2.79	0.59
1:B:362:ILE:HG22	1:B:363:LYS:N	2.17	0.59
1:B:449:ARG:NH1	1:B:452:ASP:HA	2.16	0.59
1:B:642:ARG:O	1:B:646:HIS:HB2	2.02	0.59
1:B:685:ARG:HG2	1:B:686:GLU:H	1.68	0.59
1:A:538:LEU:O	1:A:540:GLU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:GLN:HG2	1:A:824:VAL:N	2.16	0.59
1:B:318:GLN:HA	1:B:318:GLN:OE1	2.01	0.59
1:B:370:PHE:CD1	1:B:370:PHE:C	2.78	0.59
1:A:529:LYS:O	1:A:533:LEU:HD13	2.02	0.59
1:A:597:ILE:O	1:A:601:VAL:HG23	2.02	0.59
1:A:605:LEU:HD13	1:A:616:PHE:HD2	1.68	0.59
1:A:776:TYR:CE1	1:A:777:ILE:HG13	2.37	0.59
1:B:181:GLU:CD	1:B:181:GLU:H	2.10	0.59
1:B:479:PHE:CD1	1:B:479:PHE:C	2.80	0.59
1:A:823:GLN:HG2	1:A:824:VAL:H	1.66	0.59
1:A:4:PHE:HA	1:A:97:TYR:CE2	2.38	0.59
1:B:103:TYR:OH	1:B:346:ASP:HB2	2.03	0.59
1:B:163:SER:HG	1:B:165:GLU:HG2	1.67	0.59
1:A:303:LEU:HD11	1:A:319:ARG:HE	1.68	0.59
1:B:604:TYR:CD1	1:B:604:TYR:C	2.81	0.59
1:A:126:PRO:O	1:A:228:ASN:ND2	2.36	0.59
1:A:272:ASP:CG	1:A:274:ILE:HG22	2.28	0.59
1:A:389:GLN:HA	1:A:389:GLN:HE21	1.68	0.59
1:A:597:ILE:HD13	1:A:667:PHE:CE1	2.38	0.59
1:A:832:VAL:H	1:A:847:ALA:CA	2.14	0.59
1:A:835:LEU:H	1:A:867:ASP:H	1.51	0.59
1:B:402:ASN:HA	1:B:886:ALA:O	2.03	0.59
1:B:455:SER:OG	1:B:676:ASN:HA	2.02	0.59
1:B:443:ILE:HG22	1:B:592:MET:HG3	1.85	0.59
1:B:679:HIS:O	1:B:681:MET:N	2.34	0.59
1:A:253:ILE:HG22	1:A:254:GLU:N	2.17	0.59
1:B:245:HIS:CE1	1:B:267:GLY:HA3	2.37	0.59
1:A:295:GLU:O	1:A:299:ASN:N	2.35	0.58
1:A:873:GLU:HA	1:A:877:ILE:CD1	2.33	0.58
1:B:685:ARG:HG2	1:B:686:GLU:N	2.17	0.58
1:B:846:ILE:HG22	1:B:847:ALA:H	1.68	0.58
1:A:145:ARG:HB2	1:A:147:TYR:CE1	2.38	0.58
1:A:415:LEU:HD22	1:A:623:ASP:HB3	1.86	0.58
1:B:481:GLN:NE2	1:B:559:ARG:NH1	2.51	0.58
1:B:645:ASN:ND2	1:B:719:ARG:HH11	1.99	0.58
1:B:647:TRP:CD1	1:B:648:VAL:N	2.71	0.58
1:A:802:PRO:HB2	1:A:804:HIS:ND1	2.18	0.58
1:B:33:TYR:HB3	1:B:65:MET:HE3	1.85	0.58
1:A:842:GLY:O	1:A:843:ASP:HB2	2.03	0.58
1:A:407:VAL:HG12	1:A:408:MET:N	2.19	0.58
1:A:13:ASP:OD1	1:A:66:ARG:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:TYR:CD2	1:A:462:MET:HG2	2.38	0.58
1:A:663:ILE:HG21	1:A:683:MET:HE2	1.85	0.58
1:A:736:SER:HA	1:A:782:VAL:O	2.02	0.58
1:A:126:PRO:HG3	1:A:221:PHE:CD1	2.38	0.58
1:B:169:LYS:HB2	1:B:175:GLY:CA	2.33	0.58
1:B:658:ARG:C	1:B:661:PRO:HD2	2.29	0.58
1:B:830:VAL:HG12	1:B:831:TYR:N	2.19	0.58
1:A:116:GLU:HG3	1:A:324:ASN:ND2	2.18	0.58
1:A:427:PRO:O	1:A:430:ILE:HG22	2.03	0.58
1:B:74:ARG:O	1:B:77:ASP:HB2	2.03	0.58
1:B:1:MET:HE3	1:B:22:SER:O	2.03	0.58
1:B:52:ILE:H	1:B:52:ILE:CD1	2.17	0.58
1:B:579:ASP:HB3	1:B:582:ASN:ND2	2.19	0.58
1:A:679:HIS:O	1:A:679:HIS:CG	2.57	0.57
1:A:767:PHE:HA	1:A:770:GLU:HG2	1.85	0.57
1:B:78:ILE:HG22	1:B:79:GLY:N	2.17	0.57
1:B:494:ARG:O	1:B:498:ILE:HD13	2.04	0.57
1:A:83:LEU:HD12	1:A:83:LEU:N	2.19	0.57
1:A:649:ASP:O	1:A:652:ASP:HB3	2.04	0.57
1:A:772:ARG:HG3	1:A:772:ARG:HH11	1.67	0.57
1:B:406:TYR:HB3	1:B:629:ALA:HB3	1.86	0.57
1:A:270:VAL:C	1:A:271:LEU:HD23	2.29	0.57
1:A:291:ASP:HB3	1:A:302:LYS:HD2	1.85	0.57
1:A:320:TYR:HD1	1:A:321:ILE:CD1	2.14	0.57
1:A:380:ILE:HG12	2:A:999:GMP:O6	2.04	0.57
1:A:830:VAL:HG12	1:A:847:ALA:HB1	1.85	0.57
1:B:433:THR:H	1:B:462:MET:HE2	1.69	0.57
1:B:455:SER:O	1:B:462:MET:HA	2.05	0.57
1:B:830:VAL:CG1	1:B:831:TYR:N	2.66	0.57
1:A:163:SER:H	1:A:318:GLN:HE22	1.53	0.57
1:A:523:SER:HB3	1:A:526:ILE:CG1	2.35	0.57
1:B:899:ASP:C	1:B:901:PHE:H	2.12	0.57
1:A:406:TYR:HB2	1:A:629:ALA:HB3	1.86	0.57
1:A:492:ALA:HA	1:A:495:ASN:HB2	1.86	0.57
1:A:493:GLN:HB2	1:A:549:GLU:HG3	1.87	0.57
1:A:90:LEU:HD11	1:A:363:LYS:CE	2.33	0.57
1:A:767:PHE:C	1:A:767:PHE:HD1	2.12	0.57
1:B:431:ALA:HB1	1:B:454:TYR:CE2	2.39	0.57
1:A:353:ILE:HD11	1:A:357:SER:HB2	1.86	0.57
1:A:432:GLY:HA3	1:A:462:MET:HE2	1.87	0.57
1:A:589:PHE:O	1:A:592:MET:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ASN:OD1	1:A:841:PHE:HB2	2.04	0.57
1:A:604:TYR:O	1:A:607:GLU:HB3	2.05	0.57
1:B:188:TYR:CD1	1:B:190:PRO:HD3	2.40	0.57
1:B:425:ILE:HG22	1:B:425:ILE:O	2.04	0.57
1:A:335:ASP:O	1:A:339:GLN:N	2.37	0.57
1:A:356:GLN:C	1:A:358:VAL:H	2.12	0.57
1:A:595:GLN:HA	1:A:598:GLU:HB3	1.86	0.57
1:A:651:LEU:O	1:A:654:PHE:HB3	2.05	0.57
1:A:685:ARG:NH2	1:A:716:GLU:H	2.02	0.57
1:A:52:ILE:HD11	1:A:381:PRO:HG3	1.85	0.57
1:B:504:HIS:C	1:B:506:PRO:HD3	2.30	0.57
1:B:602:ASN:OD1	1:B:616:PHE:HB2	2.05	0.57
1:B:752:MET:HG2	1:B:760:LEU:HD12	1.86	0.57
1:B:807:GLY:O	1:B:810:THR:HG22	2.05	0.57
1:A:121:ASP:HB2	1:A:826:GLU:OE1	2.05	0.56
1:A:403:ARG:HH22	1:A:889:LEU:HD21	1.69	0.56
1:A:605:LEU:HB3	1:A:616:PHE:HE2	1.65	0.56
1:A:752:MET:CG	1:A:760:LEU:HD12	2.32	0.56
1:A:101:ILE:HG22	1:A:102:LYS:N	2.20	0.56
1:A:844:LYS:O	1:A:845:CYS:HB3	2.03	0.56
1:A:4:PHE:HA	1:A:97:TYR:HE2	1.71	0.56
1:A:469:GLY:O	1:A:472:PRO:HG2	2.06	0.56
1:B:305:TYR:OH	1:B:309:ILE:HB	2.05	0.56
1:B:432:GLY:O	1:B:433:THR:HB	2.06	0.56
1:B:702:TRP:CZ3	1:B:708:TYR:CD2	2.93	0.56
1:B:772:ARG:HA	1:B:868:TYR:HE2	1.69	0.56
1:A:894:LYS:HA	1:A:894:LYS:HE2	1.86	0.56
1:B:711:ASN:HB2	1:B:753:LEU:HB3	1.87	0.56
1:A:129:ALA:HB1	1:A:225:TYR:CE1	2.41	0.56
1:A:303:LEU:HD23	1:A:323:TYR:CA	2.35	0.56
1:A:308:PRO:HD2	1:A:311:LYS:CG	2.36	0.56
1:B:101:ILE:HG21	1:B:349:TYR:HD1	1.69	0.56
1:A:414:SER:HB2	1:A:417:PRO:CG	2.34	0.56
1:A:291:ASP:HB3	1:A:302:LYS:CB	2.36	0.56
1:B:205:TRP:CZ3	1:B:242:LEU:O	2.58	0.56
1:A:228:ASN:O	1:A:232:ASN:ND2	2.39	0.56
1:A:506:PRO:HG3	1:A:535:ALA:HB2	1.88	0.56
1:B:162:TRP:CE3	1:B:188:TYR:HD2	2.23	0.56
1:B:309:ILE:HD13	1:B:309:ILE:O	2.06	0.56
1:B:329:TYR:O	1:B:332:LEU:HB2	2.06	0.56
1:B:604:TYR:CD1	1:B:605:LEU:HD23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ILE:HD13	1:B:589:PHE:HB3	1.88	0.56
1:B:592:MET:HE1	1:B:674:MET:HE3	1.88	0.56
1:A:391:TYR:HD1	1:A:391:TYR:H	1.54	0.55
1:B:423:VAL:O	1:B:424:ASN:HB3	2.06	0.55
1:B:19:TYR:N	1:B:19:TYR:CD1	2.73	0.55
1:B:163:SER:OG	1:B:165:GLU:HG2	2.07	0.55
1:B:455:SER:HA	1:B:675:ASN:O	2.06	0.55
1:B:553:MET:HG3	1:B:554:THR:N	2.21	0.55
1:A:465:LYS:HD3	1:A:675:ASN:O	2.06	0.55
1:B:327:ASP:O	1:B:328:VAL:C	2.49	0.55
1:B:471:VAL:HB	1:B:472:PRO:CD	2.36	0.55
1:A:51:ASP:HB2	1:A:52:ILE:HD13	1.88	0.55
1:A:625:ILE:C	1:A:626:TYR:CD1	2.84	0.55
1:B:201:TYR:O	1:B:204:PHE:HB3	2.07	0.55
1:B:439:LEU:O	1:B:440:HIS:C	2.49	0.55
1:B:857:LEU:N	1:B:857:LEU:HD23	2.21	0.55
1:A:173:GLN:H	1:A:173:GLN:NE2	2.04	0.55
1:A:214:THR:CG2	1:A:215:GLY:H	2.18	0.55
1:A:409:SER:HA	1:A:625:ILE:O	2.06	0.55
1:A:647:TRP:CD1	1:A:648:VAL:N	2.75	0.55
1:A:750:ARG:HG2	1:A:754:GLN:OE1	2.06	0.55
1:A:416:TYR:O	1:A:419:ILE:HB	2.07	0.55
1:A:498:ILE:HG22	1:A:499:ILE:HG13	1.87	0.55
1:A:147:TYR:CD2	1:A:204:PHE:HE1	2.24	0.55
1:A:883:PHE:N	1:A:883:PHE:CD1	2.70	0.55
1:B:41:CYS:CB	1:B:45:GLN:HG3	2.31	0.55
1:B:339:GLN:HA	1:B:339:GLN:NE2	2.21	0.55
1:A:254:GLU:O	1:A:255:ASN:HB2	2.06	0.55
1:A:893:LYS:HG2	1:A:894:LYS:N	2.22	0.55
1:B:443:ILE:HG22	1:B:592:MET:CG	2.37	0.55
1:B:733:GLN:O	1:B:734:LYS:C	2.47	0.55
1:B:193:ASN:ND2	1:B:195:LYS:HD3	2.21	0.55
1:B:423:VAL:HB	1:B:425:ILE:CG1	2.36	0.55
1:B:593:ALA:HA	1:B:670:MET:CE	2.28	0.55
1:A:205:TRP:CZ3	1:A:209:THR:HG23	2.42	0.54
1:A:403:ARG:NH1	1:A:888:LYS:HB2	2.22	0.54
1:A:808:ILE:O	1:A:811:TYR:HB3	2.07	0.54
1:B:195:LYS:O	1:B:199:MET:HB2	2.07	0.54
1:B:689:ALA:HB1	1:B:711:ASN:O	2.07	0.54
1:A:291:ASP:HB3	1:A:302:LYS:CD	2.37	0.54
1:A:547:ARG:HA	1:A:550:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:ASN:C	1:A:789:ALA:H	2.14	0.54
1:A:836:ARG:NH1	1:A:864:HIS:O	2.40	0.54
1:B:117:VAL:HG13	1:B:132:PRO:O	2.07	0.54
1:B:166:ILE:O	1:B:175:GLY:HA2	2.07	0.54
1:B:321:ILE:HD12	1:B:321:ILE:N	2.23	0.54
1:B:369:ILE:HG21	1:B:577:TYR:CZ	2.42	0.54
1:A:379:VAL:HG12	1:A:380:ILE:O	2.07	0.54
1:A:425:ILE:O	1:A:472:PRO:HD3	2.07	0.54
1:A:597:ILE:HB	1:A:667:PHE:CE1	2.43	0.54
1:B:763:TYR:CD1	1:B:763:TYR:C	2.84	0.54
1:A:147:TYR:CD1	1:A:147:TYR:N	2.73	0.54
1:A:166:ILE:O	1:A:175:GLY:HA2	2.07	0.54
1:A:235:GLY:O	1:A:238:THR:HG23	2.08	0.54
1:A:514:LEU:CD1	1:A:533:LEU:HD21	2.38	0.54
1:A:598:GLU:HG3	1:A:599:ARG:N	2.21	0.54
1:A:669:GLU:O	1:A:672:GLU:HB3	2.08	0.54
1:A:796:PHE:HD1	1:A:796:PHE:N	2.05	0.54
1:B:165:GLU:H	1:B:165:GLU:CD	2.15	0.54
1:A:117:VAL:HG22	1:A:133:ILE:HA	1.89	0.54
1:A:647:TRP:CD1	1:A:647:TRP:C	2.85	0.54
1:A:855:THR:HB	1:A:857:LEU:HD21	1.90	0.54
1:B:271:LEU:HD23	1:B:271:LEU:N	2.23	0.54
1:A:72:ILE:H	1:A:72:ILE:HD12	1.73	0.54
1:A:255:ASN:C	1:A:257:TYR:H	2.14	0.54
1:A:576:ARG:HB3	1:A:577:TYR:CD1	2.43	0.54
1:A:643:ASP:O	1:A:646:HIS:HB3	2.07	0.54
1:B:456:CYS:HB3	1:B:462:MET:N	2.23	0.54
1:B:625:ILE:C	1:B:626:TYR:CD1	2.86	0.54
1:B:834:PRO:O	1:B:845:CYS:HA	2.07	0.54
1:A:40:HIS:HE1	1:A:81:GLU:OE1	1.91	0.54
1:A:536:LYS:HD3	1:A:536:LYS:C	2.33	0.54
1:B:830:VAL:CG1	1:B:847:ALA:HB1	2.38	0.54
1:B:421:ARG:CZ	1:B:476:THR:HG23	2.36	0.54
1:B:547:ARG:HB3	1:B:547:ARG:CZ	2.38	0.54
1:B:702:TRP:CD1	1:B:702:TRP:N	2.75	0.54
1:B:766:GLU:O	1:B:769:LYS:HB3	2.07	0.54
1:B:810:THR:HB	1:B:843:ASP:OD2	2.08	0.54
1:A:475:ILE:HG22	1:A:476:THR:N	2.23	0.54
1:A:837:GLU:HB2	1:A:844:LYS:HE2	1.90	0.54
1:B:689:ALA:HB3	1:B:710:LEU:HD22	1.89	0.54
1:A:162:TRP:HE3	1:A:188:TYR:CE2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD11	1:A:357:SER:O	2.08	0.54
1:A:870:VAL:HG12	1:A:871:LEU:N	2.23	0.54
1:B:282:PHE:O	1:B:283:THR:HG23	2.07	0.54
1:B:459:ASN:HD21	1:B:461:MET:CG	2.21	0.54
1:B:728:MET:HA	1:B:728:MET:CE	2.33	0.54
1:B:149:PHE:N	1:B:149:PHE:CD1	2.75	0.53
1:B:248:THR:HA	1:B:266:PHE:HD1	1.72	0.53
1:B:654:PHE:CD1	1:B:654:PHE:C	2.86	0.53
1:A:104:ASP:OD2	1:A:107:LYS:N	2.42	0.53
1:A:145:ARG:HH21	1:A:185:LYS:CD	2.21	0.53
1:A:214:THR:CG2	1:A:215:GLY:N	2.71	0.53
1:A:593:ALA:HA	1:A:670:MET:CE	2.23	0.53
1:B:53:TYR:CE1	1:B:428:GLU:CB	2.91	0.53
1:B:751:ARG:NH1	1:B:763:TYR:HB2	2.23	0.53
1:B:791:TYR:CD1	1:B:791:TYR:C	2.86	0.53
1:A:101:ILE:CG2	1:A:102:LYS:N	2.72	0.53
1:A:320:TYR:CD1	1:A:321:ILE:HD12	2.37	0.53
1:A:152:LEU:O	1:A:158:ASN:HA	2.09	0.53
1:A:596:TRP:CB	1:A:670:MET:HE3	2.39	0.53
1:B:808:ILE:O	1:B:811:TYR:HB3	2.07	0.53
1:A:116:GLU:CG	1:A:324:ASN:ND2	2.71	0.53
1:A:810:THR:HG21	1:A:845:CYS:O	2.07	0.53
1:A:899:ASP:HB2	1:A:900:MET:SD	2.49	0.53
1:A:434:PHE:CE2	1:A:460:GLY:HA2	2.44	0.53
1:A:602:ASN:OD1	1:A:617:VAL:HG23	2.07	0.53
1:B:245:HIS:HE1	1:B:267:GLY:HA3	1.74	0.53
1:B:653:LYS:HD2	1:B:656:ARG:HH11	1.73	0.53
1:A:62:PHE:HD2	1:A:67:ASP:HB3	1.73	0.53
1:A:285:GLN:HG3	1:A:286:PRO:HD2	1.91	0.53
1:A:594:LEU:O	1:A:597:ILE:HG22	2.08	0.53
1:A:788:ILE:O	1:A:791:TYR:CD2	2.62	0.53
1:B:253:ILE:CG2	1:B:260:ARG:CB	2.59	0.53
1:B:802:PRO:HD2	1:B:805:ILE:HB	1.90	0.53
1:B:167:ALA:HB1	1:B:178:VAL:HG21	1.91	0.53
1:B:499:ILE:HD11	1:B:541:MET:HB3	1.90	0.53
1:B:555:ALA:O	1:B:558:ASN:HB3	2.08	0.53
1:B:803:PHE:CZ	1:B:845:CYS:HB3	2.44	0.53
1:A:471:VAL:HB	1:A:472:PRO:CD	2.38	0.53
1:A:494:ARG:HA	1:A:497:GLU:HG2	1.91	0.53
1:A:165:GLU:O	1:A:168:ALA:HB3	2.08	0.53
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ILE:N	1:B:321:ILE:CD1	2.72	0.53
1:B:329:TYR:CD2	1:B:333:GLN:NE2	2.77	0.53
1:B:752:MET:CG	1:B:760:LEU:HD12	2.39	0.53
1:B:820:ASP:C	1:B:822:PRO:HD2	2.34	0.53
1:A:123:PHE:CZ	1:A:828:GLU:HB3	2.44	0.52
1:A:288:TYR:HA	1:A:293:ILE:CD1	2.39	0.52
1:A:796:PHE:N	1:A:796:PHE:CD1	2.75	0.52
1:A:821:ALA:N	1:A:822:PRO:CD	2.71	0.52
1:B:33:TYR:O	1:B:35:PRO:HD3	2.09	0.52
1:B:144:ASP:OD2	1:B:185:LYS:HE3	2.09	0.52
1:B:423:VAL:O	1:B:424:ASN:CB	2.57	0.52
1:A:167:ALA:HA	1:A:176:ASP:CB	2.39	0.52
1:A:323:TYR:O	1:A:324:ASN:C	2.52	0.52
1:A:636:VAL:HG12	1:A:636:VAL:O	2.09	0.52
1:A:792:ASP:O	1:A:794:GLY:N	2.43	0.52
1:B:129:ALA:O	1:B:229:ARG:HD3	2.10	0.52
1:B:581:ARG:HG3	1:B:581:ARG:NH1	2.17	0.52
1:B:4:PHE:O	1:B:19:TYR:HB2	2.09	0.52
1:B:495:ASN:OD1	1:B:521:ASP:HA	2.09	0.52
1:B:867:ASP:O	1:B:871:LEU:HB2	2.09	0.52
1:A:103:TYR:CD1	1:A:103:TYR:C	2.88	0.52
1:A:219:GLU:HA	1:A:223:ILE:HD12	1.90	0.52
1:A:511:ASP:HB2	1:A:537:SER:HB3	1.92	0.52
1:A:647:TRP:HH2	1:A:691:PRO:O	1.93	0.52
1:A:818:ASN:CA	1:A:822:PRO:HG3	2.37	0.52
1:B:164:ILE:HD12	1:B:164:ILE:N	2.17	0.52
1:B:343:LEU:C	1:B:343:LEU:HD23	2.35	0.52
1:B:776:TYR:CE2	1:B:777:ILE:HG12	2.44	0.52
1:A:104:ASP:CG	1:A:107:LYS:HD2	2.34	0.52
1:A:434:PHE:CZ	1:A:460:GLY:HA2	2.44	0.52
1:B:101:ILE:HG21	1:B:349:TYR:CD1	2.44	0.52
1:B:626:TYR:CD1	1:B:626:TYR:N	2.77	0.52
1:A:506:PRO:HG2	1:A:507:ASN:H	1.74	0.52
1:B:530:ILE:C	1:B:532:LYS:N	2.68	0.52
1:B:549:GLU:O	1:B:553:MET:HB3	2.09	0.52
1:B:744:ALA:CB	1:B:767:PHE:CE2	2.93	0.52
1:B:489:MET:SD	1:B:553:MET:CB	2.87	0.52
1:A:62:PHE:O	1:A:64:ASN:N	2.42	0.52
1:A:308:PRO:HD2	1:A:311:LYS:HB2	1.91	0.52
1:A:419:ILE:O	1:A:423:VAL:HG23	2.10	0.52
1:A:489:MET:HG3	1:A:553:MET:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ALA:HA	1:B:176:ASP:CB	2.37	0.52
1:A:421:ARG:HD2	1:A:475:ILE:HG21	1.89	0.52
1:A:647:TRP:CZ3	1:A:693:LEU:HB2	2.44	0.51
1:B:16:PHE:HE1	1:B:30:GLU:HG3	1.76	0.51
1:B:186:ILE:N	1:B:186:ILE:HD12	2.26	0.51
1:A:169:LYS:HB2	1:A:175:GLY:CA	2.39	0.51
1:A:781:SER:O	1:A:831:TYR:O	2.28	0.51
1:B:589:PHE:CD1	1:B:589:PHE:C	2.88	0.51
1:B:788:ILE:HG22	1:B:791:TYR:CG	2.45	0.51
1:A:155:PRO:HG2	1:A:156:TYR:CD1	2.45	0.51
1:A:280:PHE:CD2	1:A:343:LEU:HD13	2.46	0.51
1:A:597:ILE:HD13	1:A:667:PHE:CD1	2.46	0.51
1:B:4:PHE:CE2	1:B:103:TYR:HA	2.46	0.51
1:B:23:ASN:O	1:B:25:ARG:N	2.43	0.51
1:B:103:TYR:CE1	1:B:346:ASP:HA	2.46	0.51
1:B:728:MET:HE2	1:B:728:MET:HA	1.90	0.51
1:A:127:SER:HB2	1:A:128:GLN:OE1	2.10	0.51
1:A:167:ALA:HA	1:A:176:ASP:OD2	2.09	0.51
1:A:186:ILE:CG2	1:A:187:ILE:N	2.73	0.51
1:A:822:PRO:O	1:A:822:PRO:HG2	2.09	0.51
1:B:70:GLN:OE1	1:B:70:GLN:HA	2.09	0.51
1:B:188:TYR:CE1	1:B:190:PRO:HD3	2.45	0.51
1:B:205:TRP:CZ3	1:B:209:THR:HG23	2.45	0.51
1:A:232:ASN:HD22	1:A:232:ASN:H	1.59	0.51
1:B:6:LEU:HD12	1:B:211:VAL:HG11	1.91	0.51
1:B:53:TYR:CE1	1:B:428:GLU:HB2	2.46	0.51
1:B:108:ILE:O	1:B:110:VAL:N	2.44	0.51
1:A:274:ILE:HG23	1:A:275:ASP:H	1.75	0.51
1:A:321:ILE:CD1	1:A:321:ILE:N	2.73	0.51
1:A:413:THR:O	1:A:415:LEU:N	2.42	0.51
1:A:656:ARG:NH1	1:A:656:ARG:CB	2.74	0.51
1:A:811:TYR:HB2	1:A:846:ILE:HG23	1.91	0.51
1:A:818:ASN:O	1:A:822:PRO:HG3	2.11	0.51
1:B:788:ILE:O	1:B:790:LYS:HG3	2.11	0.51
1:A:52:ILE:HD13	1:A:52:ILE:N	2.18	0.51
1:A:274:ILE:HG23	1:A:275:ASP:N	2.26	0.51
1:A:338:ARG:HG3	1:A:340:PHE:CE1	2.45	0.51
1:A:582:ASN:O	1:A:585:ALA:HB3	2.11	0.51
1:B:472:PRO:O	1:B:473:THR:C	2.54	0.51
1:A:5:TYR:HA	1:A:19:TYR:HB3	1.92	0.51
1:A:273:TYR:OH	1:A:335:ASP:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:VAL:CG2	1:A:541:MET:HE2	2.41	0.51
1:A:899:ASP:O	1:A:900:MET:SD	2.68	0.51
1:B:83:LEU:HD12	1:B:83:LEU:H	1.75	0.51
1:B:858:ILE:HG13	1:B:859:LYS:N	2.26	0.51
1:A:680:LEU:HD23	1:A:680:LEU:N	2.22	0.51
1:B:246:ARG:N	1:B:246:ARG:CD	2.74	0.51
1:B:541:MET:HA	1:B:541:MET:CE	2.39	0.51
1:B:711:ASN:OD1	1:B:723:PRO:HB2	2.11	0.51
1:A:68:ALA:O	1:A:71:TRP:HB3	2.11	0.51
1:A:437:ALA:O	1:A:442:TYR:HE2	1.94	0.51
1:A:642:ARG:O	1:A:643:ASP:CB	2.53	0.51
1:A:763:TYR:O	1:A:763:TYR:CD1	2.57	0.51
1:B:71:TRP:CZ3	1:B:82:ALA:HB1	2.46	0.51
1:B:499:ILE:CD1	1:B:541:MET:HB3	2.41	0.51
1:A:125:GLU:CB	1:A:128:GLN:HE22	2.24	0.50
1:A:606:ASN:C	1:A:606:ASN:HD22	2.20	0.50
1:B:139:TYR:CE1	1:B:144:ASP:HA	2.46	0.50
1:B:188:TYR:HE1	1:B:190:PRO:CB	2.22	0.50
1:B:606:ASN:O	1:B:611:THR:N	2.42	0.50
1:A:191:PHE:CD1	1:A:197:LEU:HD22	2.47	0.50
1:A:191:PHE:CD1	1:A:191:PHE:N	2.78	0.50
1:A:332:LEU:H	1:A:332:LEU:HD23	1.75	0.50
1:A:491:ALA:O	1:A:495:ASN:N	2.43	0.50
1:A:744:ALA:HB2	1:A:767:PHE:HE2	1.74	0.50
1:B:8:VAL:HG12	1:B:17:GLU:HB2	1.93	0.50
1:B:499:ILE:HD13	1:B:542:LEU:N	2.27	0.50
1:B:794:GLY:C	1:B:796:PHE:H	2.19	0.50
1:A:110:VAL:HG22	1:A:212:ILE:HB	1.94	0.50
1:A:321:ILE:HD12	1:A:321:ILE:N	2.25	0.50
1:A:412:LEU:HD13	1:A:683:MET:HB2	1.93	0.50
1:A:776:TYR:CD1	1:A:777:ILE:N	2.80	0.50
1:B:115:ILE:C	1:B:115:ILE:HD12	2.36	0.50
1:B:218:VAL:O	1:B:223:ILE:HG13	2.11	0.50
1:B:255:ASN:HB3	1:B:257:TYR:CE2	2.46	0.50
1:A:184:ASP:N	1:A:184:ASP:OD1	2.45	0.50
1:A:205:TRP:CZ2	1:A:210:PRO:HD2	2.46	0.50
1:A:744:ALA:CB	1:A:767:PHE:CE2	2.94	0.50
1:A:744:ALA:CB	1:A:767:PHE:HE2	2.25	0.50
1:B:128:GLN:OE1	1:B:128:GLN:N	2.45	0.50
1:B:311:LYS:NZ	1:B:821:ALA:HA	2.26	0.50
1:A:626:TYR:CD1	1:A:626:TYR:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:HD3	1:B:246:ARG:NH1	2.26	0.50
1:B:604:TYR:HD1	1:B:605:LEU:HD23	1.76	0.50
1:A:222:ASP:O	1:A:226:VAL:HG23	2.11	0.50
1:A:858:ILE:HG13	1:A:859:LYS:N	2.25	0.50
1:A:863:LEU:HA	1:A:866:MET:HB2	1.93	0.50
1:B:188:TYR:HD1	1:B:189:MET:N	2.10	0.50
1:B:345:LEU:O	1:B:349:TYR:HD2	1.95	0.50
1:A:325:ILE:O	1:A:326:ILE:C	2.54	0.50
1:A:408:MET:HE2	1:A:685:ARG:HG3	1.94	0.50
1:B:188:TYR:CD1	1:B:189:MET:N	2.80	0.50
1:B:250:VAL:HG12	1:B:251:LYS:N	2.25	0.50
1:B:605:LEU:O	1:B:607:GLU:N	2.45	0.50
1:B:785:ALA:C	1:B:787:ASN:N	2.69	0.50
1:B:1:MET:O	1:B:22:SER:HA	2.11	0.50
1:B:253:ILE:HG22	1:B:260:ARG:O	2.11	0.50
1:B:402:ASN:CG	1:B:403:ARG:N	2.66	0.50
1:B:459:ASN:HD21	1:B:461:MET:HG3	1.76	0.50
1:A:115:ILE:HD12	1:A:115:ILE:C	2.37	0.49
1:A:229:ARG:O	1:A:232:ASN:HB2	2.11	0.49
1:A:324:ASN:O	1:A:327:ASP:HB2	2.12	0.49
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.47	0.49
1:B:119:SER:HB2	1:B:131:HIS:ND1	2.27	0.49
1:B:312:LEU:HD13	1:B:312:LEU:O	2.12	0.49
1:B:600:LYS:O	1:B:603:GLU:HB3	2.12	0.49
1:A:169:LYS:HB3	1:A:173:GLN:HB2	1.94	0.49
1:B:65:MET:HE2	1:B:88:PHE:CB	2.40	0.49
1:B:139:TYR:HE1	1:B:144:ASP:HA	1.76	0.49
1:B:343:LEU:O	1:B:345:LEU:N	2.44	0.49
1:B:391:TYR:CD1	1:B:391:TYR:N	2.80	0.49
1:B:528:GLU:C	1:B:530:ILE:H	2.21	0.49
1:A:201:TYR:O	1:A:204:PHE:HB3	2.13	0.49
1:B:456:CYS:HB3	1:B:462:MET:HA	1.95	0.49
1:B:854:ILE:CG2	1:B:859:LYS:HB2	2.37	0.49
1:A:334:ILE:O	1:A:335:ASP:C	2.53	0.49
1:A:815:ILE:CG2	1:A:815:ILE:O	2.60	0.49
1:B:431:ALA:HB3	1:B:462:MET:O	2.12	0.49
1:B:507:ASN:O	1:B:508:LEU:HD12	2.12	0.49
1:B:733:GLN:CD	1:B:733:GLN:H	2.19	0.49
1:A:328:VAL:O	1:A:332:LEU:HD23	2.12	0.49
1:A:689:ALA:HB1	1:A:711:ASN:C	2.37	0.49
1:B:53:TYR:CD1	1:B:428:GLU:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:ALA:CB	1:B:710:LEU:HD22	2.42	0.49
1:B:693:LEU:C	1:B:695:SER:H	2.21	0.49
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.94	0.49
1:A:92:TYR:CD1	1:A:92:TYR:C	2.90	0.49
1:A:116:GLU:CG	1:A:324:ASN:HD21	2.26	0.49
1:A:262:ILE:HG13	1:A:262:ILE:O	2.13	0.49
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.42	0.49
1:B:162:TRP:HB3	1:B:188:TYR:CE2	2.44	0.49
1:B:431:ALA:HB1	1:B:454:TYR:CD2	2.47	0.49
1:B:857:LEU:CD2	1:B:857:LEU:H	2.26	0.49
1:A:658:ARG:HG3	1:A:658:ARG:HH11	1.78	0.49
1:B:41:CYS:HB3	1:B:58:THR:HG23	1.94	0.49
1:B:45:GLN:OE1	1:B:45:GLN:HA	2.12	0.49
1:B:162:TRP:CE3	1:B:188:TYR:CE2	3.01	0.49
1:B:303:LEU:CD2	1:B:326:ILE:HG13	2.42	0.49
1:B:343:LEU:C	1:B:345:LEU:N	2.71	0.49
1:B:347:MET:CE	1:B:358:VAL:HG13	2.36	0.49
1:A:6:LEU:HB2	1:A:18:ARG:O	2.13	0.49
1:A:89:LYS:O	1:A:93:LEU:HG	2.13	0.49
1:A:451:SER:OG	1:A:454:TYR:HB2	2.13	0.49
1:B:410:PHE:O	1:B:624:SER:HA	2.13	0.49
1:B:456:CYS:HB3	1:B:462:MET:CA	2.42	0.49
1:B:481:GLN:NE2	1:B:559:ARG:HH11	2.08	0.49
1:A:169:LYS:HB2	1:A:175:GLY:HA3	1.94	0.49
1:A:364:THR:HG22	1:A:368:ILE:HD11	1.94	0.49
1:A:430:ILE:HG23	1:A:430:ILE:O	2.12	0.49
1:A:459:ASN:HD22	1:A:459:ASN:H	1.61	0.49
1:B:216:TRP:C	1:B:218:VAL:H	2.21	0.49
1:B:428:GLU:OE2	1:B:470:VAL:HG23	2.12	0.49
1:A:72:ILE:O	1:A:73:LYS:C	2.55	0.48
1:B:606:ASN:HB2	1:B:611:THR:C	2.37	0.48
1:B:837:GLU:OE1	1:B:837:GLU:HA	2.12	0.48
1:A:167:ALA:CA	1:A:176:ASP:HB2	2.42	0.48
1:A:455:SER:HA	1:A:675:ASN:O	2.13	0.48
1:A:614:GLU:HG3	1:A:616:PHE:HE1	1.78	0.48
1:B:61:LEU:HD13	1:B:62:PHE:N	2.28	0.48
1:B:292:TYR:C	1:B:292:TYR:CD1	2.91	0.48
1:A:112:ASN:HD22	1:A:112:ASN:C	2.18	0.48
1:A:556:GLN:OE1	1:A:557:ILE:HD13	2.12	0.48
1:A:844:LYS:O	1:A:845:CYS:CB	2.62	0.48
1:B:188:TYR:CE1	1:B:190:PRO:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:PRO:HD2	1:B:576:ARG:HD3	1.94	0.48
1:B:433:THR:HG23	1:B:434:PHE:N	2.27	0.48
1:B:474:GLU:O	1:B:477:LYS:HB3	2.13	0.48
1:B:744:ALA:O	1:B:747:GLU:HB2	2.13	0.48
1:B:884:THR:HB	1:B:889:LEU:O	2.14	0.48
1:A:8:VAL:HG11	1:A:93:LEU:HD21	1.95	0.48
1:A:291:ASP:HA	1:A:294:SER:OG	2.13	0.48
1:A:421:ARG:HB2	1:A:680:LEU:CD1	2.43	0.48
1:A:643:ASP:HB3	1:A:646:HIS:N	2.26	0.48
1:A:832:VAL:N	1:A:847:ALA:HA	2.19	0.48
1:A:897:LEU:HD12	1:A:897:LEU:N	2.27	0.48
1:A:68:ALA:O	1:A:72:ILE:HD12	2.14	0.48
1:A:104:ASP:O	1:A:105:HIS:CD2	2.66	0.48
1:A:339:GLN:HE22	1:A:342:ASN:HB2	1.77	0.48
1:A:835:LEU:CD1	1:A:845:CYS:H	2.26	0.48
1:B:857:LEU:CD2	1:B:857:LEU:N	2.76	0.48
1:A:255:ASN:OD1	1:A:256:MET:N	2.44	0.48
1:A:514:LEU:HD13	1:A:533:LEU:HD21	1.94	0.48
1:A:654:PHE:HD1	1:A:654:PHE:O	1.97	0.48
1:B:112:ASN:ND2	1:B:113:PHE:N	2.58	0.48
1:B:518:TYR:OH	1:B:541:MET:HE2	2.14	0.48
1:B:787:ASN:O	1:B:790:LYS:HG2	2.14	0.48
1:A:113:PHE:HE1	1:A:218:VAL:HG23	1.78	0.48
1:A:408:MET:O	1:A:627:VAL:HG23	2.14	0.48
1:A:655:ALA:HA	1:A:659:MET:CB	2.43	0.48
1:A:818:ASN:O	1:A:819:ILE:HB	2.12	0.48
1:B:170:LEU:HB3	1:B:172:GLU:OE1	2.14	0.48
1:B:577:TYR:N	1:B:577:TYR:CD1	2.81	0.48
1:A:289:SER:O	1:A:290:LEU:C	2.57	0.48
1:B:18:ARG:NH2	1:B:210:PRO:O	2.46	0.48
1:B:221:PHE:CD2	1:B:222:ASP:N	2.82	0.48
1:B:834:PRO:O	1:B:835:LEU:HB2	2.14	0.48
1:B:843:ASP:O	1:B:844:LYS:HE3	2.14	0.48
1:A:291:ASP:HB2	1:A:302:LYS:HB2	1.94	0.48
1:A:745:LEU:O	1:A:746:LYS:C	2.57	0.48
1:A:830:VAL:HG13	1:A:848:TRP:C	2.39	0.48
1:A:899:ASP:C	1:A:901:PHE:H	2.22	0.48
1:B:790:LYS:C	1:B:792:ASP:H	2.22	0.48
1:B:873:GLU:HA	1:B:877:ILE:CD1	2.41	0.48
1:A:9:GLU:CG	1:A:266:PHE:CD1	2.97	0.48
1:A:254:GLU:O	1:A:255:ASN:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:C	1:B:172:GLU:H	2.21	0.48
1:B:364:THR:O	1:B:368:ILE:HG12	2.13	0.48
1:B:373:LEU:O	1:B:374:LYS:C	2.57	0.48
1:A:211:VAL:HG12	1:A:212:ILE:HG13	1.96	0.47
1:B:880:LEU:HD23	1:B:883:PHE:CE2	2.49	0.47
1:A:872:LEU:HD23	1:A:876:PHE:HB3	1.94	0.47
1:B:365:TRP:O	1:B:368:ILE:HB	2.13	0.47
1:B:712:VAL:CG1	1:B:713:TRP:N	2.77	0.47
1:B:831:TYR:O	1:B:832:VAL:HB	2.14	0.47
1:B:859:LYS:HG2	1:B:863:LEU:HD11	1.96	0.47
1:A:449:ARG:NH1	1:A:452:ASP:HA	2.29	0.47
1:A:883:PHE:N	1:A:883:PHE:HD1	2.11	0.47
1:B:305:TYR:HE1	1:B:307:GLY:O	1.97	0.47
1:B:727:ILE:HG21	1:B:732:THR:OG1	2.15	0.47
1:B:832:VAL:HG22	1:B:847:ALA:CB	2.41	0.47
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.14	0.47
1:A:524:ASP:HA	1:A:527:LYS:HB2	1.96	0.47
1:A:644:THR:HG23	1:A:645:ASN:H	1.80	0.47
1:A:796:PHE:CB	1:A:797:PRO:HD2	2.22	0.47
1:A:806:ARG:NH1	1:A:806:ARG:HG2	2.29	0.47
1:A:873:GLU:HA	1:A:877:ILE:CG1	2.44	0.47
1:B:129:ALA:HB1	1:B:229:ARG:HB2	1.96	0.47
1:B:370:PHE:CD1	1:B:371:ASN:N	2.82	0.47
1:B:562:LEU:HD12	1:B:562:LEU:HA	1.56	0.47
1:B:601:VAL:O	1:B:602:ASN:C	2.57	0.47
1:B:645:ASN:OD1	1:B:645:ASN:C	2.57	0.47
1:A:188:TYR:CD1	1:A:189:MET:N	2.75	0.47
1:A:674:MET:HB2	1:A:676:ASN:ND2	2.30	0.47
1:A:831:TYR:CD2	1:A:848:TRP:CE2	3.03	0.47
1:B:166:ILE:HA	1:B:169:LYS:HG2	1.97	0.47
1:B:612:GLU:OE1	1:B:612:GLU:HA	2.15	0.47
1:A:18:ARG:NH2	1:A:210:PRO:O	2.47	0.47
1:A:99:TYR:HD2	1:A:100:GLU:O	1.97	0.47
1:A:692:PRO:O	1:A:693:LEU:CB	2.62	0.47
1:A:806:ARG:HG2	1:A:806:ARG:HH11	1.79	0.47
1:A:830:VAL:CG1	1:A:831:TYR:H	2.23	0.47
1:B:143:ASP:C	1:B:145:ARG:N	2.71	0.47
1:B:263:ILE:N	1:B:263:ILE:HD12	2.29	0.47
1:B:405:LYS:O	1:B:690:GLY:HA2	2.15	0.47
1:B:416:TYR:O	1:B:420:ILE:HG13	2.13	0.47
1:B:468:ASP:HB3	1:B:473:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:872:LEU:HD22	1:B:877:ILE:CD1	2.45	0.47
1:A:37:LEU:HD22	1:A:83:LEU:O	2.15	0.47
1:A:156:TYR:HD1	1:A:156:TYR:N	2.12	0.47
1:A:190:PRO:C	1:A:191:PHE:CD1	2.92	0.47
1:A:275:ASP:O	1:A:279:LYS:HG2	2.15	0.47
1:A:288:TYR:HA	1:A:293:ILE:HD11	1.95	0.47
1:A:331:VAL:O	1:A:334:ILE:N	2.48	0.47
1:A:791:TYR:CD1	1:A:791:TYR:C	2.92	0.47
1:A:866:MET:HE2	1:A:868:TYR:CD1	2.49	0.47
1:B:213:LEU:HD12	1:B:213:LEU:HA	1.72	0.47
1:B:551:ALA:O	1:B:554:THR:HG22	2.14	0.47
1:A:300:VAL:HG23	1:A:301:GLY:N	2.30	0.47
1:A:389:GLN:NE2	1:A:390:PRO:HD2	2.30	0.47
1:A:503:LEU:HA	1:A:506:PRO:HB3	1.97	0.47
1:A:570:LEU:HD23	1:A:575:PHE:CD2	2.50	0.47
1:A:644:THR:HG23	1:A:645:ASN:N	2.30	0.47
1:B:616:PHE:HE1	1:B:631:LYS:HB2	1.80	0.47
1:A:101:ILE:HG22	1:A:102:LYS:H	1.78	0.47
1:A:103:TYR:HE2	1:A:346:ASP:CA	2.18	0.47
1:A:211:VAL:HG12	1:A:212:ILE:CG1	2.45	0.47
1:A:420:ILE:HD12	1:A:420:ILE:N	2.30	0.47
1:A:570:LEU:HD23	1:A:570:LEU:HA	1.56	0.47
1:A:683:MET:HE2	1:A:683:MET:HB3	1.61	0.47
1:B:170:LEU:C	1:B:172:GLU:N	2.72	0.47
1:B:338:ARG:HD2	1:B:338:ARG:HA	1.57	0.47
1:B:392:PRO:HG2	1:B:587:THR:HG23	1.95	0.47
1:B:415:LEU:HD12	1:B:415:LEU:HA	1.61	0.47
1:B:744:ALA:HB1	1:B:767:PHE:CE2	2.49	0.47
1:A:113:PHE:HE1	1:A:218:VAL:CG2	2.27	0.47
1:A:115:ILE:HD12	1:A:116:GLU:N	2.29	0.47
1:A:188:TYR:HE1	1:A:190:PRO:HB3	1.80	0.47
1:A:335:ASP:O	1:A:339:GLN:HA	2.15	0.47
1:A:605:LEU:C	1:A:607:GLU:H	2.23	0.47
1:A:897:LEU:H	1:A:897:LEU:CD1	2.24	0.47
1:B:182:ILE:O	1:B:186:ILE:CD1	2.62	0.47
1:B:386:HIS:HB3	1:B:387:PRO:HD2	1.96	0.47
1:B:412:LEU:HD13	1:B:412:LEU:HA	1.76	0.47
1:B:427:PRO:O	1:B:430:ILE:HG22	2.14	0.47
1:B:775:ASN:O	1:B:778:SER:OG	2.31	0.47
1:B:804:HIS:HB2	1:B:805:ILE:H	1.55	0.47
1:B:821:ALA:N	1:B:822:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HB2	1:A:89:LYS:NZ	2.30	0.46
1:A:162:TRP:CE3	1:A:188:TYR:CE2	3.02	0.46
1:A:522:PHE:O	1:A:523:SER:CB	2.63	0.46
1:A:702:TRP:CZ3	1:A:708:TYR:CD2	3.03	0.46
1:B:112:ASN:HA	1:B:214:THR:HG22	1.96	0.46
1:B:188:TYR:O	1:B:189:MET:HG3	2.15	0.46
1:B:195:LYS:H	1:B:195:LYS:CD	2.23	0.46
1:B:216:TRP:C	1:B:218:VAL:N	2.69	0.46
1:B:268:ILE:HD12	1:B:269:SER:N	2.30	0.46
1:B:605:LEU:C	1:B:607:GLU:N	2.71	0.46
1:A:337:LYS:HG3	1:A:338:ARG:N	2.30	0.46
1:A:339:GLN:HE21	1:A:339:GLN:CA	2.27	0.46
1:A:409:SER:C	1:A:410:PHE:CD1	2.93	0.46
1:A:491:ALA:HA	1:A:494:ARG:NH2	2.29	0.46
1:A:495:ASN:OD1	1:A:521:ASP:HA	2.15	0.46
1:A:663:ILE:HD12	1:A:663:ILE:H	1.80	0.46
1:B:92:TYR:C	1:B:92:TYR:HD1	2.22	0.46
1:A:15:ILE:HG21	1:A:92:TYR:CE2	2.51	0.46
1:A:155:PRO:HG2	1:A:156:TYR:HD1	1.80	0.46
1:A:426:SER:HB2	1:A:472:PRO:HD2	1.98	0.46
1:B:118:THR:HB	1:B:134:ASP:OD2	2.15	0.46
1:B:896:SER:O	1:B:898:PHE:N	2.49	0.46
1:A:156:TYR:CD1	1:A:156:TYR:N	2.83	0.46
1:A:234:PHE:HB3	1:A:238:THR:HG21	1.98	0.46
1:A:236:GLU:O	1:A:239:ALA:N	2.48	0.46
1:A:692:PRO:O	1:A:693:LEU:HB3	2.15	0.46
1:A:763:TYR:O	1:A:764:PHE:C	2.58	0.46
1:A:878:LYS:HB3	1:A:879:PRO:CD	2.46	0.46
1:B:4:PHE:CA	1:B:97:TYR:HE2	2.25	0.46
1:B:389:GLN:CD	1:B:390:PRO:HD2	2.41	0.46
1:B:653:LYS:HA	1:B:653:LYS:HD2	1.62	0.46
1:A:178:VAL:HG12	1:A:183:ILE:CD1	2.45	0.46
1:A:604:TYR:CD1	1:A:604:TYR:C	2.93	0.46
1:A:884:THR:HG21	1:A:891:TYR:HD2	1.80	0.46
1:B:23:ASN:ND2	1:B:25:ARG:HD2	2.31	0.46
1:B:96:THR:C	1:B:97:TYR:CD1	2.93	0.46
1:B:365:TRP:HA	1:B:368:ILE:HG13	1.97	0.46
1:B:640:LYS:O	1:B:640:LYS:HG3	2.16	0.46
1:B:129:ALA:HA	1:B:225:TYR:CZ	2.51	0.46
1:B:183:ILE:HA	1:B:186:ILE:HD13	1.97	0.46
1:B:604:TYR:HD1	1:B:605:LEU:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:LEU:O	1:B:761:GLN:C	2.59	0.46
1:A:49:TYR:HA	1:A:377:ASN:O	2.16	0.46
1:A:303:LEU:HB3	1:A:323:TYR:HD1	1.80	0.46
1:A:691:PRO:HA	1:A:692:PRO:HD3	1.73	0.46
1:A:799:PRO:O	1:A:800:LYS:HB3	2.16	0.46
1:A:818:ASN:O	1:A:822:PRO:CD	2.64	0.46
1:A:835:LEU:HG	1:A:845:CYS:HA	1.98	0.46
1:A:856:ASP:HA	1:A:859:LYS:CB	2.46	0.46
1:B:35:PRO:HG2	1:B:62:PHE:HB2	1.96	0.46
1:B:71:TRP:HZ3	1:B:82:ALA:HB1	1.81	0.46
1:A:105:HIS:C	1:A:107:LYS:N	2.70	0.46
1:A:169:LYS:HA	1:A:169:LYS:NZ	2.30	0.46
1:A:240:LYS:O	1:A:242:LEU:N	2.49	0.46
1:A:897:LEU:O	1:A:900:MET:HE1	2.15	0.46
1:B:501:GLU:C	1:B:503:LEU:H	2.24	0.46
1:A:182:ILE:O	1:A:185:LYS:HB2	2.16	0.46
1:A:629:ALA:O	1:A:630:ASP:C	2.58	0.46
1:A:659:MET:HB3	1:A:660:GLU:H	1.55	0.46
1:A:757:GLU:O	1:A:761:GLN:HG3	2.15	0.46
1:B:726:LYS:HD2	1:B:726:LYS:HA	1.76	0.46
1:A:365:TRP:CE3	1:A:368:ILE:HD12	2.52	0.45
1:A:579:ASP:O	1:A:582:ASN:HB2	2.16	0.45
1:A:663:ILE:HG12	1:A:683:MET:CE	2.46	0.45
1:A:772:ARG:HA	1:A:868:TYR:CE2	2.51	0.45
1:A:863:LEU:HD12	1:A:863:LEU:H	1.81	0.45
1:A:866:MET:HE3	1:A:871:LEU:HD12	1.98	0.45
1:B:877:ILE:O	1:B:878:LYS:C	2.59	0.45
1:A:64:ASN:OD1	1:A:64:ASN:C	2.58	0.45
1:A:214:THR:HG21	1:A:273:TYR:HD1	1.82	0.45
1:A:394:ALA:CB	1:A:622:THR:HG23	2.45	0.45
1:B:566:LEU:O	1:B:569:ALA:N	2.49	0.45
1:B:605:LEU:O	1:B:608:VAL:HG12	2.16	0.45
1:B:770:GLU:O	1:B:771:PHE:C	2.58	0.45
1:B:776:TYR:CD2	1:B:777:ILE:HG12	2.52	0.45
1:A:51:ASP:C	1:A:53:TYR:H	2.24	0.45
1:A:211:VAL:HG12	1:A:212:ILE:N	2.31	0.45
1:A:650:PHE:CD1	1:A:650:PHE:C	2.93	0.45
1:B:502:ALA:HB1	1:B:531:LYS:HA	1.98	0.45
1:B:788:ILE:O	1:B:791:TYR:HB3	2.16	0.45
1:B:880:LEU:HA	1:B:883:PHE:HE2	1.72	0.45
1:A:125:GLU:HB3	1:A:128:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:CG	1:A:256:MET:H	2.24	0.45
1:A:409:SER:OG	1:A:686:GLU:HG3	2.16	0.45
1:A:491:ALA:O	1:A:495:ASN:HB2	2.16	0.45
1:A:499:ILE:CG2	1:A:542:LEU:HB2	2.46	0.45
1:A:605:LEU:C	1:A:607:GLU:N	2.73	0.45
1:A:796:PHE:C	1:A:809:LEU:HD13	2.41	0.45
1:B:304:LYS:O	1:B:319:ARG:HD3	2.17	0.45
1:B:362:ILE:O	1:B:363:LYS:C	2.59	0.45
1:B:382:GLN:HG3	1:B:383:GLY:N	2.31	0.45
1:B:828:GLU:CG	1:B:829:LYS:H	2.28	0.45
1:B:828:GLU:OE1	1:B:828:GLU:HA	2.15	0.45
1:B:897:LEU:N	1:B:897:LEU:CD1	2.80	0.45
1:A:178:VAL:CG1	1:A:183:ILE:HD11	2.45	0.45
1:A:397:LYS:HG2	1:A:398:GLU:O	2.17	0.45
1:A:540:GLU:HG3	1:A:544:ARG:CZ	2.45	0.45
1:A:861:ASP:O	1:A:862:VAL:C	2.59	0.45
1:B:61:LEU:HD13	1:B:61:LEU:C	2.40	0.45
1:B:557:ILE:HD13	1:B:557:ILE:HA	1.81	0.45
1:A:228:ASN:O	1:A:229:ARG:C	2.60	0.45
1:A:347:MET:HA	1:A:558:ASN:HD21	1.81	0.45
1:A:419:ILE:O	1:A:420:ILE:C	2.60	0.45
1:A:576:ARG:CD	1:A:577:TYR:CE1	2.96	0.45
1:A:855:THR:CB	1:A:857:LEU:HD21	2.46	0.45
1:B:48:LYS:O	1:B:49:TYR:HB2	2.17	0.45
1:B:145:ARG:HB2	1:B:147:TYR:HE1	1.82	0.45
1:B:416:TYR:HD2	1:B:567:TYR:CG	2.35	0.45
1:B:645:ASN:O	1:B:646:HIS:C	2.59	0.45
1:A:8:VAL:HG23	1:A:8:VAL:O	2.17	0.45
1:A:218:VAL:HG22	1:A:223:ILE:HD11	1.99	0.45
1:A:329:TYR:O	1:A:332:LEU:HB2	2.17	0.45
1:A:365:TRP:O	1:A:366:ASP:C	2.58	0.45
1:A:391:TYR:CD1	1:A:391:TYR:N	2.85	0.45
1:A:439:LEU:O	1:A:440:HIS:C	2.59	0.45
1:A:858:ILE:O	1:A:859:LYS:C	2.59	0.45
1:B:5:TYR:HD1	1:B:5:TYR:H	1.64	0.45
1:B:112:ASN:HA	1:B:214:THR:CG2	2.47	0.45
1:B:137:THR:HB	1:B:328:VAL:HG21	1.99	0.45
1:B:343:LEU:C	1:B:343:LEU:CD2	2.89	0.45
1:B:409:SER:HB3	1:B:626:TYR:CD2	2.52	0.45
1:A:51:ASP:OD1	1:A:53:TYR:HB2	2.17	0.45
1:A:131:HIS:N	1:A:131:HIS:CD2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:O	1:A:199:MET:C	2.59	0.45
1:A:274:ILE:O	1:A:277:TYR:HB3	2.16	0.45
1:A:342:ASN:O	1:A:345:LEU:HB2	2.16	0.45
1:B:19:TYR:N	1:B:19:TYR:HD1	2.15	0.45
1:B:205:TRP:C	1:B:207:GLN:N	2.73	0.45
1:B:431:ALA:CB	1:B:454:TYR:CD2	2.99	0.45
1:B:597:ILE:HD12	1:B:597:ILE:HA	1.91	0.45
1:B:877:ILE:HD12	1:B:877:ILE:N	2.30	0.45
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.88	0.45
1:A:298:LEU:HB2	1:A:300:VAL:HG22	1.98	0.45
1:A:439:LEU:O	1:A:442:TYR:HB2	2.17	0.45
1:A:602:ASN:CG	1:A:617:VAL:HG23	2.42	0.45
1:A:856:ASP:HA	1:A:859:LYS:HB2	1.98	0.45
1:B:162:TRP:HE3	1:B:188:TYR:CD2	2.34	0.45
1:B:167:ALA:HB1	1:B:178:VAL:CG2	2.46	0.45
1:B:198:LEU:O	1:B:199:MET:C	2.60	0.45
1:B:700:GLY:HA3	1:B:710:LEU:HD23	1.99	0.45
1:B:731:GLU:HB3	1:B:734:LYS:HD2	1.98	0.45
1:A:225:TYR:O	1:A:226:VAL:C	2.60	0.45
1:A:291:ASP:HB3	1:A:302:LYS:CG	2.46	0.45
1:A:698:ILE:HD11	1:A:752:MET:HB3	1.99	0.45
1:A:728:MET:HE2	1:A:729:GLY:H	1.80	0.45
1:A:819:ILE:C	1:A:821:ALA:H	2.25	0.45
1:B:389:GLN:HE21	1:B:389:GLN:HA	1.82	0.45
1:B:686:GLU:HG3	1:B:687:ALA:N	2.32	0.45
1:B:811:TYR:O	1:B:815:ILE:HB	2.17	0.45
2:B:999:GMP:H2'	2:B:999:GMP:O5'	2.16	0.45
1:A:507:ASN:N	1:A:534:SER:HA	2.32	0.44
1:A:596:TRP:CZ3	1:A:599:ARG:NH2	2.85	0.44
1:A:689:ALA:HB1	1:A:711:ASN:O	2.17	0.44
1:A:700:GLY:N	1:A:753:LEU:HD22	2.32	0.44
1:B:204:PHE:O	1:B:207:GLN:HB3	2.17	0.44
1:A:489:MET:O	1:A:489:MET:HG2	2.16	0.44
1:A:800:LYS:O	1:A:800:LYS:HG2	2.17	0.44
1:A:902:ASP:N	1:A:902:ASP:OD1	2.51	0.44
1:B:275:ASP:O	1:B:276:LEU:C	2.61	0.44
1:A:18:ARG:HA	1:A:27:ARG:O	2.17	0.44
1:A:137:THR:HG21	1:A:325:ILE:HA	1.99	0.44
1:A:575:PHE:O	1:A:576:ARG:C	2.60	0.44
1:B:433:THR:N	1:B:462:MET:HE2	2.31	0.44
1:B:820:ASP:O	1:B:822:PRO:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:PRO:O	1:B:835:LEU:CB	2.65	0.44
1:A:103:TYR:CD1	1:A:103:TYR:O	2.71	0.44
1:A:116:GLU:HG2	1:A:324:ASN:HD21	1.82	0.44
1:A:733:GLN:O	1:A:734:LYS:C	2.60	0.44
1:B:15:ILE:HD13	1:B:15:ILE:HA	1.69	0.44
1:B:175:GLY:C	1:B:177:GLU:H	2.26	0.44
1:A:832:VAL:O	1:A:833:LEU:HG	2.17	0.44
1:B:126:PRO:HG3	1:B:221:PHE:CD1	2.52	0.44
1:B:218:VAL:HG22	1:B:223:ILE:HG13	1.98	0.44
1:B:369:ILE:O	1:B:370:PHE:C	2.60	0.44
1:B:605:LEU:HB3	1:B:616:PHE:CE2	2.53	0.44
1:B:698:ILE:HD12	1:B:753:LEU:HD23	2.00	0.44
1:A:1:MET:HB3	1:A:22:SER:O	2.18	0.44
1:A:17:GLU:O	1:A:28:THR:HA	2.17	0.44
1:A:97:TYR:CD1	1:A:97:TYR:N	2.85	0.44
1:A:113:PHE:CD1	1:A:113:PHE:C	2.92	0.44
1:A:280:PHE:HD2	1:A:343:LEU:HD13	1.81	0.44
1:B:194:GLU:O	1:B:195:LYS:C	2.61	0.44
1:B:834:PRO:HG2	1:B:871:LEU:HB2	1.99	0.44
1:A:126:PRO:HG3	1:A:221:PHE:CE1	2.52	0.44
1:A:139:TYR:CE2	1:A:141:SER:HA	2.52	0.44
1:A:145:ARG:HB2	1:A:147:TYR:HE1	1.81	0.44
1:A:713:TRP:CZ2	1:A:723:PRO:HG3	2.53	0.44
1:A:888:LYS:O	1:A:889:LEU:HD23	2.17	0.44
1:B:412:LEU:HD22	1:B:683:MET:HB2	1.99	0.44
1:B:550:VAL:O	1:B:553:MET:HG3	2.18	0.44
1:B:647:TRP:CD1	1:B:647:TRP:C	2.95	0.44
1:B:835:LEU:HB2	1:B:844:LYS:C	2.43	0.44
1:A:1:MET:O	1:A:22:SER:HA	2.18	0.44
1:A:253:ILE:CG2	1:A:254:GLU:N	2.81	0.44
1:A:402:ASN:HB3	1:A:404:TYR:CZ	2.53	0.44
1:B:97:TYR:CD1	1:B:97:TYR:N	2.86	0.44
1:B:194:GLU:O	1:B:197:LEU:HB3	2.18	0.44
1:B:229:ARG:O	1:B:230:ILE:C	2.61	0.44
1:B:233:ILE:HG13	1:B:234:PHE:CE1	2.50	0.44
1:A:187:ILE:HG22	1:A:187:ILE:O	2.17	0.44
1:A:265:LEU:CB	1:A:268:ILE:HD11	2.47	0.44
1:A:339:GLN:NE2	1:A:339:GLN:CA	2.81	0.44
1:A:832:VAL:H	1:A:847:ALA:CB	2.31	0.44
1:B:62:PHE:C	1:B:64:ASN:H	2.25	0.44
1:B:110:VAL:HG12	1:B:111:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD13	1:B:332:LEU:HA	1.73	0.44
1:B:389:GLN:HB3	1:B:580:LEU:HD22	2.00	0.44
1:B:454:TYR:O	1:B:675:ASN:HB3	2.18	0.44
1:B:503:LEU:HD11	1:B:539:ASN:ND2	2.33	0.44
1:B:730:LEU:C	1:B:732:THR:H	2.26	0.44
1:B:880:LEU:HA	1:B:883:PHE:HD2	1.80	0.44
1:A:62:PHE:CE2	1:A:68:ALA:HA	2.53	0.43
1:A:401:PRO:O	1:A:402:ASN:HB2	2.17	0.43
1:A:407:VAL:HA	1:A:627:VAL:O	2.17	0.43
1:A:751:ARG:CZ	1:A:763:TYR:HB2	2.47	0.43
1:B:409:SER:C	1:B:410:PHE:CD1	2.96	0.43
1:B:846:ILE:HG22	1:B:847:ALA:N	2.32	0.43
1:B:879:PRO:O	1:B:882:GLY:N	2.51	0.43
1:A:555:ALA:HA	1:A:558:ASN:HB2	1.99	0.43
1:A:772:ARG:HA	1:A:868:TYR:HE2	1.83	0.43
1:B:124:PRO:O	1:B:126:PRO:HD3	2.17	0.43
1:B:291:ASP:CG	1:B:302:LYS:HD2	2.43	0.43
1:B:601:VAL:O	1:B:604:TYR:HB3	2.17	0.43
1:B:806:ARG:NH1	1:B:806:ARG:HG2	2.33	0.43
1:B:862:VAL:O	1:B:863:LEU:C	2.61	0.43
1:A:180:SER:C	1:A:182:ILE:H	2.26	0.43
1:A:855:THR:HG22	1:A:857:LEU:CD2	2.49	0.43
1:B:49:TYR:HA	1:B:377:ASN:O	2.18	0.43
1:B:404:TYR:CG	1:B:618:LEU:HD11	2.53	0.43
1:B:450:PRO:O	1:B:451:SER:O	2.35	0.43
1:B:528:GLU:C	1:B:530:ILE:N	2.77	0.43
1:B:752:MET:HG2	1:B:760:LEU:CD1	2.48	0.43
1:A:115:ILE:CD1	1:A:117:VAL:HG23	2.49	0.43
1:A:188:TYR:CE1	1:A:190:PRO:HD3	2.53	0.43
1:A:744:ALA:O	1:A:747:GLU:N	2.51	0.43
1:A:767:PHE:O	1:A:768:GLU:CB	2.65	0.43
1:A:772:ARG:HH11	1:A:772:ARG:CG	2.29	0.43
1:B:194:GLU:O	1:B:197:LEU:N	2.52	0.43
1:B:859:LYS:O	1:B:862:VAL:HB	2.18	0.43
1:A:189:MET:O	1:A:191:PHE:HE1	2.01	0.43
1:A:503:LEU:HD21	1:A:539:ASN:ND2	2.33	0.43
1:A:526:ILE:O	1:A:530:ILE:HG12	2.19	0.43
1:A:576:ARG:HB3	1:A:577:TYR:CE1	2.54	0.43
1:A:656:ARG:O	1:A:656:ARG:HG2	2.18	0.43
1:A:831:TYR:HD2	1:A:848:TRP:CE2	2.37	0.43
1:B:139:TYR:HE1	1:B:144:ASP:CA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLU:O	1:B:201:TYR:C	2.60	0.43
1:B:243:SER:HB3	1:B:247:LYS:N	2.34	0.43
1:B:253:ILE:HG22	1:B:260:ARG:CA	2.46	0.43
1:B:517:ASP:CG	1:B:520:PHE:HE2	2.27	0.43
1:B:806:ARG:HG2	1:B:806:ARG:HH11	1.83	0.43
1:A:223:ILE:HB	1:A:224:PRO:CD	2.41	0.43
1:A:331:VAL:HG12	1:A:332:LEU:N	2.34	0.43
1:A:632:ILE:O	1:A:635:LYS:HB3	2.17	0.43
1:A:883:PHE:O	1:A:884:THR:C	2.62	0.43
1:B:9:GLU:HG2	1:B:266:PHE:CD2	2.53	0.43
1:B:199:MET:O	1:B:202:LEU:HB3	2.17	0.43
1:B:243:SER:HB3	1:B:247:LYS:H	1.83	0.43
1:B:243:SER:O	1:B:246:ARG:HD2	2.18	0.43
1:B:411:ASP:HA	1:B:623:ASP:O	2.18	0.43
1:B:494:ARG:O	1:B:498:ILE:CD1	2.66	0.43
1:A:163:SER:HB3	1:A:166:ILE:CD1	2.42	0.43
1:A:804:HIS:HB2	1:A:805:ILE:H	1.68	0.43
1:B:75:MET:N	1:B:75:MET:HE2	2.34	0.43
1:B:835:LEU:HD12	1:B:839:ASN:ND2	2.33	0.43
1:A:215:GLY:HA3	1:A:218:VAL:HB	2.00	0.43
1:A:330:ARG:HA	1:A:333:GLN:NE2	2.32	0.43
1:A:797:PRO:HB2	1:A:798:GLY:H	1.65	0.43
1:A:894:LYS:O	1:A:896:SER:N	2.51	0.43
1:B:601:VAL:HG12	1:B:602:ASN:N	2.34	0.43
1:B:680:LEU:HD23	1:B:680:LEU:N	2.27	0.43
1:B:731:GLU:HA	1:B:734:LYS:HG3	2.00	0.43
1:B:831:TYR:O	1:B:832:VAL:CB	2.67	0.43
1:B:861:ASP:O	1:B:864:HIS:HB3	2.19	0.43
1:A:407:VAL:CG1	1:A:408:MET:N	2.82	0.43
1:A:663:ILE:HG12	1:A:683:MET:HE1	2.00	0.43
1:A:762:GLU:HG3	1:A:763:TYR:N	2.34	0.43
1:B:109:ARG:HB3	1:B:211:VAL:HG23	2.01	0.43
1:B:163:SER:HG	1:B:166:ILE:HG13	1.84	0.43
1:B:566:LEU:O	1:B:567:TYR:C	2.61	0.43
1:B:566:LEU:C	1:B:568:GLY:N	2.75	0.43
1:B:605:LEU:C	1:B:607:GLU:H	2.26	0.43
1:B:606:ASN:HB3	1:B:614:GLU:HB2	2.01	0.43
1:B:790:LYS:O	1:B:792:ASP:N	2.52	0.43
1:B:828:GLU:HG3	1:B:829:LYS:H	1.83	0.43
1:A:300:VAL:HG23	1:A:301:GLY:H	1.83	0.43
1:A:740:ALA:HB2	1:A:778:SER:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:O	1:B:53:TYR:N	2.52	0.43
1:B:130:LYS:H	1:B:130:LYS:HG3	1.45	0.43
1:B:511:ASP:HB2	1:B:534:SER:CB	2.48	0.43
1:A:191:PHE:CD2	1:A:197:LEU:HA	2.54	0.42
1:A:901:PHE:N	1:A:901:PHE:CD1	2.84	0.42
1:B:253:ILE:CG1	1:B:254:GLU:N	2.63	0.42
1:B:262:ILE:HD12	1:B:262:ILE:O	2.19	0.42
1:B:343:LEU:O	1:B:346:ASP:N	2.52	0.42
1:B:653:LYS:HA	1:B:656:ARG:HH12	1.84	0.42
1:B:894:LYS:O	1:B:895:ALA:C	2.62	0.42
1:A:308:PRO:HD2	1:A:311:LYS:CB	2.48	0.42
1:A:353:ILE:HD11	1:A:357:SER:C	2.44	0.42
1:A:508:LEU:HD13	1:A:531:LYS:O	2.19	0.42
1:B:293:ILE:HG22	1:B:294:SER:N	2.33	0.42
1:B:308:PRO:HD2	1:B:311:LYS:HG3	2.02	0.42
1:B:456:CYS:O	1:B:674:MET:HB3	2.18	0.42
1:B:651:LEU:O	1:B:652:ASP:C	2.61	0.42
1:B:656:ARG:HH11	1:B:656:ARG:HB3	1.83	0.42
1:B:745:LEU:HD23	1:B:745:LEU:HA	1.61	0.42
1:A:176:ASP:O	1:A:177:GLU:HB2	2.19	0.42
1:A:406:TYR:HB3	1:A:629:ALA:HB3	2.01	0.42
1:A:647:TRP:O	1:A:650:PHE:N	2.52	0.42
1:A:714:ASP:OD1	1:A:717:GLY:N	2.52	0.42
1:A:763:TYR:HE1	1:A:767:PHE:CB	2.31	0.42
1:B:112:ASN:O	1:B:113:PHE:HB3	2.19	0.42
1:B:189:MET:O	1:B:191:PHE:CE1	2.71	0.42
1:B:341:ILE:O	1:B:345:LEU:CD2	2.67	0.42
1:B:352:LYS:HD3	1:B:352:LYS:N	2.34	0.42
1:B:604:TYR:O	1:B:607:GLU:HB3	2.19	0.42
1:B:643:ASP:O	1:B:646:HIS:CB	2.68	0.42
1:B:690:GLY:O	1:B:713:TRP:NE1	2.52	0.42
1:A:15:ILE:HD13	1:A:15:ILE:HA	1.75	0.42
1:A:232:ASN:N	1:A:232:ASN:ND2	2.60	0.42
1:A:446:VAL:HG12	1:A:446:VAL:O	2.19	0.42
1:A:476:THR:O	1:A:477:LYS:C	2.60	0.42
1:B:256:MET:O	1:B:257:TYR:CD1	2.73	0.42
1:B:323:TYR:O	1:B:324:ASN:C	2.61	0.42
1:B:664:ASP:O	1:B:668:ARG:HG3	2.20	0.42
1:B:713:TRP:CZ3	1:B:723:PRO:HD3	2.54	0.42
1:B:840:PRO:HD2	1:B:865:TRP:CD1	2.55	0.42
1:A:197:LEU:CD1	1:A:197:LEU:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:H	1:A:680:LEU:CD2	2.24	0.42
1:B:52:ILE:N	1:B:52:ILE:CD1	2.80	0.42
1:B:143:ASP:C	1:B:145:ARG:H	2.27	0.42
1:B:246:ARG:N	1:B:246:ARG:HD2	2.33	0.42
1:B:305:TYR:CE1	1:B:307:GLY:O	2.73	0.42
1:B:596:TRP:CE2	1:B:670:MET:HB2	2.54	0.42
1:B:710:LEU:HD23	1:B:710:LEU:HA	1.84	0.42
1:B:730:LEU:O	1:B:732:THR:N	2.52	0.42
1:A:36:SER:HB2	2:A:999:GMP:O4'	2.20	0.42
1:A:296:PHE:C	1:A:296:PHE:CD1	2.96	0.42
1:B:112:ASN:HD22	1:B:112:ASN:C	2.27	0.42
1:B:290:LEU:HD12	1:B:290:LEU:O	2.19	0.42
1:B:591:GLN:O	1:B:595:GLN:HG2	2.19	0.42
1:B:660:GLU:N	1:B:661:PRO:CD	2.83	0.42
1:A:420:ILE:H	1:A:420:ILE:CD1	2.33	0.42
1:A:422:GLN:HE21	1:A:422:GLN:HB2	1.55	0.42
1:B:13:ASP:O	1:B:32:GLU:HA	2.20	0.42
1:B:162:TRP:HE3	1:B:188:TYR:CE2	2.38	0.42
1:B:389:GLN:HA	1:B:390:PRO:HD3	1.83	0.42
1:B:391:TYR:N	1:B:391:TYR:HD1	2.17	0.42
1:B:426:SER:OG	1:B:427:PRO:HD2	2.20	0.42
1:B:789:ALA:HA	1:B:805:ILE:HG21	2.01	0.42
1:A:188:TYR:CD1	1:A:190:PRO:HD3	2.55	0.42
1:A:255:ASN:HB3	1:A:257:TYR:CE2	2.55	0.42
1:A:344:SER:O	1:A:345:LEU:C	2.60	0.42
1:A:470:VAL:O	1:A:471:VAL:C	2.61	0.42
1:A:600:LYS:HD3	1:A:600:LYS:HA	1.82	0.42
1:A:785:ALA:C	1:A:787:ASN:H	2.27	0.42
1:A:786:ASN:O	1:A:788:ILE:N	2.53	0.42
1:B:18:ARG:HH22	1:B:211:VAL:HA	1.83	0.42
1:B:330:ARG:HD2	1:B:333:GLN:HE22	1.85	0.42
1:B:859:LYS:HD2	1:B:860:ASP:OD1	2.19	0.42
1:A:226:VAL:O	1:A:230:ILE:HG13	2.20	0.42
1:A:373:LEU:HG	1:A:378:LYS:HB2	2.01	0.42
1:A:693:LEU:C	1:A:695:SER:H	2.28	0.42
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.83	0.42
1:B:154:SER:C	1:B:156:TYR:H	2.28	0.42
1:B:246:ARG:HD2	1:B:246:ARG:H	1.85	0.42
1:B:414:SER:HB2	1:B:417:PRO:HG2	2.01	0.42
1:B:872:LEU:HD22	1:B:877:ILE:HD11	2.02	0.42
1:A:112:ASN:C	1:A:112:ASN:ND2	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ALA:C	1:A:353:ILE:HG22	2.44	0.42
1:A:420:ILE:HD12	1:A:420:ILE:H	1.84	0.42
1:A:655:ALA:O	1:A:659:MET:HB3	2.20	0.42
1:A:695:SER:HB2	1:A:754:GLN:O	2.20	0.42
1:A:767:PHE:HD1	1:A:768:GLU:N	2.18	0.42
1:B:153:ASN:HA	1:B:158:ASN:ND2	2.35	0.42
1:B:404:TYR:CD1	1:B:618:LEU:HD11	2.55	0.42
1:B:454:TYR:CD1	1:B:454:TYR:N	2.88	0.42
1:B:488:TYR:CD2	1:B:519:ARG:HG2	2.55	0.42
1:B:507:ASN:C	1:B:508:LEU:HD12	2.45	0.42
1:B:625:ILE:CD1	1:B:683:MET:SD	3.08	0.42
1:A:64:ASN:OD1	1:A:66:ARG:N	2.53	0.41
1:A:450:PRO:O	1:A:451:SER:O	2.37	0.41
1:A:489:MET:SD	1:A:553:MET:HB2	2.60	0.41
1:A:567:TYR:O	1:A:567:TYR:CD1	2.73	0.41
1:A:659:MET:O	1:A:660:GLU:C	2.63	0.41
1:A:741:VAL:O	1:A:742:GLN:C	2.63	0.41
1:A:807:GLY:HA2	1:A:845:CYS:O	2.20	0.41
1:B:680:LEU:H	1:B:680:LEU:CD2	2.27	0.41
1:B:747:GLU:O	1:B:748:CYS:C	2.63	0.41
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.83	0.41
1:A:353:ILE:CG1	1:A:357:SER:HB2	2.50	0.41
1:B:64:ASN:HB3	1:B:67:ASP:OD2	2.20	0.41
1:B:198:LEU:CD1	1:B:233:ILE:HD11	2.50	0.41
1:B:738:PRO:HG3	1:B:781:SER:HA	2.01	0.41
1:B:776:TYR:O	1:B:779:ILE:CG1	2.68	0.41
1:A:103:TYR:C	1:A:103:TYR:HD1	2.27	0.41
1:B:1:MET:HB3	1:B:22:SER:HA	2.02	0.41
1:B:172:GLU:C	1:B:174:GLY:H	2.27	0.41
1:B:305:TYR:CD1	1:B:305:TYR:C	2.98	0.41
1:B:345:LEU:HD13	1:B:345:LEU:HA	1.83	0.41
1:B:531:LYS:H	1:B:531:LYS:HG3	1.53	0.41
1:B:653:LYS:O	1:B:654:PHE:C	2.63	0.41
1:A:147:TYR:CD2	1:A:204:PHE:CE1	3.07	0.41
1:A:274:ILE:CG1	1:A:278:LYS:HE3	2.51	0.41
1:A:330:ARG:O	1:A:334:ILE:HG13	2.21	0.41
1:A:431:ALA:HB2	1:A:464:TYR:CE1	2.55	0.41
1:A:547:ARG:O	1:A:550:VAL:HB	2.20	0.41
1:A:570:LEU:HD23	1:A:575:PHE:HD2	1.85	0.41
1:B:5:TYR:HA	1:B:19:TYR:HB3	2.02	0.41
1:B:109:ARG:HD2	1:B:210:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LYS:HE3	1:B:169:LYS:HB3	1.93	0.41
1:B:402:ASN:ND2	1:B:403:ARG:H	2.18	0.41
1:B:422:GLN:HE21	1:B:422:GLN:HB2	1.48	0.41
1:B:776:TYR:O	1:B:779:ILE:HG12	2.19	0.41
1:B:858:ILE:HG13	1:B:859:LYS:H	1.84	0.41
1:A:818:ASN:C	1:A:822:PRO:HG3	2.45	0.41
1:B:150:ASP:HB3	1:B:190:PRO:HA	2.03	0.41
1:B:178:VAL:HA	1:B:179:PRO:HD3	1.87	0.41
1:B:330:ARG:HA	1:B:333:GLN:HE21	1.80	0.41
1:B:335:ASP:O	1:B:339:GLN:HA	2.20	0.41
1:A:113:PHE:CE1	1:A:218:VAL:HG23	2.55	0.41
1:A:125:GLU:HB3	1:A:128:GLN:HE22	1.83	0.41
1:A:188:TYR:C	1:A:188:TYR:CD1	2.98	0.41
1:A:240:LYS:C	1:A:242:LEU:H	2.28	0.41
1:A:400:ILE:HA	1:A:401:PRO:HD3	1.86	0.41
1:A:621:ASP:O	1:A:623:ASP:N	2.50	0.41
1:A:663:ILE:HD12	1:A:663:ILE:N	2.35	0.41
1:A:745:LEU:O	1:A:748:CYS:N	2.54	0.41
1:B:243:SER:CB	1:B:247:LYS:H	2.33	0.41
1:B:373:LEU:O	1:B:376:GLN:HB2	2.20	0.41
1:B:415:LEU:O	1:B:416:TYR:C	2.62	0.41
1:B:807:GLY:O	1:B:810:THR:CG2	2.67	0.41
1:B:858:ILE:O	1:B:859:LYS:C	2.64	0.41
1:A:253:ILE:HG22	1:A:254:GLU:H	1.84	0.41
1:A:293:ILE:N	1:A:293:ILE:HD12	2.35	0.41
1:A:343:LEU:O	1:A:346:ASP:HB3	2.20	0.41
1:A:373:LEU:O	1:A:376:GLN:HB3	2.20	0.41
1:A:406:TYR:C	1:A:407:VAL:HG23	2.46	0.41
1:B:41:CYS:SG	1:B:45:GLN:HB2	2.61	0.41
1:B:51:ASP:HB3	1:B:83:LEU:CD2	2.51	0.41
1:B:139:TYR:CD1	1:B:140:ASP:N	2.89	0.41
1:B:157:GLY:O	1:B:313:ARG:NH2	2.46	0.41
1:B:182:ILE:O	1:B:186:ILE:HD13	2.20	0.41
1:B:512:GLU:OE1	1:B:513:PRO:HD2	2.21	0.41
1:B:792:ASP:O	1:B:794:GLY:N	2.53	0.41
1:A:9:GLU:HG3	1:A:266:PHE:CE1	2.56	0.41
1:A:189:MET:O	1:A:191:PHE:CE1	2.73	0.41
1:A:364:THR:O	1:A:367:ALA:HB3	2.19	0.41
1:A:364:THR:O	1:A:368:ILE:HG13	2.20	0.41
1:A:633:ILE:HD13	1:A:633:ILE:HA	1.88	0.41
1:B:293:ILE:HG23	1:B:297:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:O	1:B:349:TYR:HB2	2.21	0.41
1:B:456:CYS:HB3	1:B:462:MET:H	1.85	0.41
1:B:475:ILE:HD11	1:B:566:LEU:CD2	2.46	0.41
1:B:570:LEU:HD23	1:B:570:LEU:HA	1.44	0.41
1:B:597:ILE:HB	1:B:667:PHE:HE1	1.82	0.41
1:B:767:PHE:O	1:B:768:GLU:HB3	2.20	0.41
1:B:896:SER:C	1:B:898:PHE:N	2.77	0.41
1:A:108:ILE:HG22	1:A:211:VAL:HG11	2.03	0.41
1:A:109:ARG:HH12	1:A:142:ILE:HG21	1.86	0.41
1:A:188:TYR:HD1	1:A:188:TYR:C	2.29	0.41
1:A:363:LYS:HD3	1:A:363:LYS:HA	1.77	0.41
1:A:369:ILE:O	1:A:370:PHE:C	2.64	0.41
1:A:434:PHE:HD1	1:A:462:MET:SD	2.43	0.41
1:A:457:SER:HA	1:A:458:PRO:HD3	1.69	0.41
1:A:656:ARG:HA	1:A:660:GLU:HG3	2.02	0.41
1:A:746:LYS:CA	1:A:749:ILE:HD12	2.51	0.41
1:A:757:GLU:HG2	1:A:761:GLN:HG3	2.03	0.41
1:A:867:ASP:O	1:A:871:LEU:HB2	2.21	0.41
1:B:78:ILE:HG22	1:B:80:LEU:N	2.36	0.41
1:B:335:ASP:CG	1:B:341:ILE:HD12	2.46	0.41
1:B:354:GLN:O	1:B:357:SER:HB2	2.21	0.41
1:B:367:ALA:O	1:B:368:ILE:C	2.64	0.41
1:B:373:LEU:HA	1:B:373:LEU:HD12	1.80	0.41
1:B:491:ALA:C	1:B:493:GLN:H	2.29	0.41
1:B:606:ASN:N	1:B:616:PHE:HE2	2.19	0.41
1:B:625:ILE:HD11	1:B:683:MET:SD	2.61	0.41
1:B:641:PHE:HE2	1:B:647:TRP:HA	1.86	0.41
1:B:815:ILE:HA	1:B:815:ILE:HD12	1.82	0.41
1:B:816:LYS:HB3	1:B:816:LYS:HE2	1.86	0.41
1:A:198:LEU:CD1	1:A:233:ILE:HD11	2.51	0.41
1:A:201:TYR:O	1:A:202:LEU:C	2.62	0.41
1:A:611:THR:O	1:A:612:GLU:OE2	2.39	0.41
1:A:751:ARG:NH1	1:A:759:SER:O	2.54	0.41
1:B:150:ASP:O	1:B:191:PHE:N	2.54	0.41
1:B:186:ILE:N	1:B:186:ILE:CD1	2.83	0.41
1:B:248:THR:HA	1:B:266:PHE:CD1	2.55	0.41
1:B:422:GLN:HE22	1:B:679:HIS:C	2.29	0.41
1:B:747:GLU:O	1:B:750:ARG:N	2.54	0.41
1:A:391:TYR:CD2	1:A:587:THR:HG21	2.55	0.40
1:A:445:ALA:HA	1:A:673:TYR:CE2	2.55	0.40
1:A:795:GLY:C	1:A:796:PHE:HD1	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:C	1:B:378:LYS:HD2	2.47	0.40
1:B:491:ALA:O	1:B:493:GLN:N	2.53	0.40
1:B:787:ASN:O	1:B:790:LYS:CG	2.70	0.40
1:B:791:TYR:CG	1:B:791:TYR:O	2.74	0.40
1:A:327:ASP:O	1:A:328:VAL:C	2.65	0.40
1:A:815:ILE:O	1:A:815:ILE:HG22	2.21	0.40
1:B:53:TYR:CE1	1:B:428:GLU:HA	2.48	0.40
1:B:81:GLU:CD	1:B:83:LEU:HD11	2.46	0.40
1:B:169:LYS:C	1:B:175:GLY:HA3	2.46	0.40
1:B:876:PHE:O	1:B:879:PRO:HG2	2.20	0.40
1:A:128:GLN:O	1:A:129:ALA:HB3	2.20	0.40
1:B:49:TYR:OH	1:B:59:ARG:HD2	2.20	0.40
1:B:64:ASN:OD1	1:B:65:MET:N	2.55	0.40
1:B:205:TRP:O	1:B:209:THR:N	2.53	0.40
1:B:419:ILE:HG22	1:B:420:ILE:N	2.34	0.40
1:A:14:SER:HA	1:A:32:GLU:HA	2.03	0.40
1:A:34:LYS:HB3	1:A:34:LYS:HE3	1.77	0.40
1:A:140:ASP:HB3	1:A:143:ASP:HB2	2.03	0.40
1:A:147:TYR:N	1:A:147:TYR:HD1	2.17	0.40
1:A:263:ILE:HD12	1:A:263:ILE:N	2.36	0.40
1:A:647:TRP:O	1:A:650:PHE:CB	2.64	0.40
1:A:667:PHE:HD1	1:A:667:PHE:HA	1.73	0.40
1:A:685:ARG:HG2	1:A:686:GLU:N	2.37	0.40
1:A:738:PRO:HG3	1:A:780:ALA:O	2.21	0.40
1:B:6:LEU:CD1	1:B:211:VAL:HG11	2.51	0.40
1:B:109:ARG:HA	1:B:142:ILE:HG12	2.03	0.40
1:B:145:ARG:HE	1:B:185:LYS:HA	1.87	0.40
1:B:327:ASP:O	1:B:330:ARG:N	2.54	0.40
1:B:422:GLN:NE2	1:B:679:HIS:C	2.79	0.40
1:B:511:ASP:CB	1:B:537:SER:OG	2.67	0.40
1:B:659:MET:C	1:B:661:PRO:HD2	2.47	0.40
1:B:713:TRP:CH2	1:B:723:PRO:HB3	2.57	0.40
1:B:818:ASN:HD22	1:B:819:ILE:H	1.70	0.40
1:A:34:LYS:CE	1:A:63:ALA:HA	2.51	0.40
1:A:218:VAL:HG22	1:A:223:ILE:CD1	2.52	0.40
1:A:249:ARG:HG2	1:A:251:LYS:HE3	2.03	0.40
1:A:274:ILE:HG12	1:A:278:LYS:HE3	2.03	0.40
1:A:351:ALA:HB3	1:A:353:ILE:CG2	2.52	0.40
1:A:356:GLN:C	1:A:358:VAL:N	2.78	0.40
1:A:746:LYS:HA	1:A:749:ILE:HD12	2.03	0.40
1:B:91:ALA:O	1:B:92:TYR:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:HA	1:B:210:PRO:HD3	1.82	0.40
1:B:430:ILE:HG23	1:B:430:ILE:O	2.22	0.40
1:B:482:ARG:HB2	1:B:559:ARG:HB2	2.03	0.40
1:B:727:ILE:HG23	1:B:728:MET:N	2.37	0.40
1:B:767:PHE:O	1:B:768:GLU:CB	2.70	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	901/903 (100%)	657 (73%)	170 (19%)	74 (8%)	0	4
1	B	901/903 (100%)	659 (73%)	177 (20%)	65 (7%)	1	6
All	All	1802/1806 (100%)	1316 (73%)	347 (19%)	139 (8%)	1	5

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	255	ASN
1	A	312	LEU
1	A	316	ASN
1	A	405	LYS
1	A	451	SER
1	A	462	MET
1	A	523	SER
1	A	539	ASN
1	A	643	ASP
1	A	680	LEU
1	A	692	PRO
1	A	766	GLU

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Mol	Chain	Res	Type
1	A	768	GLU
1	A	787	ASN
1	A	797	PRO
1	A	799	PRO
1	A	819	ILE
1	A	827	GLY
1	A	829	LYS
1	A	845	CYS
1	A	895	ALA
1	B	24	GLY
1	B	161	GLU
1	B	259	SER
1	B	388	VAL
1	B	451	SER
1	B	507	ASN
1	B	622	THR
1	B	680	LEU
1	B	731	GLU
1	B	766	GLU
1	B	768	GLU
1	B	787	ASN
1	B	791	TYR
1	B	793	VAL
1	B	799	PRO
1	B	804	HIS
1	B	818	ASN
1	B	834	PRO
1	B	835	LEU
1	B	897	LEU
1	A	24	GLY
1	A	49	TYR
1	A	101	ILE
1	A	122	GLY
1	A	376	GLN
1	A	458	PRO
1	A	507	ASN
1	A	550	VAL
1	A	637	GLY
1	A	659	MET
1	A	721	ALA
1	A	804	HIS
1	A	859	LYS

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Mol	Chain	Res	Type
1	A	862	VAL
1	A	866	MET
1	B	43	GLU
1	B	102	LYS
1	B	109	ARG
1	B	122	GLY
1	B	181	GLU
1	B	312	LEU
1	B	344	SER
1	B	415	LEU
1	B	433	THR
1	B	509	SER
1	B	646	HIS
1	B	736	SER
1	B	789	ALA
1	B	797	PRO
1	B	832	VAL
1	B	836	ARG
1	B	895	ALA
1	A	44	SER
1	A	105	HIS
1	A	181	GLU
1	A	226	VAL
1	A	256	MET
1	A	381	PRO
1	A	415	LEU
1	A	506	PRO
1	A	522	PHE
1	A	630	ASP
1	A	731	GLU
1	A	734	LYS
1	A	832	VAL
1	A	834	PRO
1	B	241	ARG
1	B	390	PRO
1	B	523	SER
1	B	605	LEU
1	B	693	LEU
1	B	821	ALA
1	B	843	ASP
1	B	873	GLU
1	A	22	SER

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Mol	Chain	Res	Type
1	A	63	ALA
1	A	183	ILE
1	A	228	ASN
1	A	278	LYS
1	A	519	ARG
1	A	538	LEU
1	A	586	ILE
1	B	52	ILE
1	B	257	TYR
1	B	414	SER
1	B	424	ASN
1	B	506	PRO
1	B	661	PRO
1	B	827	GLY
1	A	102	LYS
1	A	124	PRO
1	A	295	GLU
1	A	603	GLU
1	A	793	VAL
1	A	796	PHE
1	B	222	ASP
1	B	316	ASN
1	B	318	GLN
1	B	362	ILE
1	B	462	MET
1	B	601	VAL
1	B	643	ASP
1	B	730	LEU
1	B	758	GLU
1	B	859	LYS
1	A	3	GLU
1	A	187	ILE
1	A	622	THR
1	A	718	THR
1	B	374	LYS
1	B	659	MET
1	A	300	VAL
1	B	392	PRO
1	A	470	VAL
1	A	52	ILE
1	A	326	ILE
1	A	390	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	802/802 (100%)	617 (77%)	185 (23%)	1	5
1	B	802/802 (100%)	608 (76%)	194 (24%)	1	4
All	All	1604/1604 (100%)	1225 (76%)	379 (24%)	1	4

All (379) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	6	LEU
1	A	9	GLU
1	A	11	ILE
1	A	15	ILE
1	A	22	SER
1	A	44	SER
1	A	47	THR
1	A	48	LYS
1	A	49	TYR
1	A	52	ILE
1	A	58	THR
1	A	59	ARG
1	A	61	LEU
1	A	64	ASN
1	A	66	ARG
1	A	69	SER
1	A	78	ILE
1	A	89	LYS
1	A	95	ASP
1	A	96	THR
1	A	101	ILE
1	A	105	HIS
1	A	108	ILE
1	A	112	ASN
1	A	113	PHE
1	A	114	ASP

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Mol	Chain	Res	Type
1	A	115	ILE
1	A	121	ASP
1	A	124	PRO
1	A	125	GLU
1	A	130	LYS
1	A	141	SER
1	A	147	TYR
1	A	149	PHE
1	A	165	GLU
1	A	169	LYS
1	A	170	LEU
1	A	173	GLN
1	A	184	ASP
1	A	187	ILE
1	A	188	TYR
1	A	189	MET
1	A	191	PHE
1	A	197	LEU
1	A	199	MET
1	A	200	GLU
1	A	202	LEU
1	A	211	VAL
1	A	212	ILE
1	A	213	LEU
1	A	217	ASN
1	A	220	SER
1	A	232	ASN
1	A	238	THR
1	A	242	LEU
1	A	254	GLU
1	A	256	MET
1	A	260	ARG
1	A	262	ILE
1	A	280	PHE
1	A	285	GLN
1	A	289	SER
1	A	294	SER
1	A	309	ILE
1	A	312	LEU
1	A	314	GLU
1	A	331	VAL
1	A	332	LEU

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Mol	Chain	Res	Type
1	A	337	LYS
1	A	338	ARG
1	A	339	GLN
1	A	342	ASN
1	A	345	LEU
1	A	353	ILE
1	A	356	GLN
1	A	358	VAL
1	A	363	LYS
1	A	375	GLU
1	A	376	GLN
1	A	391	TYR
1	A	408	MET
1	A	418	SER
1	A	419	ILE
1	A	422	GLN
1	A	423	VAL
1	A	436	VAL
1	A	438	PRO
1	A	443	ILE
1	A	455	SER
1	A	459	ASN
1	A	462	MET
1	A	466	ASP
1	A	475	ILE
1	A	481	GLN
1	A	501	GLU
1	A	503	LEU
1	A	505	ASN
1	A	507	ASN
1	A	508	LEU
1	A	511	ASP
1	A	513	PRO
1	A	514	LEU
1	A	516	VAL
1	A	519	ARG
1	A	526	ILE
1	A	528	GLU
1	A	536	LYS
1	A	541	MET
1	A	549	GLU
1	A	553	MET

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Mol	Chain	Res	Type
1	A	556	GLN
1	A	559	ARG
1	A	562	LEU
1	A	573	VAL
1	A	577	TYR
1	A	587	THR
1	A	594	LEU
1	A	595	GLN
1	A	598	GLU
1	A	603	GLU
1	A	606	ASN
1	A	607	GLU
1	A	614	GLU
1	A	617	VAL
1	A	618	LEU
1	A	625	ILE
1	A	627	VAL
1	A	631	LYS
1	A	632	ILE
1	A	633	ILE
1	A	639	SER
1	A	640	LYS
1	A	644	THR
1	A	647	TRP
1	A	654	PHE
1	A	659	MET
1	A	667	PHE
1	A	671	CYS
1	A	680	LEU
1	A	685	ARG
1	A	686	GLU
1	A	693	LEU
1	A	698	ILE
1	A	703	THR
1	A	705	LYS
1	A	710	LEU
1	A	718	THR
1	A	722	GLU
1	A	728	MET
1	A	731	GLU
1	A	736	SER
1	A	741	VAL

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Mol	Chain	Res	Type
1	A	762	GLU
1	A	763	TYR
1	A	765	LYS
1	A	767	PHE
1	A	768	GLU
1	A	769	LYS
1	A	788	ILE
1	A	791	TYR
1	A	799	PRO
1	A	803	PHE
1	A	804	HIS
1	A	809	LEU
1	A	816	LYS
1	A	818	ASN
1	A	828	GLU
1	A	834	PRO
1	A	837	GLU
1	A	846	ILE
1	A	855	THR
1	A	857	LEU
1	A	859	LYS
1	A	860	ASP
1	A	863	LEU
1	A	871	LEU
1	A	872	LEU
1	A	877	ILE
1	A	880	LEU
1	A	890	ASP
1	A	896	SER
1	A	897	LEU
1	A	902	ASP
1	A	903	PHE
1	B	6	LEU
1	B	15	ILE
1	B	17	GLU
1	B	19	TYR
1	B	22	SER
1	B	26	GLU
1	B	27	ARG
1	B	30	GLU
1	B	36	SER
1	B	43	GLU

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Mol	Chain	Res	Type
1	B	44	SER
1	B	47	THR
1	B	52	ILE
1	B	57	CYS
1	B	65	MET
1	B	70	GLN
1	B	73	LYS
1	B	75	MET
1	B	86	ASP
1	B	90	LEU
1	B	92	TYR
1	B	97	TYR
1	B	105	HIS
1	B	106	THR
1	B	112	ASN
1	B	118	THR
1	B	121	ASP
1	B	130	LYS
1	B	142	ILE
1	B	147	TYR
1	B	158	ASN
1	B	165	GLU
1	B	169	LYS
1	B	173	GLN
1	B	180	SER
1	B	181	GLU
1	B	183	ILE
1	B	184	ASP
1	B	185	LYS
1	B	189	MET
1	B	195	LYS
1	B	199	MET
1	B	220	SER
1	B	232	ASN
1	B	245	HIS
1	B	246	ARG
1	B	248	THR
1	B	250	VAL
1	B	251	LYS
1	B	252	VAL
1	B	255	ASN
1	B	257	TYR

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Mol	Chain	Res	Type
1	B	259	SER
1	B	268	ILE
1	B	271	LEU
1	B	276	LEU
1	B	285	GLN
1	B	291	ASP
1	B	294	SER
1	B	296	PHE
1	B	309	ILE
1	B	312	LEU
1	B	330	ARG
1	B	337	LYS
1	B	343	LEU
1	B	344	SER
1	B	356	GLN
1	B	358	VAL
1	B	360	SER
1	B	363	LYS
1	B	370	PHE
1	B	373	LEU
1	B	375	GLU
1	B	382	GLN
1	B	388	VAL
1	B	390	PRO
1	B	399	PRO
1	B	403	ARG
1	B	407	VAL
1	B	408	MET
1	B	411	ASP
1	B	412	LEU
1	B	418	SER
1	B	419	ILE
1	B	422	GLN
1	B	430	ILE
1	B	443	ILE
1	B	444	ASN
1	B	446	VAL
1	B	452	ASP
1	B	453	VAL
1	B	456	CYS
1	B	459	ASN
1	B	466	ASP

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Mol	Chain	Res	Type
1	B	467	ARG
1	B	468	ASP
1	B	499	ILE
1	B	503	LEU
1	B	505	ASN
1	B	507	ASN
1	B	510	VAL
1	B	511	ASP
1	B	514	LEU
1	B	515	ASP
1	B	519	ARG
1	B	524	ASP
1	B	525	GLU
1	B	531	LYS
1	B	532	LYS
1	B	533	LEU
1	B	541	MET
1	B	542	LEU
1	B	547	ARG
1	B	553	MET
1	B	554	THR
1	B	556	GLN
1	B	557	ILE
1	B	559	ARG
1	B	562	LEU
1	B	573	VAL
1	B	594	LEU
1	B	595	GLN
1	B	598	GLU
1	B	604	TYR
1	B	605	LEU
1	B	611	THR
1	B	618	LEU
1	B	624	SER
1	B	627	VAL
1	B	628	SER
1	B	631	LYS
1	B	634	ASP
1	B	638	GLU
1	B	639	SER
1	B	640	LYS
1	B	642	ARG

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Mol	Chain	Res	Type
1	B	644	THR
1	B	659	MET
1	B	661	PRO
1	B	678	GLN
1	B	684	ASP
1	B	693	LEU
1	B	698	ILE
1	B	703	THR
1	B	707	ARG
1	B	716	GLU
1	B	722	GLU
1	B	724	LYS
1	B	727	ILE
1	B	728	MET
1	B	731	GLU
1	B	733	GLN
1	B	735	SER
1	B	736	SER
1	B	747	GLU
1	B	762	GLU
1	B	766	GLU
1	B	768	GLU
1	B	772	ARG
1	B	773	GLN
1	B	774	LEU
1	B	777	ILE
1	B	778	SER
1	B	790	LYS
1	B	791	TYR
1	B	792	ASP
1	B	799	PRO
1	B	804	HIS
1	B	809	LEU
1	B	815	ILE
1	B	816	LYS
1	B	818	ASN
1	B	824	VAL
1	B	834	PRO
1	B	835	LEU
1	B	837	GLU
1	B	841	PHE
1	B	844	LYS

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Mol	Chain	Res	Type
1	B	850	SER
1	B	853	GLU
1	B	854	ILE
1	B	855	THR
1	B	857	LEU
1	B	859	LYS
1	B	867	ASP
1	B	869	THR
1	B	871	LEU
1	B	872	LEU
1	B	880	LEU
1	B	881	GLU
1	B	890	ASP
1	B	897	LEU
1	B	902	ASP
1	B	903	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	112	ASN
1	A	131	HIS
1	A	173	GLN
1	A	206	GLN
1	A	232	ASN
1	A	318	GLN
1	A	324	ASN
1	A	333	GLN
1	A	339	GLN
1	A	356	GLN
1	A	377	ASN
1	A	389	GLN
1	A	402	ASN
1	A	422	GLN
1	A	480	ASN
1	A	539	ASN
1	A	546	GLN
1	A	558	ASN
1	A	761	GLN
1	A	786	ASN
1	A	818	ASN

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Mol	Chain	Res	Type
1	B	10	GLN
1	B	112	ASN
1	B	158	ASN
1	B	173	GLN
1	B	193	ASN
1	B	203	ASN
1	B	217	ASN
1	B	245	HIS
1	B	255	ASN
1	B	333	GLN
1	B	339	GLN
1	B	354	GLN
1	B	356	GLN
1	B	389	GLN
1	B	402	ASN
1	B	422	GLN
1	B	444	ASN
1	B	459	ASN
1	B	481	GLN
1	B	485	HIS
1	B	539	ASN
1	B	556	GLN
1	B	582	ASN
1	B	645	ASN
1	B	676	ASN
1	B	818	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GMP	B	999	-	22,22,22	1.73	4 (18%)	33,33,33	1.42	3 (9%)
2	GMP	A	999	-	22,22,22	1.53	2 (9%)	33,33,33	1.15	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GMP	B	999	-	-	1/6/22/22	0/3/3/3
2	GMP	A	999	-	-	0/6/22/22	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	GMP	O3'-C3'	4.33	1.53	1.43
2	A	999	GMP	C6-N1	3.94	1.46	1.38
2	B	999	GMP	C6-N1	3.03	1.44	1.38
2	B	999	GMP	C4-N3	2.91	1.40	1.34
2	B	999	GMP	C2-N1	2.22	1.43	1.37
2	A	999	GMP	C4-N3	2.10	1.39	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	GMP	C2'-C3'-C4'	-4.20	94.49	102.61
2	A	999	GMP	C5'-C4'-C3'	-3.18	107.58	115.10
2	B	999	GMP	N1-C2-N3	-2.47	118.81	123.32
2	A	999	GMP	O4'-C4'-C5'	2.44	114.37	109.22
2	B	999	GMP	O4'-C1'-C2'	-2.24	101.82	106.62
2	A	999	GMP	O2'-C2'-C1'	2.04	117.13	110.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

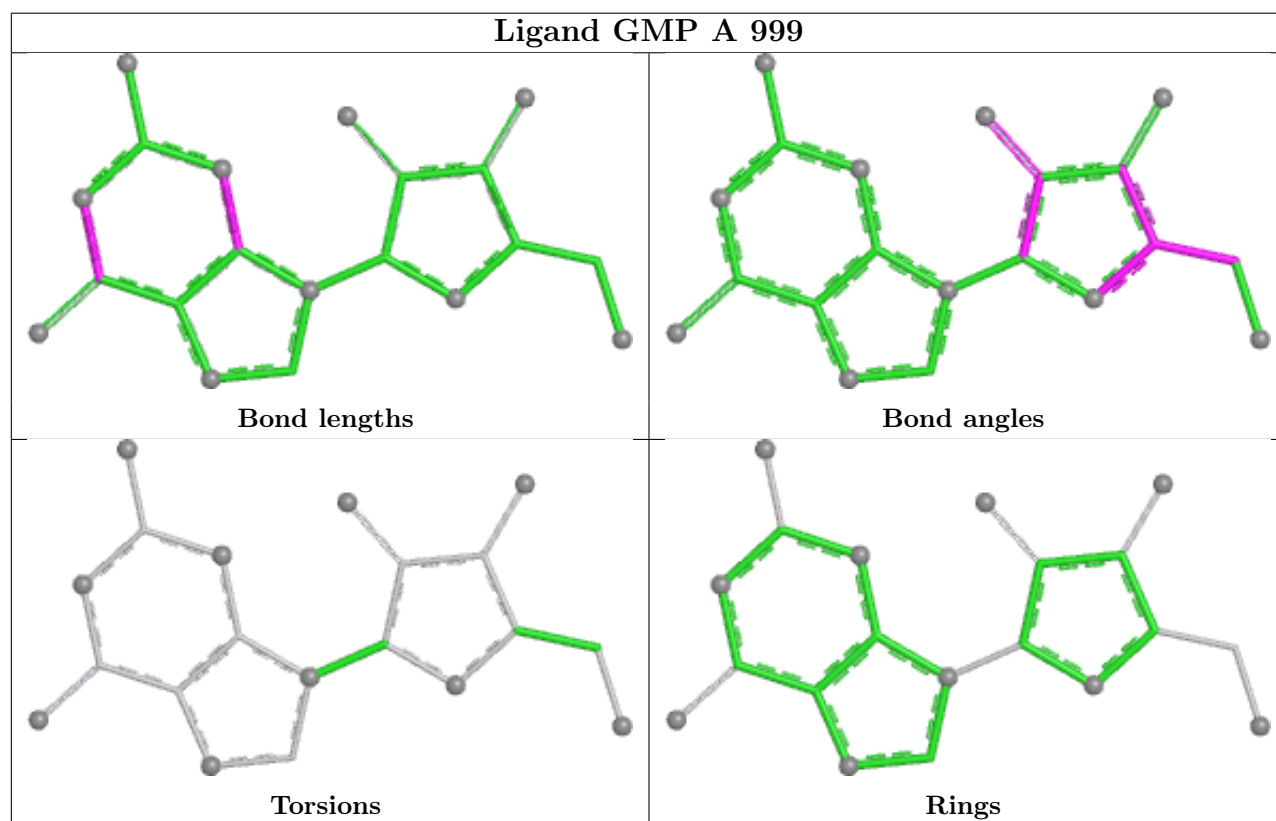
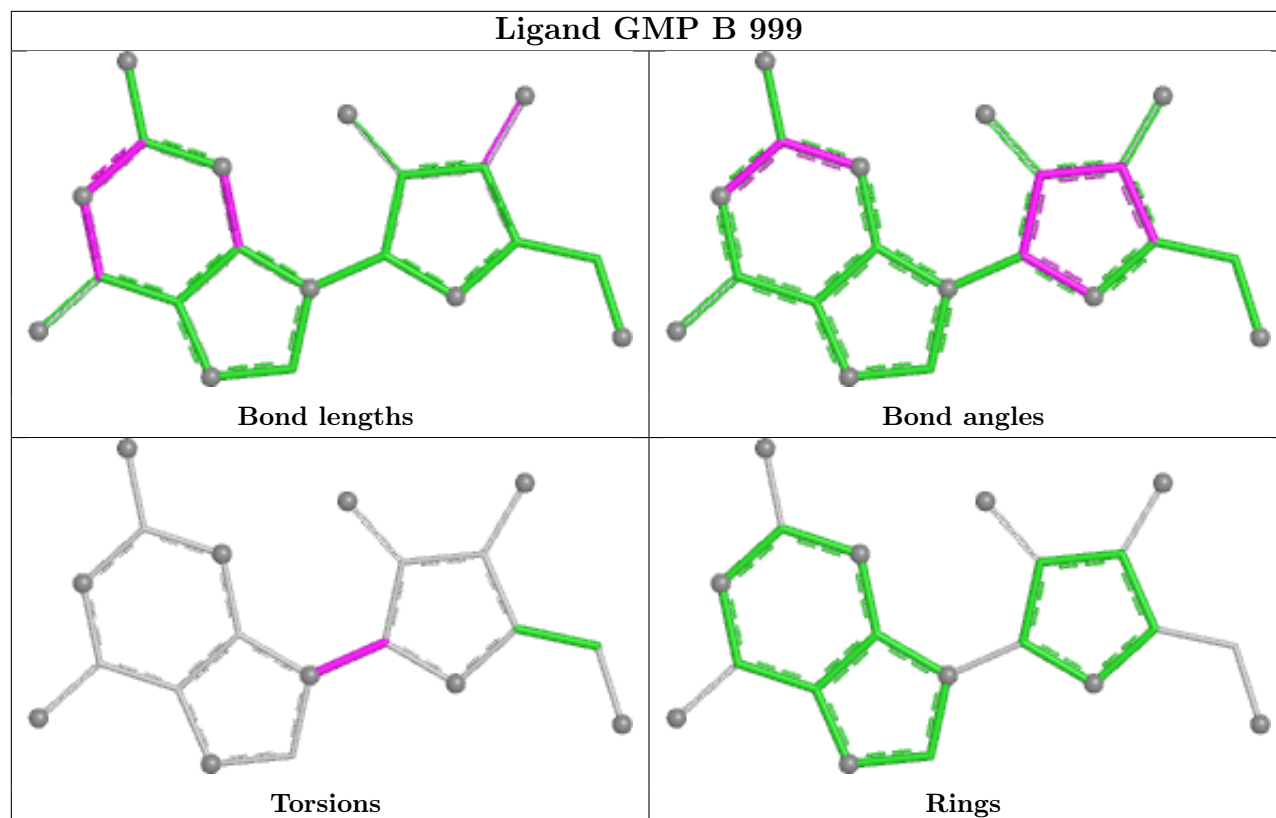
Mol	Chain	Res	Type	Atoms
2	B	999	GMP	O4'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	999	GMP	2	0
2	A	999	GMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	903/903 (100%)	-0.03	18 (1%) 65 45	40, 68, 100, 100	0
1	B	903/903 (100%)	-0.06	7 (0%) 82 67	39, 68, 100, 100	0
All	All	1806/1806 (100%)	-0.04	25 (1%) 73 54	39, 68, 100, 100	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	665	ARG	4.7
1	A	903	PHE	3.8
1	A	514	LEU	3.8
1	A	508	LEU	3.7
1	A	821	ALA	3.5
1	B	821	ALA	3.5
1	B	824	VAL	3.4
1	B	823	GLN	3.4
1	A	820	ASP	3.4
1	A	513	PRO	3.3
1	A	819	ILE	3.2
1	A	510	VAL	3.1
1	A	665	ARG	2.8
1	A	502	ALA	2.5
1	B	514	LEU	2.5
1	A	804	HIS	2.3
1	B	786	ASN	2.3
1	A	259	SER	2.2
1	A	512	GLU	2.2
1	B	793	VAL	2.1
1	A	507	ASN	2.1
1	A	789	ALA	2.1
1	A	509	SER	2.0
1	A	84	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	515	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

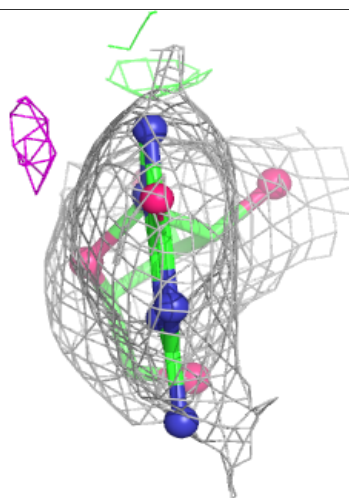
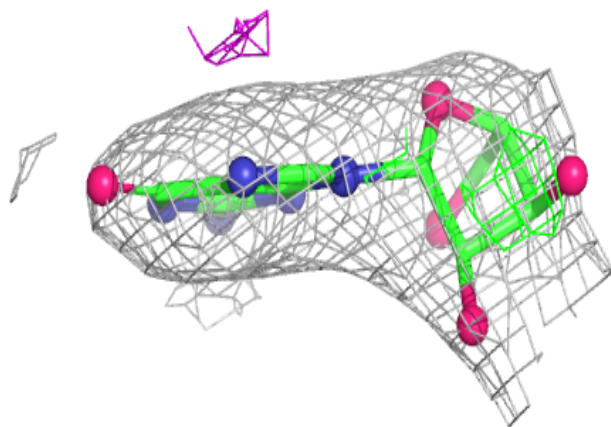
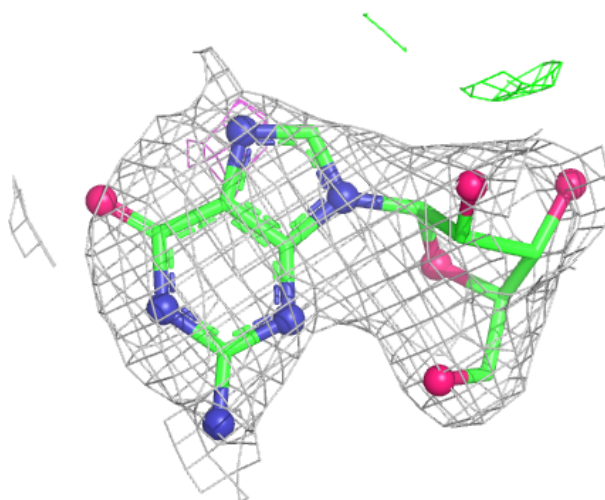
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

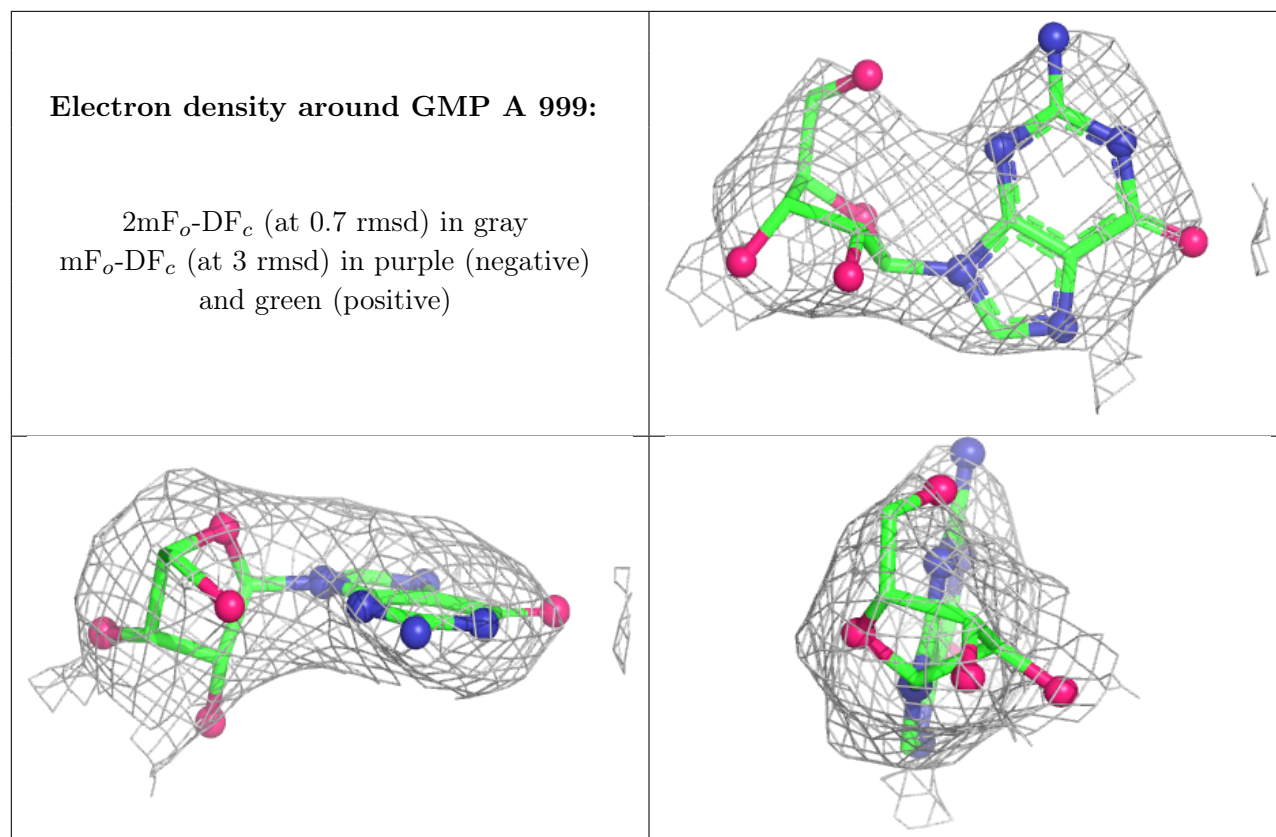
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GMP	B	999	20/20	0.93	0.11	82,82,84,84	0
2	GMP	A	999	20/20	0.95	0.11	81,82,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GMP B 999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.