



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:15 AM GMT

PDB ID : 1GC3
Title : THERMUS THERMOPHILUS ASPARTATE AMINOTRANSFERASE
TETRA MUTANT 2 COMPLEXED WITH TRYPTOPHAN
Authors : Ura, H.; Nakai, T.; Hirotsu, K.; Kuramitsu, S.
Deposited on : 2000-07-18
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

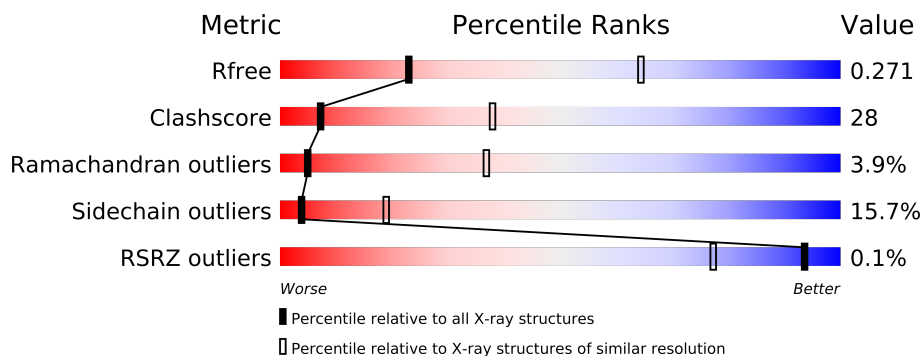
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	385	
1	B	385	
1	C	385	
1	D	385	
1	E	385	
1	F	385	
1	G	385	
1	H	385	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	TRP	A	414	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	TRP	A	914	-	X
2	TRP	C	1414	-	X
2	TRP	D	1914	-	X
2	TRP	E	2414	-	X
2	TRP	E	2914	-	X
2	TRP	G	3414	-	X
2	TRP	H	3914	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23824 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	B	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	C	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	D	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	E	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	F	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	G	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	H	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			

There are 32 discrepancies between the modelled and reference sequences:

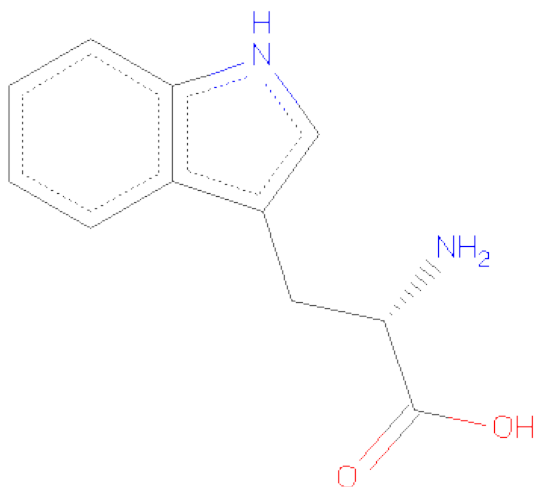
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	SER	ENGINEERED	UNP Q56232
A	16	VAL	THR	ENGINEERED	UNP Q56232
A	101	SER	LYS	ENGINEERED	UNP Q56232
A	261	ARG	SER	ENGINEERED	UNP Q56232
B	514	ASP	SER	ENGINEERED	UNP Q56232
B	516	VAL	THR	ENGINEERED	UNP Q56232
B	601	SER	LYS	ENGINEERED	UNP Q56232
B	761	ARG	SER	ENGINEERED	UNP Q56232
C	1014	ASP	SER	ENGINEERED	UNP Q56232
C	1016	VAL	THR	ENGINEERED	UNP Q56232
C	1101	SER	LYS	ENGINEERED	UNP Q56232
C	1261	ARG	SER	ENGINEERED	UNP Q56232
D	1514	ASP	SER	ENGINEERED	UNP Q56232

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1516	VAL	THR	ENGINEERED	UNP Q56232
D	1601	SER	LYS	ENGINEERED	UNP Q56232
D	1761	ARG	SER	ENGINEERED	UNP Q56232
E	2014	ASP	SER	ENGINEERED	UNP Q56232
E	2016	VAL	THR	ENGINEERED	UNP Q56232
E	2101	SER	LYS	ENGINEERED	UNP Q56232
E	2261	ARG	SER	ENGINEERED	UNP Q56232
F	2514	ASP	SER	ENGINEERED	UNP Q56232
F	2516	VAL	THR	ENGINEERED	UNP Q56232
F	2601	SER	LYS	ENGINEERED	UNP Q56232
F	2761	ARG	SER	ENGINEERED	UNP Q56232
G	3014	ASP	SER	ENGINEERED	UNP Q56232
G	3016	VAL	THR	ENGINEERED	UNP Q56232
G	3101	SER	LYS	ENGINEERED	UNP Q56232
G	3261	ARG	SER	ENGINEERED	UNP Q56232
H	3514	ASP	SER	ENGINEERED	UNP Q56232
H	3516	VAL	THR	ENGINEERED	UNP Q56232
H	3601	SER	LYS	ENGINEERED	UNP Q56232
H	3761	ARG	SER	ENGINEERED	UNP Q56232

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



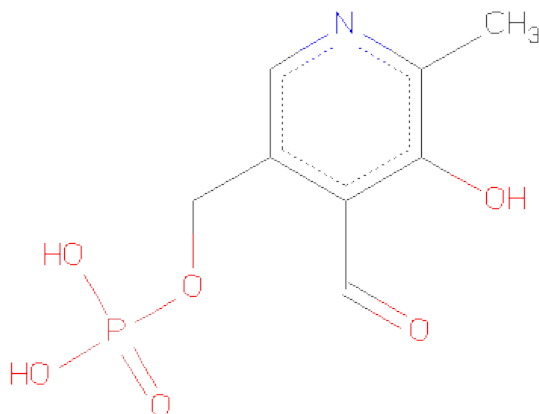
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	A	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	G	1	Total	C	N	O	0	0
			15	11	2	2		
2	H	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).

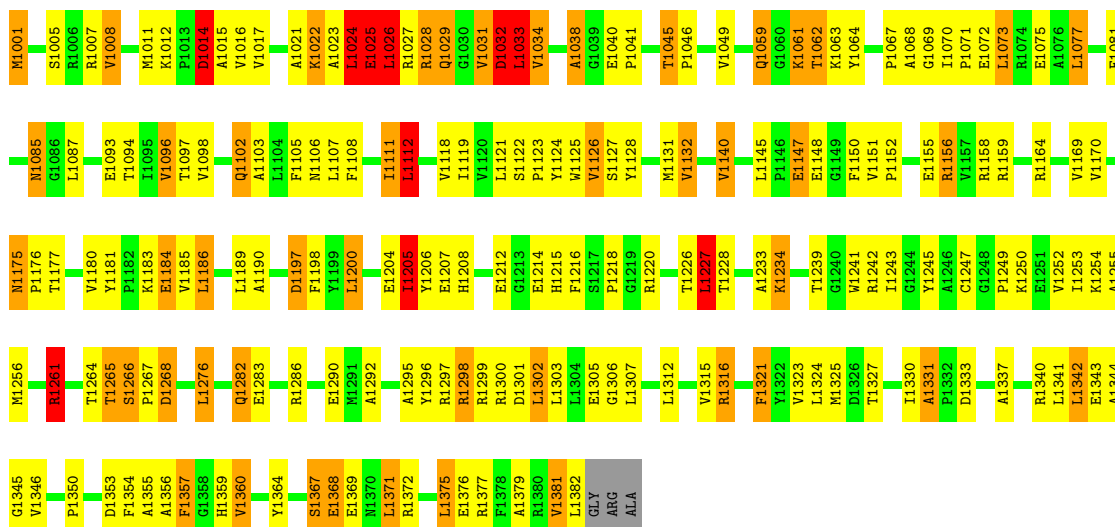


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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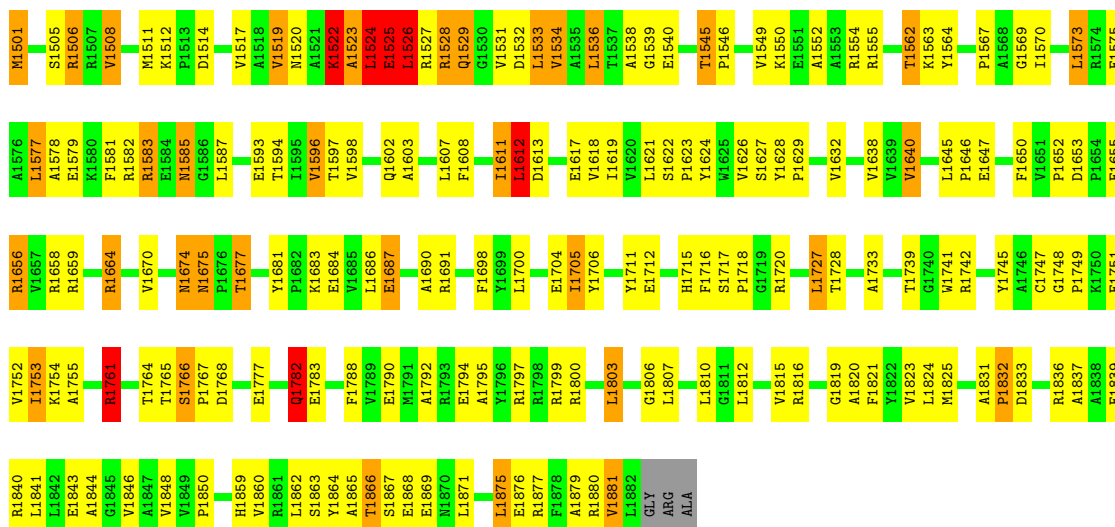
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		



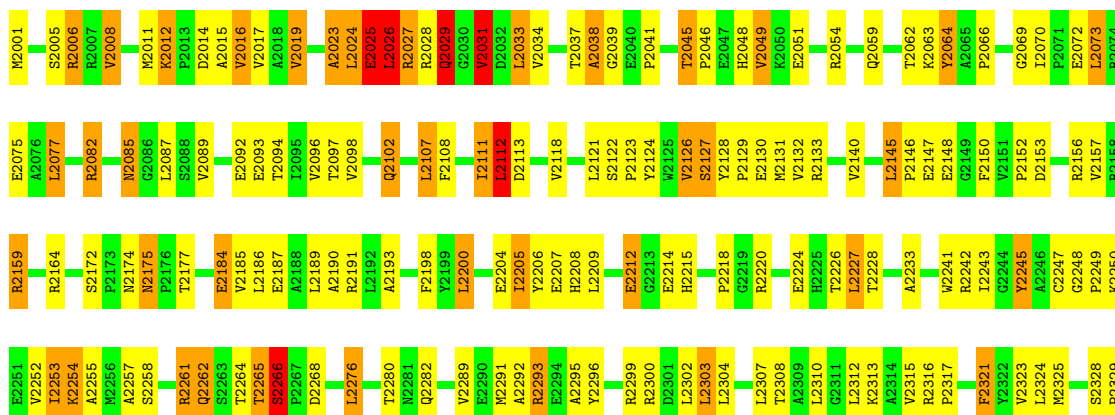
- Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain D:



- Molecule 1: ASPARTATE AMINOTRANSFERASE

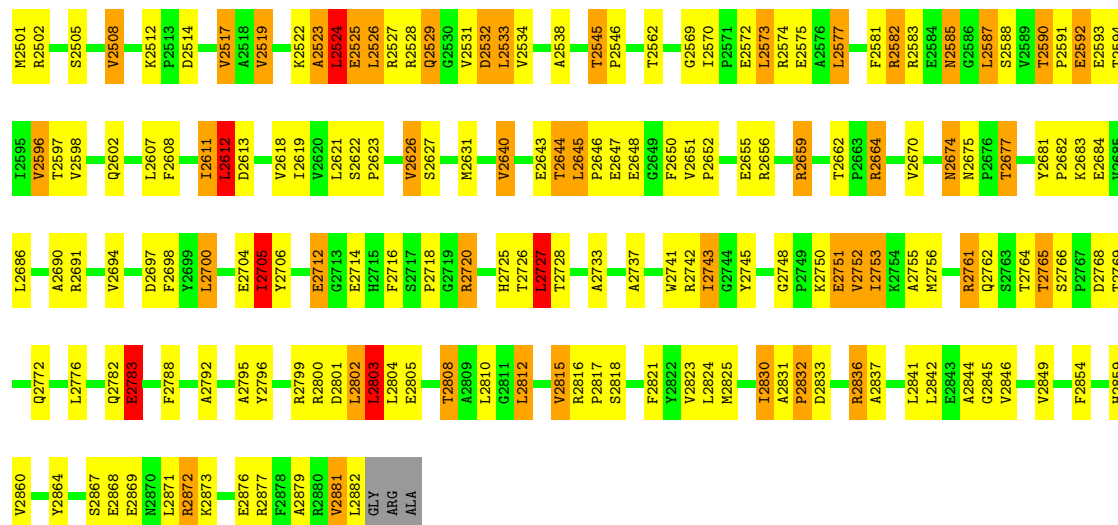
Chain E:





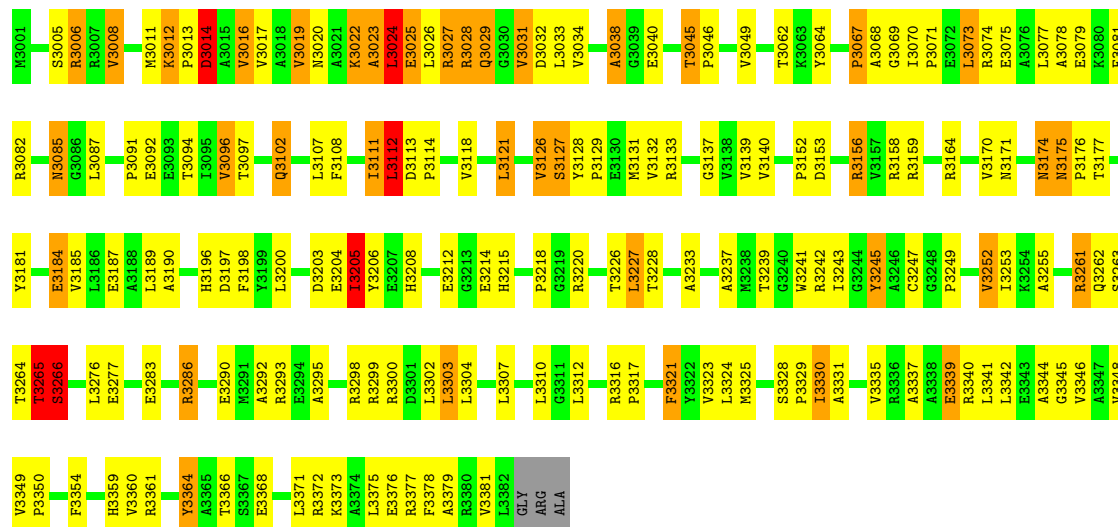
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain F:



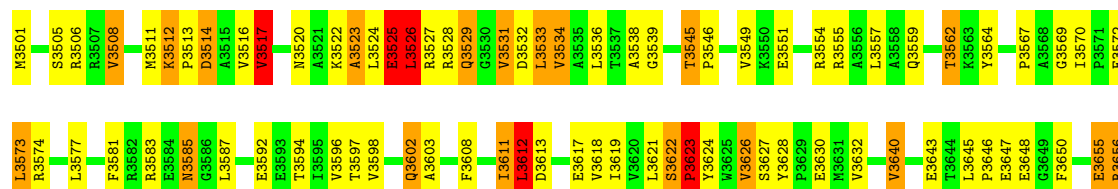
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain G:



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain H:



E3839	R3840	L3841	L3842	E3843	A3844	G3845	V3846		F3854		H3859	V3860	R3861	L3862	S3863	Y3864	A3865		E3868		L3871	R3872	K3873	A3874	L3875	E3876	R3877	A3879	R3880	V3881	L3882	GLY	ARG	ALA																									
G3748	P3749	K3750	E3751	V3752	I3753	K3754	A3755		R3761	Q3762	S3763	T3764	T3765	S3766	P3767	D3768		L3776		Q3782	E3783		R3786		E3790	P3791	A3792	A3795	Y3796		R3799	R3800	D3801	L3802	L3803	L3804		L3807		L3812		P3817		F3821	Y3822	V3823	L3824	M3825	D3826	T3827	S3828	P3829	I3830	A3831	P3832		A3837	A3838	
V3657	R3658	R3659		R3664		V3670		N3674	N3675	P3676	T3677	G3678		Y3681	P3682	K3683	E3684	V3685	L3686	E3687	A3688	L3689	A3690	R3691	L3692	A3693		F3698	Y3699	L3700		E3704	I3705	Y3706	E3707	H3708	L3709		E3714	H3715	F3716	S3717	P3718	G3719	R3720		T3726	L3727	T3728		A3733		W3741	R3742	I3743	G3744	Y3745	A3746	C3747

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.50Å 98.40Å 187.00Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30 47.58 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (8.00-3.30) 94.9 (47.58-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.33Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.203 , 0.282 0.196 , 0.271	Depositor DCC
R_{free} test set	3992 reflections (10.11%)	DCC
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 31.2	EDS
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 42518 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23824	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.0780e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	4/3009 (0.1%)	1.07	23/4092 (0.6%)
1	B	0.43	1/3009 (0.0%)	1.04	22/4092 (0.5%)
1	C	0.48	2/3009 (0.1%)	1.09	25/4092 (0.6%)
1	D	0.45	1/3009 (0.0%)	1.07	19/4092 (0.5%)
1	E	0.43	0/3009	0.98	12/4092 (0.3%)
1	F	0.42	0/3009	0.98	21/4092 (0.5%)
1	G	0.43	0/3009	0.97	17/4092 (0.4%)
1	H	0.48	3/3009 (0.1%)	0.98	21/4092 (0.5%)
All	All	0.45	11/24072 (0.0%)	1.02	160/32736 (0.5%)

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	2
1	C	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1261	ARG	CG-CD	-10.02	1.26	1.51
1	A	261	ARG	NE-CZ	7.27	1.42	1.33
1	H	3517	VAL	CB-CG2	-7.10	1.38	1.52
1	H	3761	ARG	CG-CD	6.76	1.68	1.51
1	H	3761	ARG	CZ-NH2	6.39	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	PRO	CG-CD	-6.38	1.29	1.50
1	A	67	PRO	CA-CB	-5.94	1.41	1.53
1	D	1761	ARG	NE-CZ	5.55	1.40	1.33
1	B	761	ARG	NE-CZ	5.20	1.39	1.33
1	C	1261	ARG	NE-CZ	5.10	1.39	1.33
1	A	67	PRO	N-CD	-5.02	1.40	1.47

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1261	ARG	NE-CZ-NH2	22.81	131.70	120.30
1	A	261	ARG	NE-CZ-NH1	22.08	131.34	120.30
1	D	1761	ARG	NE-CZ-NH2	21.92	131.26	120.30
1	B	761	ARG	NE-CZ-NH2	18.72	129.66	120.30
1	C	1261	ARG	NH1-CZ-NH2	-15.26	102.62	119.40
1	A	261	ARG	NE-CZ-NH2	-14.64	112.98	120.30
1	D	1761	ARG	NH1-CZ-NH2	-14.28	103.69	119.40
1	B	675	ASN	C-N-CD	12.66	155.00	128.40
1	E	2023	ALA	N-CA-C	-12.05	78.47	111.00
1	C	1023	ALA	N-CA-C	-11.98	78.64	111.00
1	C	1026	LEU	N-CA-C	-11.10	81.04	111.00
1	F	2526	LEU	N-CA-C	-10.99	81.33	111.00
1	A	23	ALA	N-CA-C	-10.41	82.89	111.00
1	E	2025	GLU	N-CA-C	-10.26	83.31	111.00
1	A	26	LEU	N-CA-C	-10.21	83.43	111.00
1	B	526	LEU	N-CA-C	-10.08	83.78	111.00
1	B	523	ALA	N-CA-C	-10.06	83.83	111.00
1	G	3023	ALA	N-CA-C	-10.06	83.85	111.00
1	B	761	ARG	NH1-CZ-NH2	-10.05	108.34	119.40
1	F	2523	ALA	N-CA-C	-9.96	84.09	111.00
1	D	1523	ALA	N-CA-C	-9.87	84.35	111.00
1	D	1526	LEU	N-CA-C	-9.84	84.44	111.00
1	E	2255	ALA	N-CA-C	-9.75	84.67	111.00
1	H	3525	GLU	N-CA-C	-9.70	84.80	111.00
1	D	1525	GLU	N-CA-C	-9.27	85.96	111.00
1	B	755	ALA	N-CA-C	-8.91	86.95	111.00
1	C	1025	GLU	N-CA-C	-8.77	87.33	111.00
1	H	3523	ALA	N-CA-C	-8.71	87.50	111.00
1	A	67	PRO	CA-CB-CG	-8.67	87.53	104.00
1	B	525	GLU	N-CA-C	-8.49	88.07	111.00
1	G	3024	LEU	N-CA-C	8.45	133.82	111.00
1	A	67	PRO	N-CD-CG	-8.41	90.58	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3261	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	H	3675	ASN	N-CA-C	-8.12	89.08	111.00
1	F	2755	ALA	N-CA-C	-7.92	89.63	111.00
1	H	3517	VAL	CG1-CB-CG2	-7.84	98.36	110.90
1	D	1755	ALA	N-CA-C	-7.77	90.02	111.00
1	A	255	ALA	N-CA-C	-7.74	90.10	111.00
1	G	3025	GLU	N-CA-C	-7.67	90.30	111.00
1	A	175	ASN	N-CA-C	-7.61	90.44	111.00
1	E	2175	ASN	N-CA-C	-7.59	90.51	111.00
1	H	3755	ALA	N-CA-C	-7.50	90.75	111.00
1	C	1024	LEU	N-CA-C	7.42	131.04	111.00
1	C	1175	ASN	N-CA-C	-7.19	91.59	111.00
1	G	3038	ALA	N-CA-C	7.17	130.37	111.00
1	G	3175	ASN	N-CA-C	-7.17	91.65	111.00
1	H	3526	LEU	N-CA-C	-7.13	91.75	111.00
1	C	1032	ASP	CB-CG-OD1	7.12	124.71	118.30
1	E	2038	ALA	N-CA-C	7.11	130.18	111.00
1	F	2651	VAL	N-CA-C	-7.10	91.83	111.00
1	A	38	ALA	N-CA-C	7.08	130.12	111.00
1	B	538	ALA	N-CA-C	7.04	130.00	111.00
1	F	2538	ALA	N-CA-C	7.03	129.97	111.00
1	H	3517	VAL	CA-CB-CG2	-6.99	100.41	110.90
1	D	1524	LEU	N-CA-C	6.97	129.83	111.00
1	D	1538	ALA	N-CA-C	6.89	129.62	111.00
1	H	3538	ALA	N-CA-C	6.81	129.38	111.00
1	B	675	ASN	C-N-CA	-6.77	93.55	122.00
1	H	3761	ARG	CG-CD-NE	-6.71	97.70	111.80
1	C	1038	ALA	N-CA-C	6.69	129.06	111.00
1	A	25	GLU	N-CA-C	-6.65	93.06	111.00
1	C	1014	ASP	N-CA-C	6.58	128.77	111.00
1	D	1675	ASN	N-CA-C	-6.56	93.28	111.00
1	G	3255	ALA	N-CA-C	-6.54	93.35	111.00
1	F	2675	ASN	N-CA-C	-6.49	93.49	111.00
1	E	2024	LEU	CA-CB-CG	6.47	130.18	115.30
1	F	2612	LEU	N-CA-C	6.42	128.33	111.00
1	F	2640	VAL	N-CA-C	-6.33	93.91	111.00
1	C	1112	LEU	N-CA-C	6.31	128.04	111.00
1	G	3140	VAL	N-CA-C	-6.31	93.95	111.00
1	B	612	LEU	N-CA-C	6.30	128.02	111.00
1	G	3112	LEU	N-CA-C	6.29	128.00	111.00
1	F	2532	ASP	N-CA-C	-6.25	94.12	111.00
1	F	2524	LEU	N-CA-C	6.25	127.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1612	LEU	N-CA-C	6.25	127.87	111.00
1	H	3705	ILE	N-CA-C	6.23	127.81	111.00
1	H	3612	LEU	N-CA-C	6.22	127.80	111.00
1	H	3534	VAL	N-CA-C	-6.18	94.31	111.00
1	G	3014	ASP	N-CA-C	6.17	127.67	111.00
1	E	2112	LEU	N-CA-C	6.17	127.65	111.00
1	G	3127	SER	N-CA-C	6.16	127.64	111.00
1	D	1782	GLN	N-CA-C	-6.14	94.43	111.00
1	B	524	LEU	N-CA-C	6.12	127.51	111.00
1	D	1585	ASN	N-CA-C	6.04	127.30	111.00
1	C	1085	ASN	N-CA-C	6.02	127.26	111.00
1	B	534	VAL	N-CA-C	-5.99	94.82	111.00
1	C	1033	LEU	CA-CB-CG	5.96	129.01	115.30
1	D	1627	SER	N-CA-C	5.96	127.10	111.00
1	H	3627	SER	N-CA-C	5.95	127.07	111.00
1	H	3640	VAL	N-CA-C	-5.91	95.03	111.00
1	A	85	ASN	N-CA-C	5.90	126.93	111.00
1	B	640	VAL	N-CA-C	-5.90	95.07	111.00
1	A	140	VAL	N-CA-C	-5.89	95.09	111.00
1	A	127	SER	N-CA-C	5.84	126.77	111.00
1	E	2085	ASN	N-CA-C	5.83	126.73	111.00
1	C	1034	VAL	N-CA-C	-5.82	95.29	111.00
1	A	121	LEU	N-CA-C	5.81	126.69	111.00
1	D	1674	ASN	N-CA-C	5.81	126.68	111.00
1	H	3585	ASN	N-CA-C	5.80	126.65	111.00
1	F	2585	ASN	N-CA-C	5.76	126.56	111.00
1	A	112	LEU	N-CA-C	5.75	126.51	111.00
1	C	1255	ALA	N-CA-C	-5.74	95.50	111.00
1	H	3623	PRO	CA-N-CD	-5.74	103.46	111.50
1	D	1640	VAL	N-CA-C	-5.71	95.59	111.00
1	B	627	SER	N-CA-C	5.70	126.39	111.00
1	A	34	VAL	N-CA-C	-5.68	95.67	111.00
1	C	1140	VAL	N-CA-C	-5.67	95.69	111.00
1	D	1653	ASP	N-CA-C	-5.67	95.70	111.00
1	A	205	ILE	N-CA-C	5.67	126.29	111.00
1	B	861	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	G	3085	ASN	N-CA-C	5.66	126.28	111.00
1	F	2783	GLU	N-CA-C	5.64	126.24	111.00
1	C	1127	SER	N-CA-C	5.64	126.23	111.00
1	F	2644	THR	N-CA-C	-5.58	95.94	111.00
1	A	209	LEU	N-CA-C	-5.56	95.99	111.00
1	F	2534	VAL	N-CA-C	-5.52	96.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1227	LEU	N-CA-C	-5.52	96.10	111.00
1	C	1032	ASP	N-CA-C	-5.51	96.14	111.00
1	F	2803	LEU	N-CA-C	-5.50	96.15	111.00
1	F	2836	ARG	N-CA-C	-5.49	96.18	111.00
1	A	113	ASP	N-CA-C	-5.47	96.23	111.00
1	B	585	ASN	N-CA-C	5.46	125.75	111.00
1	A	254	LYS	CD-CE-NZ	-5.46	99.14	111.70
1	F	2590	THR	N-CA-C	-5.43	96.34	111.00
1	E	2140	VAL	N-CA-C	-5.43	96.35	111.00
1	H	3720	ARG	N-CA-C	-5.41	96.38	111.00
1	A	67	PRO	CA-N-CD	-5.40	103.94	111.50
1	D	1533	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	1205	ILE	N-CA-C	5.33	125.39	111.00
1	E	2261	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	F	2802	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	720	ARG	N-CA-C	-5.27	96.77	111.00
1	B	514	ASP	N-CA-C	5.24	125.16	111.00
1	H	3861	ARG	N-CA-C	5.24	125.15	111.00
1	B	653	ASP	N-CA-C	-5.21	96.92	111.00
1	G	3205	ILE	N-CA-C	5.20	125.05	111.00
1	E	2209	LEU	N-CA-C	-5.19	96.98	111.00
1	G	3164	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	1132	VAL	N-CA-C	-5.18	97.00	111.00
1	C	1061	LYS	N-CA-C	-5.18	97.01	111.00
1	H	3761	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	G	3361	ARG	N-CA-C	5.17	124.95	111.00
1	B	533	LEU	CA-CB-CG	5.16	127.17	115.30
1	G	3263	SER	N-CA-C	-5.14	97.13	111.00
1	F	2705	ILE	N-CA-C	5.12	124.82	111.00
1	D	1824	LEU	N-CA-C	-5.11	97.20	111.00
1	F	2674	ASN	N-CA-C	5.11	124.78	111.00
1	A	200	LEU	N-CA-C	-5.10	97.22	111.00
1	F	2727	LEU	N-CA-C	-5.10	97.22	111.00
1	A	14	ASP	N-CA-C	5.09	124.76	111.00
1	C	1261	ARG	CD-NE-CZ	-5.08	116.50	123.60
1	C	1022	LYS	N-CA-C	5.07	124.70	111.00
1	C	1200	LEU	N-CA-C	-5.07	97.31	111.00
1	B	583	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	1534	VAL	N-CA-C	-5.06	97.33	111.00
1	H	3727	LEU	N-CA-C	-5.06	97.34	111.00
1	B	674	ASN	N-CA-C	5.06	124.65	111.00
1	G	3153	ASP	N-CA-C	-5.05	97.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	3514	ASP	N-CA-C	5.04	124.61	111.00
1	E	2200	LEU	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ARG	Sidechain
1	A	64	TYR	Sidechain
1	C	1261	ARG	Sidechain
1	D	1761	ARG	Sidechain
1	E	2064	TYR	Sidechain
1	H	3761	ARG	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2948	0	2965	166	0
1	B	2948	0	2962	207	0
1	C	2948	0	2962	186	0
1	D	2948	0	2962	172	0
1	E	2948	0	2962	193	0
1	F	2948	0	2962	141	0
1	G	2948	0	2962	176	0
1	H	2948	0	2962	181	0
2	A	30	0	18	10	0
2	C	15	0	9	8	0
2	D	15	0	9	11	0
2	E	30	0	18	14	0
2	G	15	0	9	6	0
2	H	15	0	9	1	0
3	A	15	0	6	2	0
3	B	15	0	7	3	0
3	C	15	0	6	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	15	0	6	2	0
3	E	15	0	7	2	0
3	F	15	0	7	0	0
3	G	15	0	6	2	0
3	H	15	0	6	2	0
All	All	23824	0	23822	1342	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (1342) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:1414:TRP:CZ3	1:D:1564:TYR:HB3	1.83	1.14
1:A:67:PRO:HB3	1:A:261:ARG:HG3	1.26	1.14
1:G:3261:ARG:CZ	1:H:3517:VAL:HG21	1.78	1.13
1:A:67:PRO:HG2	1:A:68:ALA:N	1.61	1.12
1:G:3067:PRO:HG3	1:G:3261:ARG:NH1	1.66	1.10
1:C:1067:PRO:HB3	1:C:1261:ARG:HD2	1.33	1.07
1:C:1261:ARG:HH21	1:D:1517:VAL:HG21	1.14	1.06
1:H:3567:PRO:HB3	1:H:3761:ARG:HG3	1.03	1.02
1:E:2258:SER:HA	1:E:2261:ARG:HD2	1.37	1.02
1:B:583:ARG:HG2	1:B:583:ARG:HH11	1.21	1.01
1:B:645:LEU:HB2	1:B:648:GLU:HG2	1.44	1.00
1:E:2191:ARG:HD2	1:H:3528:ARG:NH2	1.76	0.99
1:D:1806:GLY:HA3	1:D:1875:LEU:HD21	1.43	0.99
1:H:3567:PRO:CB	1:H:3761:ARG:HG3	1.91	0.98
1:B:597:THR:HB	1:B:602:GLN:HG2	1.44	0.96
1:E:2064:TYR:CG	2:E:2914:TRP:HZ3	1.83	0.96
1:H:3567:PRO:HB3	1:H:3761:ARG:CG	1.96	0.94
1:A:67:PRO:HG2	1:A:68:ALA:H	1.24	0.94
1:E:2331:ALA:HB3	1:E:2337:ALA:HB2	1.50	0.93
1:B:567:PRO:HG3	1:B:761:ARG:HH21	1.34	0.93
1:C:1067:PRO:HG3	1:C:1261:ARG:NH1	1.83	0.93
1:E:2097:THR:HB	1:E:2102:GLN:HG2	1.50	0.92
1:H:3545:THR:HG21	1:H:3741:TRP:HE1	1.35	0.92
1:A:261:ARG:HE	1:B:517:VAL:HG21	1.34	0.91
1:B:786:ARG:O	1:B:790:GLU:HG2	1.70	0.91
1:C:1017:VAL:HG11	1:D:1761:ARG:NH2	1.85	0.90
1:B:514:ASP:HB3	1:B:517:VAL:HB	1.51	0.90
1:E:2248:GLY:N	1:E:2253:ILE:HD11	1.87	0.90
1:G:3067:PRO:HG3	1:G:3261:ARG:HH11	1.36	0.89
1:B:782:GLN:HG2	1:B:786:ARG:HH21	1.35	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1017:VAL:HG11	1:D:1761:ARG:CZ	2.02	0.88
1:D:1748:GLY:N	1:D:1753:ILE:HD11	1.87	0.87
1:C:1261:ARG:NH2	1:D:1517:VAL:HG21	1.89	0.87
1:F:2727:LEU:HD11	1:F:2752:VAL:HG21	1.55	0.86
1:G:3261:ARG:NH2	1:H:3517:VAL:CG2	2.38	0.86
1:E:2145:LEU:HD22	1:E:2156:ARG:HH22	1.40	0.86
1:A:111:ILE:HG13	1:A:112:LEU:H	1.40	0.86
1:H:3748:GLY:N	1:H:3753:ILE:HD11	1.90	0.86
1:C:1045:THR:HG21	1:C:1241:TRP:HE1	1.39	0.86
1:C:1261:ARG:HH21	1:D:1517:VAL:CG2	1.89	0.85
1:C:1017:VAL:HG21	1:D:1761:ARG:HE	1.41	0.85
1:F:2525:GLU:HA	1:F:2528:ARG:HB3	1.58	0.85
1:E:2293:ARG:HB2	1:E:2293:ARG:HH11	1.39	0.84
1:B:611:ILE:HG13	1:B:612:LEU:H	1.41	0.84
1:E:2039:GLY:HA3	2:E:2414:TRP:HD1	1.40	0.84
1:A:249:PRO:HB2	1:A:252:VAL:HG12	1.59	0.84
1:D:1545:THR:HG21	1:D:1741:TRP:HE1	1.41	0.84
1:A:67:PRO:CB	1:A:261:ARG:HG3	2.07	0.84
1:H:3611:ILE:HG13	1:H:3612:LEU:H	1.42	0.84
1:A:312:LEU:HD22	1:A:325:MET:SD	2.18	0.84
2:C:1414:TRP:CZ3	1:D:1564:TYR:CB	2.61	0.83
1:G:3111:ILE:HG13	1:G:3112:LEU:H	1.43	0.83
1:F:2611:ILE:HG13	1:F:2612:LEU:H	1.43	0.83
1:G:3286:ARG:O	1:G:3290:GLU:HG2	1.77	0.82
1:A:64:TYR:CG	2:A:914:TRP:CH2	2.68	0.82
1:G:3174:ASN:ND2	1:G:3177:THR:H	1.76	0.82
1:E:2111:ILE:HG13	1:E:2112:LEU:H	1.45	0.82
1:E:2064:TYR:CG	2:E:2914:TRP:CZ3	2.68	0.81
1:D:1611:ILE:HG13	1:D:1612:LEU:H	1.43	0.81
1:C:1111:ILE:HG13	1:C:1112:LEU:H	1.44	0.81
1:C:1025:GLU:O	1:C:1026:LEU:HG	1.81	0.81
1:A:248:GLY:N	1:A:253:ILE:HD11	1.96	0.81
1:A:67:PRO:HG3	1:A:261:ARG:NH1	1.95	0.80
1:F:2802:LEU:HD21	1:F:2872:ARG:NH1	1.96	0.80
1:C:1067:PRO:HB3	1:C:1261:ARG:CD	2.12	0.80
1:H:3674:ASN:HD22	1:H:3675:ASN:N	1.79	0.80
1:A:25:GLU:O	1:A:26:LEU:HG	1.81	0.80
1:D:1522:LYS:O	1:D:1526:LEU:HD12	1.82	0.80
1:G:3016:VAL:HG21	2:G:3414:TRP:CD1	2.17	0.79
1:A:22:LYS:O	1:A:26:LEU:HD12	1.82	0.79
1:A:67:PRO:HD3	1:A:261:ARG:NH2	1.98	0.79
1:B:758:SER:HA	1:B:761:ARG:HH11	1.46	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1567:PRO:HB3	1:D:1761:ARG:CG	2.14	0.78
1:G:3261:ARG:CZ	1:H:3517:VAL:CG2	2.60	0.78
1:D:1831:ALA:HB3	1:D:1837:ALA:HB2	1.65	0.78
1:D:1628:TYR:O	1:D:1632:VAL:HG23	1.84	0.78
1:D:1524:LEU:O	1:D:1525:GLU:HG3	1.84	0.78
1:C:1097:THR:HB	1:C:1102:GLN:HG2	1.66	0.78
1:D:1567:PRO:HB3	1:D:1761:ARG:HG3	1.66	0.77
1:G:3024:LEU:O	1:G:3028:ARG:HB2	1.85	0.77
1:D:1539:GLY:HA3	2:D:1914:TRP:HA	1.67	0.77
1:H:3622:SER:CB	1:H:3623:PRO:HD2	2.15	0.77
1:B:758:SER:HA	1:B:761:ARG:HD2	1.66	0.77
1:B:708:HIS:O	1:B:793:ARG:HD3	1.85	0.77
1:H:3831:ALA:HB3	1:H:3837:ALA:HB2	1.67	0.77
1:G:3067:PRO:CG	1:G:3261:ARG:NH1	2.46	0.76
1:F:2831:ALA:HB3	1:F:2837:ALA:HB2	1.66	0.76
1:D:1608:PHE:O	1:D:1612:LEU:HB2	1.84	0.76
1:H:3597:THR:HB	1:H:3602:GLN:HG2	1.68	0.76
1:G:3331:ALA:HB3	1:G:3337:ALA:HB2	1.67	0.76
1:D:1803:LEU:HG	1:D:1871:LEU:HD22	1.67	0.76
1:G:3286:ARG:HG3	1:G:3286:ARG:HH11	1.50	0.76
1:A:67:PRO:HD3	1:A:261:ARG:CZ	2.14	0.76
1:F:2597:THR:HB	1:F:2602:GLN:HG2	1.68	0.75
1:D:1536:LEU:HD12	1:D:1866:THR:HG21	1.65	0.75
1:G:3350:PRO:HA	1:G:3360:VAL:HG23	1.67	0.75
1:C:1324:LEU:HD22	1:C:1359:HIS:HB3	1.66	0.75
1:H:3512:LYS:HG2	1:H:3513:PRO:HD2	1.68	0.75
1:H:3871:LEU:O	1:H:3875:LEU:HB2	1.87	0.75
1:H:3786:ARG:O	1:H:3790:GLU:HG2	1.86	0.75
1:B:567:PRO:HG3	1:B:761:ARG:NH2	2.01	0.75
1:F:2569:GLY:HA3	1:F:2596:VAL:HG13	1.67	0.74
1:H:3622:SER:OG	1:H:3643:GLU:HA	1.86	0.74
1:E:2025:GLU:O	1:E:2027:ARG:N	2.20	0.74
1:C:1046:PRO:HB2	1:C:1049:VAL:HG23	1.68	0.74
1:G:3069:GLY:HA3	1:G:3096:VAL:HG13	1.69	0.74
1:G:3261:ARG:NH2	1:H:3517:VAL:HG23	2.02	0.74
1:D:1812:LEU:HD22	1:D:1825:MET:SD	2.27	0.74
1:H:3622:SER:OG	1:H:3623:PRO:HD2	1.87	0.74
1:E:2045:THR:HG21	1:E:2241:TRP:HE1	1.53	0.73
1:C:1145:LEU:HB2	1:C:1148:GLU:HG2	1.68	0.73
1:E:2023:ALA:O	1:E:2025:GLU:O	2.06	0.73
1:A:331:ALA:HB3	1:A:337:ALA:HB2	1.70	0.73
1:F:2502:ARG:HH12	1:G:3082:ARG:NH2	1.85	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:2524:LEU:HA	1:F:2527:ARG:HB3	1.70	0.73
1:H:3533:LEU:H	1:H:3533:LEU:HD22	1.53	0.73
1:G:3174:ASN:HD21	1:G:3177:THR:H	1.34	0.73
1:G:3067:PRO:HD3	1:G:3261:ARG:CZ	2.18	0.73
1:A:23:ALA:HB1	1:A:27:ARG:HH21	1.54	0.73
1:A:108:PHE:O	1:A:112:LEU:HB2	1.89	0.73
1:A:45:THR:HG21	1:A:241:TRP:HE1	1.52	0.73
1:C:1072:GLU:HB3	1:C:1276:LEU:HD11	1.71	0.73
1:B:832:PRO:HB2	1:B:836:ARG:NH2	2.04	0.73
1:H:3608:PHE:O	1:H:3612:LEU:HB2	1.90	0.72
1:C:1205:ILE:HD11	1:C:1234:LYS:HD3	1.71	0.72
1:G:3014:ASP:HB3	1:G:3017:VAL:HG22	1.69	0.72
1:F:2742:ARG:O	1:F:2743:ILE:HD12	1.88	0.72
1:G:3242:ARG:HH12	1:H:3564:TYR:HE2	1.37	0.72
1:C:1298:ARG:NH1	1:C:1298:ARG:HB3	2.04	0.72
1:A:128:TYR:O	1:A:132:VAL:HG23	1.89	0.72
1:C:1016:VAL:HG11	2:C:1414:TRP:CD1	2.25	0.72
1:E:2108:PHE:HB3	1:E:2112:LEU:HD23	1.70	0.72
1:D:1765:THR:O	1:D:1766:SER:HB3	1.89	0.72
1:H:3674:ASN:HD22	1:H:3675:ASN:H	1.36	0.71
1:C:1087:LEU:HD23	1:C:1247:CYS:SG	2.30	0.71
1:G:3006:ARG:HG3	1:G:3006:ARG:HH11	1.54	0.71
1:D:1567:PRO:CB	1:D:1761:ARG:HG3	2.20	0.71
1:C:1024:LEU:HA	1:C:1027:ARG:HB3	1.71	0.71
1:E:2028:ARG:O	1:E:2029:GLN:HB3	1.90	0.71
1:H:3569:GLY:HA3	1:H:3596:VAL:HG13	1.73	0.71
1:E:2371:LEU:O	1:E:2375:LEU:HB2	1.89	0.71
1:F:2545:THR:HG21	1:F:2741:TRP:HE1	1.55	0.71
1:B:868:GLU:O	1:B:872:ARG:HG3	1.91	0.71
1:B:546:PRO:HB2	1:B:549:VAL:HG13	1.72	0.71
1:A:130:GLU:HB3	1:B:762:GLN:OE1	1.91	0.70
1:E:2082:ARG:NH1	1:E:2082:ARG:HB3	2.06	0.70
2:C:1414:TRP:HZ3	1:D:1564:TYR:HB3	1.52	0.70
1:E:2064:TYR:CB	2:E:2914:TRP:HZ3	2.03	0.70
1:B:534:VAL:HG11	1:B:874:ALA:HB2	1.73	0.70
1:E:2006:ARG:O	1:E:2006:ARG:HG2	1.90	0.70
1:B:758:SER:CA	1:B:761:ARG:HH11	2.04	0.70
1:D:1528:ARG:O	1:D:1529:GLN:HB2	1.91	0.70
1:C:1128:TYR:O	1:C:1132:VAL:HG23	1.91	0.70
1:E:2258:SER:HA	1:E:2261:ARG:CD	2.16	0.70
1:C:1344:ALA:O	1:C:1377:ARG:HD2	1.92	0.70
1:G:3017:VAL:HG11	1:H:3761:ARG:HD2	1.74	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1265:THR:O	1:C:1266:SER:HB3	1.92	0.70
1:G:3261:ARG:NH2	1:H:3517:VAL:HG21	2.00	0.69
1:A:12:LYS:HG3	1:A:13:PRO:HD2	1.74	0.69
1:A:27:ARG:HA	1:A:31:VAL:O	1.92	0.69
1:B:765:THR:O	1:B:766:SER:HB3	1.92	0.69
1:E:2293:ARG:HB2	1:E:2293:ARG:NH1	2.06	0.69
1:E:2064:TYR:CD1	2:E:2914:TRP:CZ3	2.80	0.69
1:E:2039:GLY:HA3	2:E:2414:TRP:CD1	2.27	0.69
1:C:1069:GLY:HA3	1:C:1096:VAL:HG13	1.74	0.69
1:G:3205:ILE:HG22	1:G:3206:TYR:CD2	2.27	0.69
1:F:2753:ILE:O	1:F:2753:ILE:HG22	1.92	0.69
1:C:1155:GLU:O	1:C:1158:ARG:HB3	1.93	0.69
1:B:807:LEU:HD21	1:B:825:MET:SD	2.33	0.69
1:C:1181:TYR:HB2	1:C:1186:LEU:HD21	1.72	0.69
1:C:1156:ARG:HA	1:C:1159:ARG:HG2	1.75	0.69
1:E:2069:GLY:HA3	1:E:2096:VAL:HG12	1.74	0.68
1:F:2650:PHE:HE1	1:F:2815:VAL:HG21	1.58	0.68
1:D:1525:GLU:O	1:D:1526:LEU:HG	1.94	0.68
1:G:3067:PRO:HG2	1:G:3068:ALA:N	2.09	0.68
1:G:3025:GLU:O	1:G:3029:GLN:HG2	1.93	0.68
1:E:2025:GLU:H	1:E:2028:ARG:H	1.41	0.68
1:D:1799:ARG:HB3	1:D:1871:LEU:HD11	1.75	0.68
1:F:2833:ASP:HB3	1:F:2836:ARG:HH21	1.57	0.68
1:E:2191:ARG:HD2	1:H:3528:ARG:HH22	1.56	0.68
1:B:803:LEU:HG	1:B:871:LEU:HD22	1.76	0.68
1:F:2801:ASP:O	1:F:2805:GLU:HG2	1.93	0.68
1:B:569:GLY:HA3	1:B:596:VAL:CG1	2.24	0.68
1:D:1717:SER:H	1:D:1720:ARG:HH11	1.42	0.68
1:G:3045:THR:HG21	1:G:3241:TRP:HE1	1.59	0.67
1:A:1:MET:O	1:B:698:PHE:HA	1.94	0.67
2:C:1414:TRP:CH2	1:D:1564:TYR:HB3	2.28	0.67
1:B:524:LEU:H	1:B:524:LEU:HD23	1.58	0.67
1:G:3127:SER:O	1:G:3131:MET:HG2	1.94	0.67
1:B:545:THR:HG21	1:B:741:TRP:HE1	1.60	0.67
1:C:1212:GLU:HG3	1:C:1316:ARG:HH22	1.58	0.67
1:A:371:LEU:O	1:A:375:LEU:HB2	1.95	0.67
1:C:1286:ARG:HH11	1:C:1286:ARG:HG3	1.59	0.67
1:C:1212:GLU:CG	1:C:1316:ARG:HH22	2.07	0.67
1:A:64:TYR:HB3	2:A:914:TRP:HH2	1.60	0.67
1:C:1005:SER:OG	1:C:1008:VAL:HB	1.94	0.67
1:H:3569:GLY:HA3	1:H:3596:VAL:CG1	2.25	0.67
1:G:3242:ARG:NH1	1:H:3564:TYR:HE2	1.92	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:3045:THR:HG22	1:G:3237:ALA:O	1.95	0.67
1:E:2026:LEU:HA	1:E:2031:VAL:HG13	1.77	0.67
1:B:831:ALA:HB3	1:B:837:ALA:HB2	1.77	0.67
1:A:261:ARG:NE	1:B:517:VAL:HG21	2.07	0.67
1:E:2340:ARG:HE	1:E:2381:VAL:HG22	1.58	0.67
1:C:1234:LYS:H	1:C:1234:LYS:HD2	1.61	0.66
1:C:1021:ALA:O	1:C:1024:LEU:HG	1.95	0.66
1:E:2069:GLY:HA3	1:E:2096:VAL:CG1	2.25	0.66
1:A:242:ARG:NH1	1:B:564:TYR:HE2	1.93	0.66
1:G:3046:PRO:HB2	1:G:3049:VAL:HG23	1.78	0.66
1:A:97:THR:HB	1:A:102:GLN:HG2	1.77	0.66
1:B:782:GLN:CG	1:B:786:ARG:HH21	2.09	0.66
1:F:2802:LEU:HD21	1:F:2872:ARG:HH11	1.60	0.66
1:G:3081:PHE:O	1:G:3085:ASN:HB2	1.94	0.66
1:C:1085:ASN:HB3	1:C:1087:LEU:HD13	1.78	0.66
1:B:840:ARG:HH11	1:B:881:VAL:HG13	1.61	0.66
1:H:3840:ARG:HE	1:H:3881:VAL:HG22	1.60	0.66
1:C:1204:GLU:HG2	1:C:1215:HIS:CE1	2.31	0.66
1:H:3670:VAL:HG23	1:H:3681:TYR:HE1	1.61	0.66
1:B:758:SER:HA	1:B:761:ARG:CD	2.25	0.66
1:D:1712:GLU:HG2	1:D:1816:ARG:HH22	1.60	0.66
1:E:2185:VAL:O	1:E:2189:LEU:HG	1.95	0.66
1:C:1175:ASN:HD22	3:C:1413:PLP:H2A1	1.60	0.66
1:H:3608:PHE:HD2	1:H:3612:LEU:CD2	2.08	0.66
1:A:205:ILE:HG12	1:A:230:ASN:HA	1.78	0.66
1:C:1253:ILE:O	1:C:1253:ILE:HG22	1.96	0.66
1:G:3067:PRO:HD3	1:G:3261:ARG:NH2	2.11	0.65
1:G:3017:VAL:HG21	1:H:3761:ARG:HH11	1.62	0.65
1:H:3587:LEU:HD23	1:H:3747:CYS:SG	2.36	0.65
1:A:332:PRO:HB2	1:A:336:ARG:NH2	2.11	0.65
1:B:758:SER:O	1:B:761:ARG:HG3	1.96	0.65
1:B:655:GLU:O	1:B:658:ARG:HB3	1.96	0.65
1:G:3024:LEU:HA	1:G:3027:ARG:HB3	1.77	0.65
1:A:6:ARG:HH21	1:A:10:ALA:HB2	1.61	0.65
1:B:611:ILE:HG13	1:B:612:LEU:N	2.12	0.65
1:H:3621:LEU:O	1:H:3624:TYR:HB3	1.96	0.65
1:H:3525:GLU:N	1:H:3528:ARG:HB3	2.11	0.65
1:F:2533:LEU:HD22	1:F:2533:LEU:H	1.60	0.65
1:D:1704:GLU:HG2	1:D:1715:HIS:CE1	2.32	0.65
1:G:3064:TYR:HE2	1:H:3742:ARG:NH1	1.94	0.65
1:F:2720:ARG:HH11	1:F:2720:ARG:HG2	1.61	0.65
1:G:3132:VAL:HG11	1:G:3139:VAL:HG22	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:2748:GLY:N	1:F:2753:ILE:HD11	2.11	0.65
1:C:1067:PRO:HG3	1:C:1261:ARG:CZ	2.26	0.65
1:F:2569:GLY:HA3	1:F:2596:VAL:CG1	2.26	0.65
1:D:1546:PRO:HG3	1:D:1788:PHE:CD1	2.31	0.65
1:E:2289:VAL:HG12	1:E:2293:ARG:HH12	1.62	0.64
1:D:1569:GLY:HA3	1:D:1596:VAL:HG13	1.77	0.64
1:E:2092:GLU:OE1	1:E:2250:LYS:HE3	1.97	0.64
1:A:111:ILE:HG13	1:A:112:LEU:N	2.11	0.64
1:F:2608:PHE:O	1:F:2612:LEU:HB2	1.98	0.64
1:G:3174:ASN:ND2	1:G:3177:THR:N	2.45	0.64
1:E:2204:GLU:HG2	1:E:2215:HIS:CE1	2.32	0.64
1:C:1145:LEU:HB3	1:C:1147:GLU:HG2	1.79	0.64
1:E:2082:ARG:HB3	1:E:2082:ARG:HH11	1.63	0.64
1:G:3074:ARG:NH2	1:G:3092:GLU:HA	2.12	0.64
1:B:608:PHE:HB3	1:B:612:LEU:HD23	1.79	0.64
1:H:3623:PRO:O	1:H:3676:PRO:HD2	1.98	0.64
1:C:1111:ILE:HG13	1:C:1112:LEU:N	2.13	0.64
1:F:2646:PRO:HB3	1:F:2650:PHE:CZ	2.33	0.64
1:D:1569:GLY:HA3	1:D:1596:VAL:CG1	2.28	0.64
1:G:3067:PRO:CD	1:G:3261:ARG:CZ	2.75	0.64
1:A:67:PRO:CD	1:A:261:ARG:CZ	2.76	0.64
1:A:24:LEU:O	1:A:25:GLU:HB3	1.97	0.63
1:G:3330:ILE:HD11	1:G:3381:VAL:HG21	1.79	0.63
1:F:2720:ARG:HH11	1:F:2720:ARG:CG	2.11	0.63
1:A:69:GLY:HA3	1:A:96:VAL:CG1	2.29	0.63
1:A:212:GLU:HG3	1:A:316:ARG:HH22	1.63	0.63
1:B:782:GLN:C	1:B:786:ARG:HD3	2.19	0.63
1:D:1505:SER:OG	1:D:1508:VAL:HB	1.99	0.63
1:A:64:TYR:CD1	2:A:914:TRP:CH2	2.87	0.63
1:C:1017:VAL:CG1	1:D:1761:ARG:NH2	2.60	0.62
1:A:156:ARG:HA	1:A:159:ARG:HG2	1.80	0.62
1:D:1611:ILE:HG13	1:D:1612:LEU:N	2.13	0.62
1:D:1670:VAL:HG23	1:D:1681:TYR:HE1	1.63	0.62
1:A:350:PRO:HA	1:A:360:VAL:HG23	1.81	0.62
1:C:1028:ARG:O	1:C:1029:GLN:HB2	1.99	0.62
1:H:3512:LYS:HG2	1:H:3513:PRO:CD	2.29	0.62
1:A:67:PRO:HB3	1:A:261:ARG:CG	2.18	0.62
1:B:608:PHE:O	1:B:612:LEU:HB2	1.99	0.62
1:G:3111:ILE:HG13	1:G:3112:LEU:N	2.13	0.62
1:G:3078:ALA:O	1:G:3082:ARG:HG3	2.00	0.62
1:D:1597:THR:HB	1:D:1602:GLN:HG2	1.82	0.62
1:H:3628:TYR:O	1:H:3632:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:527:ARG:HA	1:B:531:VAL:O	2.00	0.62
1:A:146:PRO:HB3	1:A:150:PHE:CZ	2.35	0.62
1:A:67:PRO:CD	1:A:261:ARG:NH1	2.63	0.62
1:D:1585:ASN:O	1:D:1720:ARG:CZ	2.48	0.62
1:E:2085:ASN:HB3	1:E:2087:LEU:HD13	1.82	0.61
1:H:3873:LYS:HD3	1:H:3877:ARG:HH21	1.65	0.61
1:E:2008:VAL:O	1:E:2011:MET:HG2	2.00	0.61
1:C:1064:TYR:HB3	2:D:1914:TRP:CZ3	2.35	0.61
1:H:3545:THR:HG21	1:H:3741:TRP:NE1	2.10	0.61
1:C:1064:TYR:CB	2:D:1914:TRP:CH2	2.82	0.61
1:E:2087:LEU:HD23	1:E:2247:CYS:SG	2.40	0.61
1:G:3025:GLU:HA	1:G:3025:GLU:OE1	2.00	0.61
1:D:1585:ASN:HB3	1:D:1587:LEU:HD13	1.81	0.61
1:H:3753:ILE:HG22	1:H:3753:ILE:O	2.01	0.61
1:D:1536:LEU:O	1:D:1863:SER:HB3	2.00	0.61
1:E:2204:GLU:O	1:E:2206:TYR:N	2.33	0.61
1:A:67:PRO:CG	1:A:261:ARG:NH1	2.63	0.61
1:F:2611:ILE:HG13	1:F:2612:LEU:N	2.14	0.61
1:F:2502:ARG:HH12	1:G:3082:ARG:HH22	1.48	0.61
1:A:269:THR:HA	1:A:272:GLN:HG3	1.82	0.61
1:A:87:LEU:HD23	1:A:247:CYS:SG	2.40	0.61
1:C:1234:LYS:N	1:C:1234:LYS:HD2	2.16	0.61
1:G:3265:THR:O	1:G:3266:SER:HB3	1.99	0.61
1:H:3611:ILE:HG13	1:H:3612:LEU:N	2.13	0.61
2:G:3414:TRP:HZ3	1:H:3564:TYR:CB	2.13	0.61
1:B:871:LEU:O	1:B:875:LEU:HB2	2.00	0.61
1:G:3300:ARG:O	1:G:3304:LEU:HD23	2.01	0.60
1:E:2108:PHE:HD2	1:E:2112:LEU:CD2	2.14	0.60
1:A:332:PRO:HB2	1:A:336:ARG:HH21	1.66	0.60
1:B:747:CYS:HA	1:B:753:ILE:HD11	1.82	0.60
1:C:1022:LYS:HG3	1:C:1025:GLU:HG3	1.82	0.60
1:F:2524:LEU:HD22	1:F:2524:LEU:H	1.65	0.60
1:B:524:LEU:HA	1:B:527:ARG:HB3	1.82	0.60
1:B:583:ARG:HG2	1:B:583:ARG:NH1	2.00	0.60
1:D:1514:ASP:HB3	1:D:1517:VAL:HG12	1.84	0.60
1:C:1064:TYR:CB	2:D:1914:TRP:CZ3	2.84	0.60
1:B:806:GLY:HA3	1:B:875:LEU:HD11	1.83	0.60
1:E:2127:SER:O	1:E:2131:MET:HG2	2.01	0.60
1:E:2111:ILE:HG13	1:E:2112:LEU:N	2.14	0.60
1:E:2145:LEU:HD22	1:E:2156:ARG:NH2	2.15	0.60
1:D:1508:VAL:O	1:D:1511:MET:HG2	2.02	0.60
1:A:5:SER:HB3	1:B:611:ILE:O	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:2039:GLY:CA	2:E:2414:TRP:HD1	2.14	0.60
1:E:2085:ASN:CB	1:E:2087:LEU:HD13	2.32	0.60
1:H:3526:LEU:O	1:H:3531:VAL:HG22	2.02	0.59
1:E:2150:PHE:CE1	1:E:2315:VAL:HG21	2.37	0.59
1:C:1350:PRO:HA	1:C:1360:VAL:HG23	1.84	0.59
1:E:2224:GLU:OE1	1:G:3079:GLU:HG2	2.03	0.59
1:G:3373:LYS:HD3	1:G:3377:ARG:HH21	1.67	0.59
1:D:1871:LEU:O	1:D:1875:LEU:HB2	2.03	0.59
1:B:717:SER:HB2	1:B:720:ARG:HH11	1.67	0.59
1:E:2012:LYS:HE2	1:E:2130:GLU:OE2	2.02	0.59
1:D:1567:PRO:HB3	1:D:1761:ARG:HG2	1.85	0.59
1:E:2248:GLY:H	1:E:2253:ILE:HD11	1.66	0.59
1:E:2027:ARG:HH11	1:E:2027:ARG:HG3	1.67	0.59
1:F:2761:ARG:HD3	1:F:2762:GLN:HE21	1.68	0.59
1:E:2156:ARG:HA	1:E:2159:ARG:HG2	1.83	0.59
1:A:262:GLN:OE1	1:B:630:GLU:HB3	2.03	0.59
1:D:1567:PRO:HG3	1:D:1761:ARG:CZ	2.33	0.59
1:H:3585:ASN:HB3	1:H:3587:LEU:HD13	1.84	0.59
1:A:25:GLU:O	1:A:25:GLU:HG2	2.03	0.59
1:D:1524:LEU:HA	1:D:1527:ARG:HB3	1.85	0.59
1:B:533:LEU:HD22	1:B:533:LEU:H	1.68	0.59
1:C:1212:GLU:CD	1:C:1316:ARG:HH22	2.05	0.59
1:A:69:GLY:HA3	1:A:96:VAL:HG13	1.85	0.59
1:C:1249:PRO:HB2	1:C:1252:VAL:HG12	1.85	0.59
1:H:3868:GLU:O	1:H:3872:ARG:HG3	2.03	0.58
1:F:2830:ILE:HD11	1:F:2881:VAL:HG11	1.84	0.58
1:E:2191:ARG:HH11	1:H:3528:ARG:NH2	2.01	0.58
1:E:2145:LEU:HB2	1:E:2148:GLU:CG	2.33	0.58
1:C:1181:TYR:HB2	1:C:1186:LEU:CD2	2.33	0.58
1:E:2034:VAL:O	1:E:2346:VAL:HA	2.02	0.58
1:D:1656:ARG:HA	1:D:1659:ARG:HG2	1.85	0.58
1:E:2175:ASN:HD22	3:E:2413:PLP:H2A1	1.68	0.58
1:C:1014:ASP:HB3	1:C:1017:VAL:HB	1.84	0.58
1:F:2694:VAL:HG23	1:F:2725:HIS:CE1	2.39	0.58
1:A:340:ARG:HE	1:A:381:VAL:HG22	1.67	0.58
1:C:1355:ALA:HA	1:C:1357:PHE:CE1	2.38	0.58
1:E:2016:VAL:HA	1:E:2019:VAL:HG23	1.85	0.58
1:C:1064:TYR:HB2	2:D:1914:TRP:CH2	2.38	0.58
1:D:1675:ASN:HD22	3:D:1913:PLP:H2A1	1.68	0.58
1:E:2264:THR:O	1:E:2265:THR:HB	2.03	0.58
1:C:1045:THR:HG21	1:C:1241:TRP:NE1	2.16	0.58
1:G:3121:LEU:CD2	1:G:3152:PRO:HB3	2.34	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:3067:PRO:HG2	1:G:3068:ALA:H	1.68	0.58
1:B:717:SER:H	1:B:720:ARG:NH1	2.00	0.58
1:D:1749:PRO:HB2	1:D:1752:VAL:HG12	1.85	0.58
1:E:2145:LEU:HB2	1:E:2148:GLU:HG2	1.85	0.58
1:B:799:ARG:HG2	1:B:868:GLU:HG3	1.86	0.58
1:C:1064:TYR:CG	2:D:1914:TRP:CZ3	2.92	0.58
1:C:1081:PHE:O	1:C:1085:ASN:HB2	2.04	0.58
1:A:6:ARG:NH2	1:A:10:ALA:HB2	2.19	0.58
1:A:34:VAL:O	1:A:346:VAL:HA	2.04	0.58
1:C:1340:ARG:NH2	1:C:1381:VAL:O	2.37	0.58
1:C:1205:ILE:HG23	1:C:1206:TYR:CD2	2.38	0.57
1:B:508:VAL:O	1:B:511:MET:HG2	2.04	0.57
1:C:1198:PHE:HA	1:D:1501:MET:O	2.04	0.57
1:D:1748:GLY:H	1:D:1753:ILE:HD11	1.70	0.57
1:A:72:GLU:HB3	1:A:276:LEU:HD11	1.86	0.57
1:F:2645:LEU:HB2	1:F:2648:GLU:HG2	1.86	0.57
1:A:242:ARG:HH12	1:B:564:TYR:HE2	1.51	0.57
1:E:2212:GLU:HG3	1:E:2316:ARG:HH22	1.68	0.57
1:E:2111:ILE:O	1:F:2505:SER:HB3	2.03	0.57
1:B:832:PRO:HB2	1:B:836:ARG:HH21	1.70	0.57
2:C:1414:TRP:CZ3	1:D:1564:TYR:CG	2.92	0.57
1:H:3525:GLU:O	1:H:3526:LEU:HG	2.05	0.57
1:A:283:GLU:OE1	1:A:286:ARG:NH1	2.38	0.57
1:A:67:PRO:CD	1:A:261:ARG:NH2	2.66	0.57
1:E:2015:ALA:O	1:E:2019:VAL:HG22	2.05	0.57
1:G:3198:PHE:HA	1:H:3501:MET:O	2.05	0.57
1:A:216:PHE:HE1	1:A:220:ARG:HH11	1.53	0.57
1:G:3303:LEU:HG	1:G:3371:LEU:HD22	1.87	0.57
1:H:3749:PRO:HB2	1:H:3752:VAL:HG12	1.87	0.57
1:H:3524:LEU:HA	1:H:3527:ARG:HB3	1.87	0.57
1:H:3622:SER:HB2	1:H:3623:PRO:HD2	1.85	0.57
1:G:3378:PHE:O	1:G:3381:VAL:HG22	2.05	0.57
1:C:1312:LEU:HD11	1:C:1382:LEU:HD11	1.86	0.57
1:A:73:LEU:O	1:A:77:LEU:HB2	2.05	0.57
1:C:1027:ARG:HA	1:C:1031:VAL:O	2.04	0.57
1:E:2034:VAL:HG11	1:E:2374:ALA:HB2	1.86	0.57
1:E:2300:ARG:O	1:E:2304:LEU:HD23	2.04	0.57
1:F:2674:ASN:CG	1:F:2677:THR:HG23	2.25	0.57
1:B:705:ILE:HG23	1:B:706:TYR:CD2	2.39	0.57
1:H:3821:PHE:CD1	1:H:3865:ALA:HB2	2.39	0.57
1:H:3525:GLU:H	1:H:3528:ARG:H	1.53	0.56
1:C:1025:GLU:N	1:C:1028:ARG:H	2.03	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:2026:LEU:CA	1:E:2031:VAL:HG13	2.35	0.56
1:A:45:THR:HG21	1:A:241:TRP:NE1	2.18	0.56
1:B:799:ARG:HB3	1:B:871:LEU:HD11	1.87	0.56
1:C:1121:LEU:CD2	1:C:1152:PRO:HB3	2.34	0.56
1:E:2128:TYR:O	1:E:2132:VAL:HG23	2.05	0.56
1:E:2064:TYR:HB3	2:E:2914:TRP:HZ3	1.69	0.56
1:G:3111:ILE:O	1:H:3505:SER:HB3	2.05	0.56
1:H:3527:ARG:HA	1:H:3531:VAL:O	2.04	0.56
1:E:2064:TYR:CE1	2:E:2914:TRP:CE3	2.94	0.56
1:G:3129:PRO:HA	1:G:3132:VAL:HG12	1.86	0.56
1:H:3505:SER:OG	1:H:3508:VAL:HB	2.05	0.56
1:E:2005:SER:HB3	1:F:2611:ILE:O	2.04	0.56
1:A:64:TYR:HE2	1:B:742:ARG:NH1	2.02	0.56
1:C:1356:ALA:O	1:C:1359:HIS:HB2	2.05	0.56
1:A:238:MET:HG2	1:A:241:TRP:CD1	2.40	0.56
1:F:2803:LEU:HG	1:F:2871:LEU:HD22	1.87	0.56
1:E:2198:PHE:HA	1:F:2501:MET:O	2.06	0.56
1:A:145:LEU:HB2	1:A:148:GLU:HG2	1.88	0.56
1:G:3073:LEU:O	1:G:3077:LEU:HB2	2.05	0.56
1:F:2833:ASP:HB3	1:F:2836:ARG:NH2	2.19	0.56
1:E:2184:GLU:HA	1:E:2187:GLU:HB2	1.88	0.56
1:G:3012:LYS:HG3	1:G:3013:PRO:N	2.21	0.56
1:A:64:TYR:CB	2:A:914:TRP:CH2	2.88	0.56
1:G:3006:ARG:NH1	1:G:3006:ARG:HG3	2.21	0.56
1:B:799:ARG:HB3	1:B:871:LEU:CD1	2.35	0.56
1:B:546:PRO:HB2	1:B:549:VAL:CG1	2.35	0.56
1:D:1712:GLU:CG	1:D:1816:ARG:HH22	2.18	0.56
1:F:2825:MET:O	1:F:2859:HIS:HA	2.06	0.56
1:C:1064:TYR:HE2	1:D:1742:ARG:HH12	1.54	0.56
1:C:1093:GLU:HG2	1:C:1250:LYS:HG3	1.87	0.56
1:D:1539:GLY:HA3	2:D:1914:TRP:CA	2.35	0.56
1:H:3534:VAL:HG22	1:H:3873:LYS:HD2	1.88	0.56
1:H:3727:LEU:HD11	1:H:3752:VAL:HG21	1.88	0.56
1:B:621:LEU:HD22	1:B:652:PRO:HB3	1.87	0.56
1:C:1126:VAL:HG23	1:C:1354:PHE:CZ	2.40	0.56
1:E:2184:GLU:HA	1:E:2187:GLU:CB	2.36	0.56
1:B:797:ARG:O	1:B:800:ARG:HB3	2.06	0.56
1:G:3019:VAL:HG21	1:G:3349:VAL:HG22	1.87	0.56
1:A:345:GLY:HA3	1:A:377:ARG:HH11	1.71	0.56
1:C:1150:PHE:HE1	1:C:1315:VAL:HG21	1.71	0.56
1:G:3328:SER:HB3	1:G:3329:PRO:HD3	1.88	0.56
1:G:3330:ILE:O	1:G:3340:ARG:HD3	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1597:THR:HG21	1:D:1603:ALA:HA	1.88	0.55
1:A:303:LEU:O	1:A:307:LEU:HB2	2.06	0.55
1:F:2810:LEU:HD22	1:F:2882:LEU:HD12	1.87	0.55
1:E:2303:LEU:HD22	1:E:2307:LEU:CD1	2.36	0.55
1:H:3685:VAL:O	1:H:3689:LEU:HG	2.07	0.55
1:E:2064:TYR:HE2	1:F:2742:ARG:NH1	2.04	0.55
1:H:3803:LEU:HD13	1:H:3871:LEU:HD22	1.88	0.55
1:A:242:ARG:NH1	1:B:564:TYR:CE2	2.73	0.55
1:E:2016:VAL:HA	1:E:2019:VAL:CG2	2.37	0.55
1:E:2310:LEU:HD11	1:E:2379:ALA:HB2	1.87	0.55
1:H:3684:GLU:CD	1:H:3684:GLU:H	2.09	0.55
1:E:2330:ILE:HG13	1:E:2382:LEU:HD21	1.87	0.55
1:A:64:TYR:HB3	2:A:914:TRP:CH2	2.41	0.55
1:D:1764:THR:O	1:D:1765:THR:HB	2.06	0.55
1:C:1001:MET:O	1:D:1698:PHE:HA	2.07	0.55
1:C:1071:PRO:O	1:C:1075:GLU:HG3	2.06	0.55
1:G:3022:LYS:HD2	1:G:3022:LYS:O	2.05	0.55
1:F:2622:SER:HA	1:F:2623:PRO:C	2.26	0.55
1:H:3645:LEU:HB3	1:H:3647:GLU:OE2	2.06	0.55
1:B:685:VAL:O	1:B:689:LEU:HG	2.07	0.55
1:B:748:GLY:N	1:B:753:ILE:HD11	2.22	0.55
1:B:876:GLU:O	1:B:879:ALA:HB3	2.07	0.55
1:F:2816:ARG:NH2	1:F:2818:SER:OG	2.39	0.55
1:G:3242:ARG:NH1	1:H:3564:TYR:CE2	2.73	0.55
2:G:3414:TRP:CZ3	1:H:3564:TYR:CD1	2.95	0.55
1:A:169:VAL:HG22	1:A:201:VAL:HB	1.89	0.55
1:C:1331:ALA:HB3	1:C:1337:ALA:HB2	1.88	0.55
1:D:1823:VAL:HG23	1:D:1864:TYR:HE2	1.71	0.55
1:C:1069:GLY:HA3	1:C:1096:VAL:CG1	2.37	0.55
1:H:3572:GLU:HB3	1:H:3776:LEU:HD11	1.88	0.55
1:A:321:PHE:HA	1:A:364:TYR:CZ	2.41	0.55
1:E:2129:PRO:O	1:E:2133:ARG:HD2	2.06	0.55
1:A:39:GLY:HA3	2:A:414:TRP:HA	1.88	0.55
1:F:2821:PHE:HA	1:F:2864:TYR:CZ	2.41	0.55
1:H:3551:GLU:HG2	1:H:3554:ARG:HH11	1.71	0.55
1:B:650:PHE:HE1	1:B:815:VAL:HG21	1.71	0.55
1:H:3748:GLY:N	1:H:3753:ILE:CD1	2.66	0.55
1:B:717:SER:CB	1:B:720:ARG:NH1	2.70	0.55
1:G:3064:TYR:HE2	1:H:3742:ARG:HH12	1.56	0.54
1:D:1523:ALA:O	1:D:1526:LEU:HB2	2.07	0.54
1:B:622:SER:HA	1:B:623:PRO:C	2.28	0.54
1:H:3812:LEU:HD13	1:H:3825:MET:SD	2.47	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:127:SER:O	1:A:131:MET:HG2	2.06	0.54
1:C:1205:ILE:HD11	1:C:1234:LYS:CD	2.36	0.54
1:H:3868:GLU:HG3	1:H:3872:ARG:HE	1.73	0.54
1:A:121:LEU:CD2	1:A:152:PRO:HB3	2.37	0.54
1:A:28:ARG:HD2	1:A:28:ARG:O	2.07	0.54
1:D:1704:GLU:O	1:D:1706:TYR:N	2.41	0.54
1:B:585:ASN:HB3	1:B:587:LEU:CD1	2.38	0.54
1:F:2812:LEU:HD11	1:F:2882:LEU:HD11	1.89	0.54
1:C:1150:PHE:CE1	1:C:1315:VAL:HG21	2.42	0.54
1:G:3323:VAL:HG23	1:G:3364:TYR:HE2	1.73	0.54
1:G:3286:ARG:CG	1:G:3286:ARG:HH11	2.20	0.54
1:D:1850:PRO:HA	1:D:1860:VAL:HG23	1.89	0.54
1:C:1107:LEU:HD21	1:C:1227:LEU:HD13	1.90	0.54
1:A:126:VAL:HG23	1:A:354:PHE:CE2	2.42	0.54
1:E:2064:TYR:CE1	2:E:2914:TRP:HE3	2.26	0.54
1:C:1108:PHE:HB3	1:C:1112:LEU:HD23	1.89	0.54
1:B:534:VAL:O	1:B:846:VAL:HA	2.07	0.54
1:D:1638:VAL:HG21	1:D:1664:ARG:NH2	2.22	0.54
1:D:1536:LEU:CD1	1:D:1866:THR:HG21	2.34	0.54
1:D:1821:PHE:HA	1:D:1864:TYR:CZ	2.43	0.54
1:C:1298:ARG:HH11	1:C:1298:ARG:HB3	1.71	0.54
1:D:1582:ARG:HA	1:D:1587:LEU:O	2.08	0.54
1:A:286:ARG:O	1:A:290:GLU:HG2	2.08	0.54
1:C:1371:LEU:O	1:C:1375:LEU:HB2	2.07	0.54
1:E:2048:HIS:CD2	1:E:2049:VAL:HG12	2.43	0.54
1:B:717:SER:CB	1:B:720:ARG:HH11	2.21	0.54
1:B:684:GLU:HA	1:B:687:GLU:HB2	1.89	0.54
1:G:3132:VAL:HG13	1:G:3133:ARG:N	2.23	0.54
1:G:3253:ILE:HG22	1:G:3253:ILE:O	2.08	0.54
1:C:1108:PHE:O	1:C:1112:LEU:HB2	2.07	0.53
1:G:3204:GLU:O	1:G:3206:TYR:N	2.41	0.53
1:F:2761:ARG:HD2	1:F:2762:GLN:HG2	1.89	0.53
1:E:2122:SER:HA	1:E:2123:PRO:C	2.28	0.53
1:G:3064:TYR:CE2	1:H:3742:ARG:NH1	2.75	0.53
1:G:3264:THR:O	1:G:3265:THR:HB	2.08	0.53
1:E:2242:ARG:HH22	3:E:2413:PLP:P	2.31	0.53
1:B:597:THR:HG21	1:B:603:ALA:HA	1.90	0.53
1:G:3087:LEU:HD23	1:G:3247:CYS:SG	2.47	0.53
1:F:2573:LEU:HD22	1:F:2577:LEU:HD22	1.90	0.53
1:E:2014:ASP:HB3	1:E:2017:VAL:HB	1.89	0.53
1:C:1064:TYR:HE2	1:D:1742:ARG:NH1	2.06	0.53
1:G:3005:SER:OG	1:G:3008:VAL:HB	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:2524:LEU:HD12	1:F:2527:ARG:HG2	1.90	0.53
1:F:2823:VAL:HG23	1:F:2864:TYR:HE2	1.73	0.53
1:A:212:GLU:CG	1:A:316:ARG:HH22	2.21	0.53
1:B:567:PRO:CG	1:B:761:ARG:NH2	2.70	0.53
1:E:2026:LEU:HD23	1:E:2026:LEU:N	2.22	0.53
1:C:1323:VAL:HG23	1:C:1364:TYR:HE2	1.74	0.53
1:F:2626:VAL:HG23	1:F:2854:PHE:CZ	2.44	0.53
1:B:602:GLN:O	1:B:602:GLN:HG3	2.09	0.53
1:E:2064:TYR:HB3	2:E:2914:TRP:CZ3	2.43	0.53
1:C:1024:LEU:HD12	1:C:1024:LEU:O	2.08	0.53
1:H:3799:ARG:HB3	1:H:3871:LEU:CD1	2.38	0.53
1:E:2323:VAL:HG23	1:E:2364:TYR:HE2	1.72	0.53
1:H:3821:PHE:HA	1:H:3864:TYR:CZ	2.43	0.53
1:H:3817:PRO:HG2	1:H:3823:VAL:HG22	1.91	0.53
1:G:3249:PRO:HB2	1:G:3252:VAL:HG12	1.91	0.53
1:F:2704:GLU:O	1:F:2706:TYR:N	2.42	0.53
1:E:2033:LEU:H	1:E:2033:LEU:HD22	1.74	0.53
1:E:2064:TYR:CB	2:E:2914:TRP:CZ3	2.88	0.53
1:H:3823:VAL:HG23	1:H:3864:TYR:HE2	1.73	0.53
1:B:583:ARG:CG	1:B:583:ARG:HH11	2.09	0.53
1:H:3675:ASN:HD22	3:H:3913:PLP:H2A1	1.74	0.53
1:F:2602:GLN:HG3	1:F:2602:GLN:O	2.08	0.53
1:B:823:VAL:HG23	1:B:864:TYR:HE2	1.74	0.53
1:H:3645:LEU:O	1:H:3648:GLU:HG2	2.09	0.53
1:F:2712:GLU:CD	1:F:2816:ARG:HH12	2.11	0.53
1:E:2344:ALA:O	1:E:2377:ARG:HD2	2.09	0.53
1:C:1299:ARG:HA	1:C:1302:LEU:HD23	1.91	0.53
1:H:3545:THR:CG2	1:H:3741:TRP:HE1	2.16	0.53
1:B:782:GLN:HB3	1:B:786:ARG:HD2	1.90	0.53
1:B:782:GLN:HB3	1:B:786:ARG:CD	2.38	0.53
1:D:1525:GLU:HA	1:D:1528:ARG:HB3	1.89	0.53
1:B:704:GLU:O	1:B:706:TYR:N	2.42	0.53
1:F:2581:PHE:O	1:F:2585:ASN:HB2	2.09	0.53
1:E:2098:VAL:O	1:E:2098:VAL:HG12	2.08	0.53
1:F:2627:SER:O	1:F:2631:MET:HG2	2.08	0.53
1:H:3646:PRO:HB3	1:H:3650:PHE:CZ	2.44	0.53
1:H:3523:ALA:O	1:H:3526:LEU:HB2	2.09	0.52
1:B:758:SER:HA	1:B:761:ARG:CG	2.39	0.52
1:F:2525:GLU:CA	1:F:2528:ARG:HB3	2.35	0.52
1:B:608:PHE:HD2	1:B:612:LEU:CD2	2.22	0.52
1:E:2085:ASN:HB3	1:E:2087:LEU:CD1	2.39	0.52
1:A:323:VAL:HG23	1:A:364:TYR:HE2	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:3551:GLU:HG2	1:H:3554:ARG:NH1	2.23	0.52
1:E:2046:PRO:HB3	1:E:2048:HIS:CE1	2.45	0.52
1:E:2299:ARG:HB3	1:E:2371:LEU:HD11	1.91	0.52
1:D:1717:SER:H	1:D:1720:ARG:NH1	2.07	0.52
1:C:1296:TYR:O	1:C:1300:ARG:HB2	2.09	0.52
1:H:3626:VAL:HG23	1:H:3854:PHE:CZ	2.45	0.52
1:H:3546:PRO:HB2	1:H:3549:VAL:HG23	1.91	0.52
1:D:1539:GLY:CA	2:D:1914:TRP:HA	2.39	0.52
1:B:546:PRO:O	1:B:549:VAL:HG22	2.09	0.52
1:D:1534:VAL:O	1:D:1846:VAL:HA	2.10	0.52
1:H:3581:PHE:O	1:H:3585:ASN:HB2	2.10	0.52
1:A:128:TYR:N	1:A:129:PRO:HD2	2.24	0.52
1:E:2369:GLU:O	1:E:2369:GLU:HG2	2.10	0.52
1:G:3376:GLU:O	1:G:3379:ALA:HB3	2.08	0.52
1:B:534:VAL:HB	1:B:846:VAL:HG23	1.91	0.52
1:C:1059:GLN:HB2	1:C:1061:LYS:HG2	1.92	0.52
1:E:2064:TYR:CE2	1:F:2742:ARG:NH1	2.78	0.52
1:F:2751:GLU:HG2	1:F:2752:VAL:N	2.24	0.52
1:E:2108:PHE:CD2	1:E:2112:LEU:CD2	2.92	0.52
1:B:747:CYS:CA	1:B:753:ILE:HD11	2.39	0.52
1:C:1098:VAL:CG2	1:C:1267:PRO:HG3	2.39	0.52
1:C:1364:TYR:HA	1:C:1371:LEU:HD11	1.92	0.52
1:H:3522:LYS:O	1:H:3526:LEU:HD12	2.09	0.52
1:E:2026:LEU:HA	1:E:2031:VAL:CG1	2.40	0.52
1:E:2261:ARG:O	1:E:2265:THR:HA	2.09	0.52
1:F:2505:SER:OG	1:F:2508:VAL:HB	2.09	0.52
1:E:2299:ARG:HB3	1:E:2371:LEU:CD1	2.39	0.52
1:C:1212:GLU:HG3	1:C:1316:ARG:NH2	2.25	0.52
1:G:3303:LEU:HD22	1:G:3307:LEU:CD1	2.40	0.52
1:E:2207:GLU:HG3	1:E:2208:HIS:N	2.25	0.52
1:F:2572:GLU:HB3	1:F:2776:LEU:HD11	1.92	0.52
1:H:3506:ARG:O	1:H:3506:ARG:HG2	2.10	0.52
1:E:2300:ARG:NH1	1:E:2317:PRO:O	2.42	0.52
1:F:2845:GLY:HA3	1:F:2877:ARG:HH11	1.75	0.52
1:C:1073:LEU:O	1:C:1077:LEU:HB2	2.10	0.52
1:C:1264:THR:O	1:C:1265:THR:HB	2.10	0.51
1:B:585:ASN:O	1:B:720:ARG:CZ	2.58	0.51
1:F:2592:GLU:HB2	1:F:2750:LYS:NZ	2.25	0.51
1:A:151:VAL:HG22	1:A:181:TYR:HD2	1.74	0.51
1:G:3040:GLU:HB3	1:G:3239:THR:HG21	1.92	0.51
1:B:669:VAL:HG22	1:B:701:VAL:HB	1.91	0.51
1:F:2607:LEU:HG	1:F:2756:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1345:GLY:O	1:C:1377:ARG:NH1	2.43	0.51
1:D:1705:ILE:HG23	1:D:1706:TYR:CD2	2.45	0.51
1:F:2764:THR:O	1:F:2765:THR:HB	2.10	0.51
1:B:674:ASN:CG	1:B:677:THR:HG23	2.29	0.51
1:E:2249:PRO:O	1:E:2253:ILE:HG13	2.10	0.51
1:C:1072:GLU:CB	1:C:1276:LEU:HD11	2.40	0.51
1:B:675:ASN:ND2	3:B:913:PLP:O3	2.44	0.51
1:C:1183:LYS:HG3	1:C:1216:PHE:CD1	2.46	0.51
1:E:2064:TYR:CD1	2:E:2914:TRP:CE3	2.99	0.51
1:C:1064:TYR:HB3	2:D:1914:TRP:CH2	2.46	0.51
1:G:3344:ALA:O	1:G:3377:ARG:HD3	2.09	0.51
1:D:1519:VAL:HG11	1:D:1848:VAL:O	2.11	0.51
1:G:3158:ARG:HH12	1:G:3196:HIS:HE1	1.59	0.51
1:A:175:ASN:HD22	3:A:413:PLP:H2A1	1.74	0.51
1:G:3171:ASN:ND2	1:G:3203:ASP:O	2.44	0.51
1:B:608:PHE:CD2	1:B:612:LEU:CD2	2.94	0.51
1:H:3674:ASN:CG	1:H:3677:THR:HG23	2.32	0.51
1:G:3026:LEU:HD12	1:G:3031:VAL:HG21	1.93	0.51
1:B:839:GLU:O	1:B:843:GLU:HG3	2.10	0.51
1:G:3345:GLY:HA3	1:G:3377:ARG:HH11	1.76	0.51
1:A:2:ARG:HH21	1:B:725:HIS:CE1	2.29	0.51
1:G:3303:LEU:HD22	1:G:3307:LEU:HD12	1.93	0.51
1:H:3506:ARG:CZ	1:H:3506:ARG:HB3	2.41	0.51
1:E:2001:MET:HA	1:F:2697:ASP:O	2.10	0.51
1:H:3516:VAL:HG21	2:H:3914:TRP:CD1	2.46	0.51
1:G:3069:GLY:HA3	1:G:3096:VAL:CG1	2.39	0.51
1:G:3299:ARG:NH1	1:G:3366:THR:O	2.44	0.51
1:E:2376:GLU:O	1:E:2379:ALA:HB3	2.11	0.51
1:A:361:ARG:HH22	2:A:414:TRP:HD1	1.58	0.51
1:H:3608:PHE:CD2	1:H:3612:LEU:CD2	2.92	0.50
1:B:821:PHE:HA	1:B:864:TYR:CZ	2.46	0.50
1:C:1151:VAL:HG22	1:C:1181:TYR:HD2	1.76	0.50
1:A:85:ASN:HB3	1:A:87:LEU:HD13	1.93	0.50
1:D:1514:ASP:HB3	1:D:1517:VAL:CG1	2.40	0.50
1:H:3764:THR:O	1:H:3765:THR:HB	2.11	0.50
1:G:3085:ASN:O	1:G:3220:ARG:NE	2.39	0.50
1:A:183:LYS:HG3	1:A:216:PHE:CD1	2.46	0.50
1:H:3807:LEU:HD21	1:H:3825:MET:SD	2.50	0.50
1:E:2046:PRO:CB	1:E:2048:HIS:CE1	2.94	0.50
1:B:520:ASN:O	1:B:524:LEU:HG	2.12	0.50
1:G:3121:LEU:HD22	1:G:3152:PRO:HB3	1.92	0.50
1:E:2121:LEU:HD22	1:E:2152:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:THR:O	1:A:266:SER:HB2	2.11	0.50
1:G:3175:ASN:HD22	3:G:3413:PLP:H2A1	1.76	0.50
1:A:67:PRO:HG3	1:A:261:ARG:HH11	1.76	0.50
1:B:757:ALA:O	1:B:761:ARG:HG2	2.11	0.50
1:G:3118:VAL:HG21	1:G:3132:VAL:HG23	1.93	0.50
1:E:2108:PHE:O	1:E:2112:LEU:HB2	2.12	0.50
1:C:1027:ARG:HB2	1:C:1033:LEU:HD21	1.92	0.50
1:C:1170:VAL:HG23	1:C:1181:TYR:HE1	1.76	0.50
1:F:2574:ARG:NH2	1:F:2592:GLU:HA	2.26	0.50
1:G:3175:ASN:ND2	3:G:3413:PLP:O3	2.44	0.50
1:F:2621:LEU:CD2	1:F:2652:PRO:HB3	2.42	0.50
1:E:2254:LYS:HA	1:E:2257:ALA:HB3	1.92	0.50
1:H:3709:LEU:HD22	1:H:3796:TYR:CE1	2.46	0.50
1:D:1807:LEU:HD11	1:D:1862:LEU:CD1	2.41	0.50
1:C:1122:SER:HB3	1:C:1124:TYR:CD2	2.47	0.50
1:G:3185:VAL:O	1:G:3189:LEU:HG	2.12	0.50
1:F:2720:ARG:HB3	1:F:2720:ARG:NH1	2.27	0.50
1:B:675:ASN:ND2	3:B:913:PLP:H2A1	2.26	0.50
1:D:1876:GLU:O	1:D:1879:ALA:HB3	2.11	0.50
1:H:3567:PRO:HG3	1:H:3761:ARG:HD3	1.94	0.50
1:B:840:ARG:HA	1:B:843:GLU:HG3	1.93	0.50
1:C:1126:VAL:HG23	1:C:1354:PHE:CE1	2.47	0.50
1:F:2598:VAL:HG12	1:F:2598:VAL:O	2.12	0.50
1:C:1292:ALA:O	1:C:1295:ALA:HB3	2.12	0.50
1:A:249:PRO:HB2	1:A:252:VAL:CG1	2.39	0.50
1:F:2800:ARG:NH1	1:F:2817:PRO:O	2.45	0.50
1:B:743:ILE:HD12	1:B:771:ALA:O	2.12	0.50
1:G:3067:PRO:HG3	1:G:3261:ARG:CZ	2.37	0.50
1:E:2019:VAL:HG21	1:E:2349:VAL:HG22	1.94	0.50
1:F:2844:ALA:O	1:F:2877:ARG:HD2	2.12	0.50
1:E:2073:LEU:O	1:E:2077:LEU:HB2	2.12	0.50
1:H:3524:LEU:O	1:H:3524:LEU:HG	2.12	0.49
1:H:3526:LEU:C	1:H:3531:VAL:HG22	2.33	0.49
1:B:783:GLU:N	1:B:786:ARG:HD3	2.27	0.49
1:G:3108:PHE:O	1:G:3112:LEU:HB2	2.13	0.49
1:H:3622:SER:CB	1:H:3623:PRO:CD	2.87	0.49
1:D:1536:LEU:HD12	1:D:1866:THR:CG2	2.40	0.49
1:B:840:ARG:O	1:B:843:GLU:HB2	2.12	0.49
1:D:1670:VAL:HG23	1:D:1681:TYR:CE1	2.45	0.49
1:A:356:ALA:O	1:A:359:HIS:HB2	2.11	0.49
1:H:3585:ASN:O	1:H:3720:ARG:NE	2.44	0.49
1:B:747:CYS:HA	1:B:753:ILE:CD1	2.41	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:3570:ILE:HG13	1:H:3573:LEU:HB2	1.94	0.49
1:B:627:SER:O	1:B:631:MET:HG2	2.12	0.49
1:H:3707:GLU:HG3	1:H:3708:HIS:N	2.28	0.49
1:H:3622:SER:O	1:H:3623:PRO:C	2.51	0.49
1:H:3598:VAL:HG23	1:H:3602:GLN:OE1	2.12	0.49
1:E:2026:LEU:O	1:E:2031:VAL:HG13	2.12	0.49
1:E:2364:TYR:HA	1:E:2371:LEU:HD21	1.94	0.49
1:B:747:CYS:C	1:B:753:ILE:HD11	2.32	0.49
1:B:705:ILE:HG23	1:B:706:TYR:N	2.27	0.49
1:G:3372:ARG:O	1:G:3376:GLU:HG3	2.11	0.49
1:B:617:GLU:OE1	1:B:664:ARG:NH1	2.45	0.49
1:C:1204:GLU:O	1:C:1206:TYR:N	2.45	0.49
1:H:3747:CYS:C	1:H:3753:ILE:HD11	2.33	0.49
1:G:3082:ARG:HG2	1:G:3087:LEU:O	2.11	0.49
1:E:2312:LEU:HD22	1:E:2325:MET:SD	2.52	0.49
1:A:64:TYR:CD2	2:A:914:TRP:CZ3	3.01	0.49
1:B:546:PRO:HG3	1:B:788:PHE:CD1	2.46	0.49
1:A:183:LYS:HG3	1:A:216:PHE:CG	2.47	0.49
1:C:1301:ASP:O	1:C:1305:GLU:HG3	2.13	0.49
1:A:198:PHE:HA	1:B:501:MET:O	2.13	0.49
1:B:526:LEU:HD21	1:B:842:LEU:HD22	1.94	0.49
1:H:3536:LEU:HB3	1:H:3863:SER:H	1.76	0.49
1:E:2045:THR:HG21	1:E:2241:TRP:NE1	2.26	0.49
1:E:2082:ARG:HG2	1:E:2087:LEU:O	2.13	0.49
1:D:1711:TYR:HB2	1:D:1712:GLU:OE2	2.12	0.49
1:H:3821:PHE:CG	1:H:3865:ALA:HB2	2.47	0.49
1:F:2582:ARG:HH11	1:F:2583:ARG:N	2.09	0.49
1:D:1582:ARG:HB3	1:D:1582:ARG:NH1	2.27	0.49
1:E:2001:MET:O	1:F:2698:PHE:HA	2.13	0.49
1:D:1687:GLU:HG3	1:D:1691:ARG:HH21	1.77	0.49
1:A:292:ALA:O	1:A:295:ALA:HB3	2.12	0.49
1:H:3528:ARG:O	1:H:3529:GLN:HB2	2.12	0.49
1:F:2608:PHE:CD2	1:F:2612:LEU:CD2	2.95	0.49
1:B:569:GLY:HA3	1:B:596:VAL:HG13	1.95	0.49
1:E:2150:PHE:HE1	1:E:2315:VAL:HG21	1.77	0.49
1:F:2864:TYR:HA	1:F:2871:LEU:HD21	1.95	0.49
1:H:3554:ARG:HA	1:H:3557:LEU:HD12	1.95	0.49
1:E:2070:ILE:HG13	1:E:2073:LEU:HB2	1.95	0.49
1:B:880:ARG:HH22	1:D:1843:GLU:HG3	1.77	0.49
1:H:3555:ARG:O	1:H:3559:GLN:HG3	2.12	0.49
1:E:2248:GLY:CA	1:E:2253:ILE:HD11	2.43	0.49
1:E:2253:ILE:HG22	1:E:2253:ILE:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1831:ALA:HB1	1:D:1832:PRO:HD2	1.95	0.49
1:E:2350:PRO:HA	1:E:2360:VAL:HG23	1.95	0.49
1:B:873:LYS:O	1:B:876:GLU:HB3	2.13	0.49
1:B:683:LYS:HZ3	1:B:687:GLU:CD	2.16	0.49
1:H:3687:GLU:O	1:H:3691:ARG:HG3	2.13	0.49
1:E:2145:LEU:O	1:E:2148:GLU:HG3	2.12	0.48
1:G:3005:SER:HB3	1:H:3611:ILE:O	2.13	0.48
1:C:1029:GLN:O	1:C:1029:GLN:HG2	2.13	0.48
1:E:2025:GLU:O	1:E:2026:LEU:HG	2.12	0.48
1:A:175:ASN:ND2	3:A:413:PLP:O3	2.46	0.48
1:B:782:GLN:HB3	1:B:786:ARG:NH2	2.28	0.48
1:F:2590:THR:HB	1:F:2591:PRO:HD2	1.95	0.48
1:D:1792:ALA:O	1:D:1795:ALA:HB3	2.13	0.48
1:D:1799:ARG:HB3	1:D:1871:LEU:CD1	2.41	0.48
1:C:1008:VAL:O	1:C:1011:MET:HG2	2.14	0.48
1:E:2224:GLU:O	1:E:2224:GLU:HG2	2.13	0.48
1:E:2041:PRO:HB3	1:E:2296:TYR:OH	2.13	0.48
1:C:1321:PHE:HA	1:C:1364:TYR:CZ	2.48	0.48
1:H:3839:GLU:O	1:H:3843:GLU:HG2	2.14	0.48
1:G:3190:ALA:HB2	1:G:3218:PRO:HB3	1.95	0.48
1:F:2690:ALA:HB2	1:F:2718:PRO:HB3	1.95	0.48
1:E:2190:ALA:HB2	1:E:2218:PRO:HB3	1.95	0.48
1:D:1803:LEU:HD12	1:D:1864:TYR:HD2	1.78	0.48
1:B:598:VAL:HG23	1:B:602:GLN:OE1	2.12	0.48
1:B:567:PRO:CG	1:B:761:ARG:HH21	2.17	0.48
1:G:3129:PRO:O	1:G:3132:VAL:HG12	2.13	0.48
1:F:2545:THR:HA	1:F:2737:ALA:HB3	1.95	0.48
1:A:102:GLN:HG3	1:A:102:GLN:O	2.14	0.48
1:B:705:ILE:HG23	1:B:706:TYR:H	1.77	0.48
1:B:792:ALA:O	1:B:795:ALA:HB3	2.13	0.48
1:D:1821:PHE:CG	1:D:1865:ALA:HB2	2.49	0.48
1:G:3045:THR:HA	1:G:3237:ALA:HB3	1.94	0.48
1:F:2769:THR:HA	1:F:2772:GLN:HG3	1.94	0.48
1:E:2072:GLU:HB3	1:E:2276:LEU:HD11	1.96	0.48
1:D:1628:TYR:N	1:D:1629:PRO:HD2	2.29	0.48
1:H:3799:ARG:HB3	1:H:3871:LEU:HD11	1.95	0.48
1:B:531:VAL:HA	1:D:1840:ARG:HH22	1.78	0.48
1:A:82:ARG:HG2	1:A:87:LEU:O	2.13	0.48
1:B:690:ALA:HB2	1:B:718:PRO:HB3	1.95	0.48
1:G:3070:ILE:HG13	1:G:3073:LEU:HB2	1.95	0.48
1:A:345:GLY:HA3	1:A:377:ARG:NH1	2.28	0.48
1:G:3102:GLN:HG3	1:G:3102:GLN:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:570:ILE:HG13	1:B:573:LEU:HB2	1.94	0.48
1:B:540:GLU:HB3	1:B:739:THR:HG21	1.96	0.48
1:C:1175:ASN:ND2	3:C:1413:PLP:O3	2.47	0.48
1:G:3085:ASN:HB3	1:G:3087:LEU:HD13	1.94	0.48
1:E:2321:PHE:HA	1:E:2364:TYR:CZ	2.48	0.48
1:E:2087:LEU:CD2	1:E:2247:CYS:SG	3.02	0.48
1:F:2810:LEU:HD21	1:F:2879:ALA:HA	1.95	0.48
1:C:1098:VAL:HG22	1:C:1267:PRO:HG3	1.96	0.48
1:G:3097:THR:HB	1:G:3102:GLN:HG2	1.96	0.48
1:F:2546:PRO:HG3	1:F:2788:PHE:CG	2.48	0.48
1:G:3067:PRO:CD	1:G:3261:ARG:NH1	2.76	0.48
1:G:3026:LEU:O	1:G:3031:VAL:HB	2.13	0.48
1:D:1704:GLU:HG2	1:D:1715:HIS:NE2	2.29	0.48
1:D:1598:VAL:HG23	1:D:1602:GLN:OE1	2.13	0.48
1:C:1107:LEU:HG	1:C:1256:MET:CE	2.44	0.48
1:B:573:LEU:O	1:B:577:LEU:HB2	2.14	0.48
1:A:184:GLU:HA	1:A:187:GLU:CB	2.44	0.48
1:C:1064:TYR:CE2	1:D:1742:ARG:NH1	2.82	0.48
1:C:1024:LEU:CD1	1:C:1024:LEU:O	2.62	0.48
1:B:806:GLY:CA	1:B:875:LEU:HD11	2.44	0.48
1:C:1186:LEU:HD12	1:C:1218:PRO:HG3	1.96	0.48
1:G:3345:GLY:HA3	1:G:3377:ARG:NH1	2.29	0.48
1:C:1367:SER:O	1:C:1371:LEU:HD22	2.14	0.48
1:F:2607:LEU:HG	1:F:2756:MET:CE	2.43	0.48
1:E:2330:ILE:HG22	1:E:2337:ALA:HB1	1.96	0.48
1:E:2026:LEU:H	1:E:2029:GLN:CD	2.17	0.48
1:C:1190:ALA:HB2	1:C:1218:PRO:HB3	1.96	0.48
1:B:705:ILE:HG23	1:B:706:TYR:HD2	1.77	0.48
1:B:800:ARG:NH1	1:B:817:PRO:O	2.46	0.48
1:E:2303:LEU:HD22	1:E:2307:LEU:HD12	1.96	0.48
1:B:525:GLU:HG2	1:B:529:GLN:HE21	1.79	0.48
1:H:3574:ARG:NH2	1:H:3592:GLU:HA	2.29	0.48
1:D:1622:SER:HA	1:D:1623:PRO:C	2.34	0.48
1:C:1032:ASP:C	1:C:1032:ASP:OD1	2.52	0.48
1:E:2261:ARG:HG3	1:E:2262:GLN:HG2	1.96	0.47
1:G:3371:LEU:O	1:G:3375:LEU:HG	2.14	0.47
1:D:1690:ALA:HB2	1:D:1718:PRO:HB3	1.96	0.47
1:G:3266:SER:O	1:H:3742:ARG:HG3	2.14	0.47
1:H:3534:VAL:O	1:H:3846:VAL:HA	2.13	0.47
1:F:2570:ILE:HG13	1:F:2573:LEU:HB2	1.96	0.47
1:F:2800:ARG:O	1:F:2804:LEU:HD23	2.14	0.47
1:G:3014:ASP:CB	1:G:3017:VAL:HG22	2.41	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:ARG:O	1:A:27:ARG:HG2	2.14	0.47
1:H:3597:THR:HG21	1:H:3603:ALA:HA	1.97	0.47
1:G:3312:LEU:HD22	1:G:3325:MET:SD	2.54	0.47
1:F:2502:ARG:HH12	1:G:3082:ARG:CZ	2.26	0.47
1:F:2712:GLU:CG	1:F:2816:ARG:HH12	2.27	0.47
1:H:3551:GLU:HA	1:H:3554:ARG:HD2	1.96	0.47
1:H:3704:GLU:O	1:H:3706:TYR:N	2.47	0.47
1:C:1145:LEU:HB2	1:C:1148:GLU:CG	2.40	0.47
1:E:2077:LEU:HD21	1:E:2245:TYR:HB3	1.96	0.47
1:H:3687:GLU:HG2	1:H:3691:ARG:NH2	2.29	0.47
1:D:1797:ARG:O	1:D:1800:ARG:HB3	2.15	0.47
1:H:3525:GLU:CA	1:H:3528:ARG:HB3	2.45	0.47
1:H:3587:LEU:CD2	1:H:3747:CYS:SG	3.03	0.47
1:A:248:GLY:CA	1:A:253:ILE:HD11	2.45	0.47
1:G:3132:VAL:HG11	1:G:3139:VAL:CG2	2.44	0.47
1:E:2027:ARG:HA	1:E:2031:VAL:O	2.14	0.47
1:F:2527:ARG:HE	1:F:2533:LEU:CD2	2.27	0.47
1:G:3121:LEU:HD12	1:G:3121:LEU:H	1.80	0.47
1:B:796:TYR:O	1:B:800:ARG:HB2	2.15	0.47
1:B:541:PRO:HB3	1:B:796:TYR:OH	2.15	0.47
1:B:804:LEU:O	1:B:808:THR:HB	2.14	0.47
1:B:684:GLU:H	1:B:684:GLU:CD	2.18	0.47
1:E:2292:ALA:O	1:E:2295:ALA:HB3	2.14	0.47
1:E:2265:THR:O	1:E:2266:SER:HB2	2.13	0.47
1:B:645:LEU:O	1:B:648:GLU:HG3	2.15	0.47
1:F:2608:PHE:HB3	1:F:2612:LEU:HD23	1.97	0.47
1:D:1546:PRO:HB2	1:D:1549:VAL:HG23	1.95	0.47
1:E:2130:GLU:HB3	1:F:2762:GLN:OE1	2.15	0.47
1:C:1070:ILE:HG13	1:C:1073:LEU:HB2	1.96	0.47
1:A:190:ALA:HB2	1:A:218:PRO:HB3	1.96	0.47
1:G:3067:PRO:CB	1:G:3261:ARG:HD2	2.45	0.47
1:G:3017:VAL:HG21	1:H:3761:ARG:NH1	2.28	0.47
1:H:3831:ALA:HB1	1:H:3832:PRO:HD2	1.97	0.47
1:G:3325:MET:O	1:G:3359:HIS:HA	2.15	0.47
1:B:684:GLU:HA	1:B:687:GLU:HG3	1.95	0.47
1:F:2792:ALA:O	1:F:2795:ALA:HB3	2.15	0.47
1:A:300:ARG:NH1	1:A:317:PRO:O	2.48	0.47
1:A:64:TYR:CG	2:A:914:TRP:CZ3	3.03	0.47
1:G:3242:ARG:HG2	1:H:3768:ASP:HA	1.95	0.47
1:G:3027:ARG:NH1	1:G:3028:ARG:HH11	2.12	0.47
1:H:3825:MET:O	1:H:3859:HIS:HA	2.15	0.47
1:A:46:PRO:HB2	1:A:49:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:3205:ILE:CG2	1:G:3206:TYR:CD2	2.96	0.47
1:E:2328:SER:HB3	1:E:2329:PRO:HD3	1.97	0.47
1:C:1242:ARG:NH1	1:D:1564:TYR:HE2	2.13	0.47
2:C:1414:TRP:CE3	1:D:1564:TYR:CD1	3.03	0.47
1:D:1593:GLU:HB3	1:D:1748:GLY:O	2.15	0.47
1:A:126:VAL:HG23	1:A:354:PHE:CZ	2.49	0.47
1:G:3158:ARG:NH1	1:G:3196:HIS:HE1	2.12	0.47
1:E:2153:ASP:O	1:E:2157:VAL:HG23	2.15	0.47
1:D:1581:PHE:O	1:D:1585:ASN:HB2	2.14	0.47
1:B:621:LEU:CD2	1:B:652:PRO:HB3	2.45	0.47
1:D:1622:SER:HB3	1:D:1624:TYR:CD2	2.50	0.47
1:D:1674:ASN:HB3	1:D:1677:THR:HG23	1.96	0.47
1:A:174:ASN:CG	1:A:177:THR:HG23	2.34	0.47
1:D:1545:THR:HG21	1:D:1741:TRP:NE1	2.19	0.46
2:G:3414:TRP:CE3	1:H:3564:TYR:CD1	3.03	0.46
1:H:3803:LEU:HD11	1:H:3862:LEU:HD13	1.97	0.46
1:G:3045:THR:HG21	1:G:3241:TRP:NE1	2.28	0.46
1:F:2876:GLU:O	1:F:2879:ALA:HB3	2.15	0.46
1:F:2691:ARG:O	1:F:2694:VAL:HG12	2.15	0.46
1:B:607:LEU:HG	1:B:756:MET:HE1	1.96	0.46
1:E:2064:TYR:CZ	2:E:2914:TRP:HE3	2.33	0.46
1:B:782:GLN:CB	1:B:786:ARG:HD2	2.45	0.46
1:B:525:GLU:CG	1:B:529:GLN:HE21	2.27	0.46
1:C:1108:PHE:CD2	1:C:1112:LEU:CD2	2.97	0.46
1:A:25:GLU:O	1:A:25:GLU:CG	2.63	0.46
1:F:2527:ARG:HE	1:F:2533:LEU:HD21	1.80	0.46
1:D:1717:SER:N	1:D:1720:ARG:HH11	2.12	0.46
1:E:2300:ARG:HH22	1:E:2316:ARG:NH1	2.13	0.46
1:F:2582:ARG:HD2	1:F:2582:ARG:C	2.35	0.46
1:B:519:VAL:HG11	1:B:849:VAL:HG22	1.96	0.46
1:H:3742:ARG:HH22	3:H:3913:PLP:P	2.38	0.46
1:B:694:VAL:HG13	1:B:725:HIS:CE1	2.50	0.46
1:G:3019:VAL:HG11	1:G:3348:VAL:O	2.14	0.46
1:H:3690:ALA:HB2	1:H:3718:PRO:HB3	1.97	0.46
1:A:307:LEU:HD22	1:A:312:LEU:HB2	1.97	0.46
1:G:3132:VAL:CG1	1:G:3133:ARG:N	2.79	0.46
1:D:1587:LEU:HD23	1:D:1747:CYS:SG	2.56	0.46
1:C:1286:ARG:NH1	1:C:1286:ARG:HG3	2.27	0.46
1:E:2019:VAL:HG11	1:E:2348:VAL:O	2.15	0.46
1:E:2345:GLY:O	1:E:2377:ARG:NH1	2.48	0.46
1:D:1684:GLU:HA	1:D:1687:GLU:CB	2.46	0.46
1:A:122:SER:HA	1:A:123:PRO:C	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:2514:ASP:HB3	1:F:2517:VAL:CG1	2.46	0.46
1:E:2093:GLU:HB3	1:E:2248:GLY:O	2.16	0.46
1:C:1064:TYR:CD1	2:D:1914:TRP:CZ3	3.04	0.46
1:E:2112:LEU:HD11	1:E:2118:VAL:CG2	2.45	0.46
1:B:764:THR:O	1:B:765:THR:HB	2.14	0.46
1:B:717:SER:HB2	1:B:720:ARG:NH1	2.28	0.46
1:F:2519:VAL:HG21	1:F:2849:VAL:HG22	1.97	0.46
1:H:3583:ARG:NH1	1:H:3782:GLN:HE21	2.14	0.46
1:E:2324:LEU:HA	1:E:2324:LEU:HD23	1.69	0.46
1:G:3020:ASN:O	1:G:3024:LEU:HG	2.15	0.46
1:H:3803:LEU:O	1:H:3807:LEU:HB2	2.16	0.46
1:A:70:ILE:HG13	1:A:73:LEU:HB2	1.96	0.46
1:C:1041:PRO:HB3	1:C:1296:TYR:OH	2.15	0.46
1:D:1646:PRO:HB3	1:D:1650:PHE:CZ	2.51	0.46
1:A:254:LYS:HG2	1:A:254:LYS:O	2.16	0.46
1:G:3292:ALA:O	1:G:3295:ALA:HB3	2.16	0.46
1:H:3612:LEU:HD11	1:H:3618:VAL:CG2	2.46	0.46
1:F:2524:LEU:CD1	1:F:2527:ARG:HG2	2.46	0.46
1:H:3533:LEU:HD22	1:H:3533:LEU:N	2.27	0.46
1:C:1122:SER:HB3	1:C:1124:TYR:HD2	1.81	0.46
1:F:2769:THR:O	1:F:2772:GLN:HB2	2.16	0.46
1:D:1622:SER:HB3	1:D:1624:TYR:HD2	1.81	0.46
1:H:3655:GLU:O	1:H:3658:ARG:HB3	2.16	0.46
1:F:2528:ARG:O	1:F:2529:GLN:HG2	2.15	0.46
1:F:2845:GLY:HA3	1:F:2877:ARG:NH1	2.31	0.46
1:D:1570:ILE:HG13	1:D:1573:LEU:HB2	1.97	0.46
1:E:2354:PHE:O	1:E:2355:ALA:HB3	2.16	0.46
1:F:2608:PHE:HD2	1:F:2612:LEU:CD2	2.29	0.45
1:F:2523:ALA:HB3	1:F:2524:LEU:HD22	1.97	0.45
1:H:3841:LEU:O	1:H:3846:VAL:HG12	2.16	0.45
1:B:625:TRP:HB2	1:B:675:ASN:CB	2.46	0.45
1:B:607:LEU:HG	1:B:756:MET:CE	2.45	0.45
1:C:1040:GLU:HB3	1:C:1239:THR:HG21	1.98	0.45
1:C:1097:THR:HG21	1:C:1103:ALA:HA	1.97	0.45
1:E:2184:GLU:H	1:E:2184:GLU:CD	2.18	0.45
1:B:800:ARG:O	1:B:800:ARG:HD2	2.15	0.45
1:D:1520:ASN:O	1:D:1524:LEU:HD23	2.16	0.45
1:A:253:ILE:O	1:A:253:ILE:HG22	2.16	0.45
1:C:1307:LEU:CD2	1:C:1325:MET:SD	3.04	0.45
1:C:1268:ASP:HA	1:D:1742:ARG:HG2	1.98	0.45
1:D:1608:PHE:HD2	1:D:1612:LEU:CD2	2.29	0.45
1:H:3602:GLN:O	1:H:3602:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:882:LEU:HA	1:B:882:LEU:HD23	1.83	0.45
1:E:2205:ILE:HG23	1:E:2206:TYR:CD2	2.52	0.45
1:A:264:THR:O	1:A:265:THR:HB	2.16	0.45
1:E:2077:LEU:HD21	1:E:2245:TYR:CB	2.46	0.45
1:D:1782:GLN:O	1:D:1783:GLU:HB2	2.17	0.45
1:D:1803:LEU:HD12	1:D:1864:TYR:CD2	2.52	0.45
1:G:3128:TYR:N	1:G:3129:PRO:HD2	2.32	0.45
2:G:3414:TRP:CZ3	1:H:3564:TYR:HB2	2.51	0.45
1:E:2048:HIS:O	1:E:2051:GLU:HB3	2.17	0.45
1:F:2593:GLU:HB3	1:F:2748:GLY:O	2.16	0.45
1:B:531:VAL:HG13	1:D:1840:ARG:HH12	1.82	0.45
1:A:2:ARG:NH2	1:B:725:HIS:CE1	2.85	0.45
1:H:3750:LYS:HB2	1:H:3750:LYS:HE3	1.80	0.45
1:C:1205:ILE:HG23	1:C:1206:TYR:N	2.32	0.45
1:B:758:SER:HA	1:B:761:ARG:HG2	1.98	0.45
1:G:3132:VAL:HG22	1:G:3137:GLY:HA3	1.97	0.45
1:D:1524:LEU:C	1:D:1525:GLU:HG3	2.37	0.45
1:F:2502:ARG:NH1	1:G:3082:ARG:NH1	2.65	0.45
1:B:832:PRO:CB	1:B:836:ARG:HH21	2.29	0.45
1:F:2545:THR:HG21	1:F:2741:TRP:NE1	2.28	0.45
1:F:2833:ASP:CB	1:F:2836:ARG:HH21	2.29	0.45
1:G:3077:LEU:HD21	1:G:3245:TYR:HB3	1.99	0.45
1:B:880:ARG:NH1	1:D:1843:GLU:OE1	2.50	0.45
1:C:1341:LEU:O	1:C:1346:VAL:HG12	2.17	0.45
1:C:1185:VAL:O	1:C:1189:LEU:HG	2.17	0.45
1:D:1612:LEU:HD11	1:D:1618:VAL:CG2	2.47	0.45
1:C:1112:LEU:HD21	1:C:1118:VAL:HG21	1.99	0.45
1:F:2881:VAL:HG12	1:F:2882:LEU:N	2.32	0.45
1:F:2674:ASN:OD1	1:F:2677:THR:HG23	2.16	0.45
1:C:1122:SER:HA	1:C:1123:PRO:C	2.37	0.45
1:C:1327:THR:HB	1:C:1337:ALA:HB1	1.98	0.45
1:H:3792:ALA:O	1:H:3795:ALA:HB3	2.17	0.45
1:C:1105:PHE:HA	1:C:1131:MET:HE2	1.97	0.45
1:G:3025:GLU:O	1:G:3028:ARG:N	2.50	0.45
1:F:2527:ARG:O	1:F:2527:ARG:HG3	2.16	0.45
1:B:562:THR:O	1:B:562:THR:OG1	2.35	0.45
1:B:830:ILE:HD11	1:B:841:LEU:HD21	1.99	0.45
1:E:2126:VAL:HG23	1:E:2354:PHE:CZ	2.52	0.45
1:D:1748:GLY:CA	1:D:1753:ILE:HD11	2.45	0.44
1:D:1596:VAL:O	1:D:1767:PRO:HG2	2.17	0.44
1:D:1727:LEU:HD11	1:D:1752:VAL:HG11	1.98	0.44
1:B:669:VAL:CG2	1:B:701:VAL:HB	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:727:LEU:HD11	1:B:752:VAL:HG21	1.99	0.44
1:H:3656:ARG:HA	1:H:3659:ARG:HG2	2.00	0.44
1:A:5:SER:O	1:A:9:GLN:HG3	2.17	0.44
1:C:1064:TYR:CD1	2:D:1914:TRP:CE3	3.05	0.44
1:F:2761:ARG:CD	1:F:2762:GLN:HG2	2.47	0.44
1:D:1877:ARG:HG2	1:D:1880:ARG:NH2	2.32	0.44
2:C:1414:TRP:CE3	1:D:1564:TYR:CG	3.06	0.44
1:B:612:LEU:HD11	1:B:618:VAL:CG2	2.47	0.44
1:E:2108:PHE:CB	1:E:2112:LEU:HD23	2.42	0.44
1:H:3670:VAL:HG23	1:H:3681:TYR:CE1	2.47	0.44
1:G:3299:ARG:HB3	1:G:3371:LEU:HD11	1.99	0.44
1:H:3573:LEU:O	1:H:3577:LEU:HB2	2.17	0.44
1:A:14:ASP:HB3	1:A:17:VAL:HG12	1.99	0.44
1:E:2107:LEU:HD21	1:E:2227:LEU:HD13	2.00	0.44
1:G:3262:GLN:OE1	1:H:3630:GLU:HB3	2.17	0.44
1:A:204:GLU:O	1:A:206:TYR:N	2.50	0.44
1:G:3108:PHE:CD2	1:G:3112:LEU:CD2	2.99	0.44
2:G:3414:TRP:CZ3	1:H:3564:TYR:CB	2.98	0.44
1:D:1585:ASN:CB	1:D:1587:LEU:HD13	2.48	0.44
1:A:143:GLU:HG3	1:A:144:THR:N	2.33	0.44
1:B:798:ARG:HH11	1:B:798:ARG:HG3	1.83	0.44
1:C:1261:ARG:NH2	1:D:1517:VAL:HG11	2.33	0.44
1:A:12:LYS:HE3	1:A:12:LYS:HB2	1.72	0.44
1:B:851:GLY:HA3	1:B:856:ALA:O	2.16	0.44
1:C:1205:ILE:HG23	1:C:1206:TYR:HD2	1.80	0.44
1:C:1112:LEU:HD11	1:C:1118:VAL:CG2	2.47	0.44
1:D:1866:THR:OG1	1:D:1867:SER:N	2.51	0.44
1:G:3034:VAL:HG22	1:G:3373:LYS:HD2	1.99	0.44
1:A:340:ARG:NH2	1:A:381:VAL:O	2.50	0.44
1:G:3077:LEU:HD11	1:G:3245:TYR:CG	2.53	0.44
1:D:1684:GLU:HA	1:D:1687:GLU:HB2	1.99	0.44
1:D:1619:ILE:HA	1:D:1640:VAL:O	2.18	0.44
1:C:1242:ARG:HH22	3:C:1413:PLP:P	2.41	0.44
1:D:1821:PHE:CD1	1:D:1865:ALA:HB2	2.53	0.44
1:E:2145:LEU:CD2	1:E:2156:ARG:HH22	2.21	0.44
1:A:5:SER:OG	1:A:8:VAL:HB	2.18	0.44
1:H:3765:THR:O	1:H:3766:SER:HB2	2.17	0.44
1:C:1151:VAL:HG22	1:C:1181:TYR:CD2	2.52	0.44
1:B:524:LEU:H	1:B:524:LEU:CD2	2.21	0.44
1:B:617:GLU:HG3	1:B:664:ARG:HB3	1.99	0.44
1:C:1184:GLU:CD	1:C:1184:GLU:H	2.20	0.44
1:E:2312:LEU:HD11	1:E:2382:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:2097:THR:HB	1:E:2102:GLN:CG	2.36	0.44
1:A:321:PHE:CG	1:A:365:ALA:HB2	2.53	0.44
1:H:3508:VAL:O	1:H:3511:MET:HG2	2.18	0.44
1:H:3621:LEU:N	1:H:3621:LEU:HD12	2.33	0.44
1:G:3300:ARG:NH1	1:G:3317:PRO:O	2.51	0.44
1:G:3170:VAL:HG23	1:G:3181:TYR:HE1	1.82	0.44
1:F:2643:GLU:HG3	1:F:2644:THR:N	2.33	0.44
1:A:22:LYS:HE2	1:A:26:LEU:HD11	1.98	0.43
1:E:2029:GLN:CG	1:E:2029:GLN:O	2.66	0.43
1:A:286:ARG:HG2	1:A:286:ARG:O	2.18	0.43
1:F:2799:ARG:HB3	1:F:2871:LEU:CD1	2.48	0.43
1:C:1216:PHE:HD1	1:C:1220:ARG:HH11	1.66	0.43
1:B:848:VAL:HG21	1:B:860:VAL:HG21	1.99	0.43
1:E:2089:VAL:HA	1:E:2093:GLU:OE1	2.18	0.43
1:A:112:LEU:HD11	1:A:118:VAL:CG2	2.49	0.43
1:G:3077:LEU:HD21	1:G:3245:TYR:CB	2.47	0.43
1:D:1579:GLU:O	1:D:1583:ARG:HB2	2.18	0.43
1:C:1024:LEU:O	1:C:1028:ARG:HB2	2.18	0.43
1:C:1212:GLU:CD	1:C:1316:ARG:HH12	2.21	0.43
1:C:1125:TRP:HA	1:C:1354:PHE:CE2	2.53	0.43
1:F:2796:TYR:O	1:F:2800:ARG:HB2	2.19	0.43
1:G:3208:HIS:O	1:G:3293:ARG:NH2	2.51	0.43
1:E:2268:ASP:HA	1:F:2742:ARG:HG2	2.00	0.43
1:C:1028:ARG:O	1:C:1029:GLN:CB	2.66	0.43
1:H:3674:ASN:OD1	1:H:3677:THR:HG23	2.19	0.43
1:G:3027:ARG:HA	1:G:3031:VAL:O	2.18	0.43
1:A:321:PHE:HA	1:A:364:TYR:OH	2.19	0.43
1:G:3321:PHE:HA	1:G:3364:TYR:CZ	2.53	0.43
1:C:1107:LEU:HG	1:C:1256:MET:HE1	2.00	0.43
1:F:2804:LEU:O	1:F:2808:THR:HB	2.18	0.43
1:C:1307:LEU:HD21	1:C:1325:MET:SD	2.58	0.43
1:D:1522:LYS:HA	1:D:1525:GLU:OE2	2.18	0.43
1:G:3204:GLU:HG2	1:G:3215:HIS:CE1	2.53	0.43
1:E:2124:TYR:CE1	1:E:2129:PRO:HG3	2.53	0.43
1:F:2573:LEU:O	1:F:2577:LEU:HB2	2.19	0.43
1:G:3310:LEU:HD11	1:G:3379:ALA:HA	2.01	0.43
1:C:1034:VAL:O	1:C:1346:VAL:HA	2.19	0.43
1:A:233:ALA:HB1	1:A:239:THR:HG22	2.00	0.43
1:G:3112:LEU:HD11	1:G:3118:VAL:CG2	2.47	0.43
1:F:2612:LEU:HD11	1:F:2618:VAL:CG2	2.47	0.43
1:C:1007:ARG:HG3	1:C:1008:VAL:N	2.33	0.43
1:E:2051:GLU:O	1:E:2054:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:2748:GLY:N	1:F:2753:ILE:CD1	2.81	0.43
1:C:1176:PRO:HD3	1:C:1354:PHE:CD2	2.54	0.43
1:F:2705:ILE:HG23	1:F:2706:TYR:CD2	2.53	0.43
1:B:662:THR:HB	1:B:664:ARG:NH2	2.33	0.43
1:F:2546:PRO:HG3	1:F:2788:PHE:CD1	2.54	0.43
1:G:3324:LEU:HA	1:G:3324:LEU:HD23	1.83	0.43
1:H:3514:ASP:O	1:H:3517:VAL:HG12	2.18	0.43
1:G:3014:ASP:HB3	1:G:3017:VAL:HG13	2.01	0.43
1:E:2265:THR:O	1:E:2266:SER:CB	2.67	0.43
1:E:2112:LEU:HD21	1:E:2118:VAL:HG21	2.01	0.43
1:C:1026:LEU:O	1:C:1031:VAL:HB	2.18	0.43
1:G:3312:LEU:HD21	1:G:3330:ILE:HD12	2.01	0.43
1:G:3205:ILE:HG22	1:G:3206:TYR:HD2	1.79	0.43
1:B:825:MET:O	1:B:859:HIS:HA	2.19	0.43
1:G:3341:LEU:O	1:G:3346:VAL:HG12	2.19	0.43
1:G:3126:VAL:HG23	1:G:3354:PHE:CZ	2.53	0.43
1:C:1372:ARG:HD3	1:C:1372:ARG:HA	1.84	0.43
1:D:1705:ILE:HG23	1:D:1706:TYR:HD2	1.82	0.43
1:E:2204:GLU:HG2	1:E:2215:HIS:HE1	1.77	0.43
1:B:717:SER:N	1:B:720:ARG:NH1	2.66	0.43
1:G:3283:GLU:H	1:G:3283:GLU:CD	2.22	0.43
1:H:3585:ASN:CB	1:H:3587:LEU:HD13	2.49	0.43
1:A:28:ARG:HA	1:A:28:ARG:HD2	1.82	0.43
1:A:198:PHE:HD2	1:A:199:TYR:O	2.02	0.43
1:B:752:VAL:O	1:B:756:MET:HG3	2.19	0.43
1:D:1655:GLU:O	1:D:1658:ARG:HB3	2.18	0.43
1:G:3335:VAL:O	1:G:3339:GLU:HG2	2.19	0.43
1:G:3067:PRO:HB3	1:G:3261:ARG:CD	2.49	0.43
1:E:2066:PRO:O	1:E:2266:SER:OG	2.37	0.43
1:E:2330:ILE:HG13	1:E:2382:LEU:CD2	2.49	0.43
1:A:248:GLY:H	1:A:253:ILE:HD11	1.79	0.43
1:H:3608:PHE:HB3	1:H:3612:LEU:HD23	2.01	0.43
1:H:3622:SER:HB2	1:H:3623:PRO:CD	2.48	0.43
1:A:12:LYS:HG3	1:A:13:PRO:CD	2.47	0.43
1:F:2841:LEU:O	1:F:2846:VAL:HG12	2.19	0.43
1:C:1376:GLU:O	1:C:1379:ALA:HB3	2.19	0.43
1:A:119:ILE:HA	1:A:140:VAL:O	2.19	0.43
1:B:758:SER:HA	1:B:761:ARG:NH1	2.24	0.42
1:B:545:THR:HG22	1:B:737:ALA:O	2.19	0.42
1:E:2146:PRO:HB3	1:E:2150:PHE:CZ	2.54	0.42
1:E:2341:LEU:O	1:E:2346:VAL:HG12	2.19	0.42
1:A:34:VAL:HG11	1:A:374:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1124:TYR:O	1:C:1354:PHE:CD2	2.72	0.42
1:H:3645:LEU:HB2	1:H:3648:GLU:HG2	2.00	0.42
1:E:2121:LEU:O	1:E:2124:TYR:HB3	2.19	0.42
1:A:184:GLU:HA	1:A:187:GLU:HB2	2.01	0.42
1:B:848:VAL:CG2	1:B:860:VAL:HG21	2.49	0.42
1:D:1823:VAL:HG23	1:D:1864:TYR:CE2	2.53	0.42
1:B:758:SER:CA	1:B:761:ARG:HD2	2.44	0.42
1:C:1345:GLY:HA3	1:C:1377:ARG:NH1	2.34	0.42
1:F:2720:ARG:HH11	1:F:2720:ARG:CB	2.32	0.42
1:B:717:SER:OG	1:B:720:ARG:NH1	2.52	0.42
1:C:1226:THR:CG2	1:C:1227:LEU:N	2.81	0.42
1:B:619:ILE:HA	1:B:640:VAL:O	2.20	0.42
1:C:1062:THR:OG1	1:C:1062:THR:O	2.37	0.42
1:A:23:ALA:HB3	1:A:24:LEU:H	1.68	0.42
1:A:341:LEU:O	1:A:346:VAL:HG12	2.20	0.42
1:A:321:PHE:CD1	1:A:365:ALA:HB2	2.54	0.42
1:A:170:VAL:HG23	1:A:181:TYR:HE1	1.84	0.42
1:C:1015:ALA:HB2	1:C:1353:ASP:OD1	2.19	0.42
1:G:3067:PRO:CG	1:G:3261:ARG:CZ	2.94	0.42
1:H:3598:VAL:HG21	1:H:3764:THR:HG21	2.00	0.42
1:E:2085:ASN:HB2	1:E:2087:LEU:HD13	2.00	0.42
1:B:534:VAL:CG1	1:B:874:ALA:HB2	2.46	0.42
1:D:1683:LYS:HG3	1:D:1716:PHE:CG	2.54	0.42
1:C:1121:LEU:HD22	1:C:1152:PRO:HB3	2.01	0.42
1:E:2077:LEU:HD11	1:E:2245:TYR:CG	2.54	0.42
1:D:1540:GLU:HB3	1:D:1739:THR:HG21	2.02	0.42
1:A:64:TYR:CE2	1:B:742:ARG:NH1	2.85	0.42
1:B:843:GLU:C	1:B:845:GLY:H	2.23	0.42
1:A:2:ARG:HE	1:B:725:HIS:CD2	2.37	0.42
1:F:2670:VAL:HG23	1:F:2681:TYR:HE1	1.83	0.42
1:A:112:LEU:HD21	1:A:118:VAL:HG21	2.01	0.42
1:G:3112:LEU:HD21	1:G:3118:VAL:HG21	2.02	0.42
1:B:841:LEU:O	1:B:846:VAL:HG12	2.19	0.42
1:C:1286:ARG:O	1:C:1290:GLU:HG2	2.20	0.42
1:H:3534:VAL:CG2	1:H:3873:LYS:HD2	2.48	0.42
1:B:804:LEU:HD11	1:B:816:ARG:HA	2.01	0.42
1:G:3227:LEU:HD11	1:G:3252:VAL:HG21	2.02	0.42
1:A:187:GLU:HG3	1:A:191:ARG:NH2	2.34	0.42
1:C:1119:ILE:HA	1:C:1140:VAL:O	2.20	0.42
1:F:2656:ARG:HA	1:F:2659:ARG:HG2	2.02	0.42
1:G:3212:GLU:OE2	1:G:3316:ARG:NH2	2.51	0.42
1:H:3827:THR:CG2	1:H:3860:VAL:HB	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:ARG:NH2	1:A:92:GLU:HA	2.35	0.42
1:G:3067:PRO:CD	1:G:3261:ARG:NH2	2.78	0.42
1:H:3524:LEU:O	1:H:3525:GLU:CG	2.68	0.42
1:A:249:PRO:O	1:A:253:ILE:HG13	2.20	0.42
1:H:3612:LEU:HD21	1:H:3618:VAL:HG21	2.02	0.42
1:B:792:ALA:HB1	1:B:796:TYR:CE1	2.55	0.42
1:H:3776:LEU:O	1:H:3776:LEU:HD23	2.19	0.42
1:C:1306:GLY:C	1:C:1375:LEU:HD21	2.39	0.42
1:B:611:ILE:CG1	1:B:612:LEU:H	2.20	0.42
1:A:45:THR:HA	1:A:46:PRO:HD3	1.88	0.42
1:E:2323:VAL:HG23	1:E:2364:TYR:CE2	2.54	0.42
1:A:330:ILE:HD11	1:A:341:LEU:HD21	2.02	0.42
1:E:2345:GLY:HA3	1:E:2377:ARG:NH1	2.35	0.42
1:D:1841:LEU:O	1:D:1846:VAL:HG12	2.20	0.42
1:H:3617:GLU:CD	1:H:3664:ARG:HG3	2.40	0.42
1:F:2587:LEU:HA	1:F:2587:LEU:HD12	1.89	0.42
1:E:2325:MET:O	1:E:2359:HIS:HA	2.20	0.42
1:D:1748:GLY:N	1:D:1753:ILE:CD1	2.73	0.42
1:A:111:ILE:CG1	1:A:112:LEU:H	2.19	0.42
1:B:612:LEU:HD21	1:B:618:VAL:HG21	2.02	0.42
1:G:3118:VAL:HB	1:G:3132:VAL:HG21	2.02	0.42
1:C:1111:ILE:CG1	1:C:1112:LEU:H	2.21	0.42
1:C:1102:GLN:O	1:C:1102:GLN:HG3	2.20	0.42
1:E:2026:LEU:C	1:E:2031:VAL:HG13	2.41	0.42
1:A:45:THR:HG22	1:A:237:ALA:O	2.19	0.42
1:E:2224:GLU:CG	1:E:2224:GLU:O	2.68	0.42
1:B:717:SER:H	1:B:720:ARG:HH11	1.65	0.42
1:A:255:ALA:HB1	1:B:508:VAL:HG11	2.02	0.42
1:E:2186:LEU:HB3	1:E:2218:PRO:HG3	2.02	0.42
1:E:2276:LEU:O	1:E:2280:THR:HG23	2.20	0.42
1:E:2302:LEU:HD11	1:E:2372:ARG:HH21	1.84	0.42
1:F:2662:THR:HB	1:F:2664:ARG:NH2	2.35	0.42
1:H:3619:ILE:HA	1:H:3640:VAL:O	2.19	0.42
1:E:2362:LEU:HD11	1:E:2378:PHE:CE1	2.55	0.42
1:A:20:ASN:O	1:A:24:LEU:HG	2.20	0.42
1:D:1825:MET:O	1:D:1859:HIS:HA	2.20	0.42
1:B:675:ASN:HD22	3:B:913:PLP:H2A1	1.85	0.42
1:G:3014:ASP:HB3	1:G:3017:VAL:CG2	2.44	0.41
1:G:3107:LEU:HD23	1:G:3111:ILE:HG12	2.01	0.41
1:A:64:TYR:CE2	2:A:914:TRP:CZ3	3.08	0.41
1:D:1578:ALA:O	1:D:1582:ARG:HG3	2.20	0.41
1:D:1681:TYR:HB2	1:D:1686:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:533:LEU:CD2	1:B:533:LEU:H	2.33	0.41
1:A:265:THR:O	1:A:266:SER:CB	2.68	0.41
1:F:2619:ILE:HA	1:F:2640:VAL:O	2.20	0.41
1:B:782:GLN:HG2	1:B:786:ARG:NH2	2.17	0.41
1:D:1840:ARG:NH2	1:D:1881:VAL:O	2.49	0.41
1:B:690:ALA:O	1:B:694:VAL:HG23	2.19	0.41
1:D:1621:LEU:O	1:D:1624:TYR:HB3	2.20	0.41
1:D:1573:LEU:O	1:D:1577:LEU:HB2	2.20	0.41
1:G:3184:GLU:H	1:G:3184:GLU:CD	2.23	0.41
1:G:3023:ALA:O	1:G:3025:GLU:N	2.46	0.41
1:B:821:PHE:CG	1:B:865:ALA:HB2	2.54	0.41
1:H:3840:ARG:NH2	1:H:3881:VAL:O	2.52	0.41
1:B:717:SER:HA	1:B:718:PRO:HD3	1.92	0.41
1:E:2346:VAL:HG13	1:E:2346:VAL:O	2.20	0.41
1:B:749:PRO:HB2	1:B:752:VAL:HG12	2.01	0.41
1:D:1844:ALA:O	1:D:1877:ARG:HD3	2.21	0.41
1:C:1242:ARG:HG2	1:D:1768:ASP:HA	2.02	0.41
1:E:2153:ASP:OD2	1:E:2156:ARG:HD3	2.20	0.41
1:D:1525:GLU:CA	1:D:1528:ARG:HB3	2.51	0.41
1:C:1085:ASN:CB	1:C:1087:LEU:HD13	2.48	0.41
1:F:2830:ILE:O	1:F:2830:ILE:HD13	2.20	0.41
1:C:1297:ARG:O	1:C:1300:ARG:HB3	2.20	0.41
1:E:2112:LEU:HD11	1:E:2118:VAL:HG23	2.03	0.41
1:F:2802:LEU:HD23	1:F:2868:GLU:OE2	2.20	0.41
1:B:694:VAL:HA	1:B:725:HIS:NE2	2.36	0.41
1:E:2174:ASN:OD1	1:E:2175:ASN:N	2.53	0.41
1:G:3071:PRO:O	1:G:3075:GLU:HG3	2.20	0.41
1:F:2824:LEU:HA	1:F:2824:LEU:HD23	1.80	0.41
1:H:3842:LEU:HD23	1:H:3842:LEU:HA	1.73	0.41
1:B:626:VAL:HG23	1:B:854:PHE:CE2	2.55	0.41
1:C:1206:TYR:HE2	3:C:1413:PLP:C2A	2.33	0.41
1:C:1324:LEU:HD23	1:C:1324:LEU:HA	1.77	0.41
1:H:3678:GLY:HA3	1:H:3817:PRO:HB3	2.01	0.41
1:H:3823:VAL:HG23	1:H:3864:TYR:CE2	2.54	0.41
1:D:1562:THR:O	1:D:1562:THR:OG1	2.36	0.41
1:H:3562:THR:OG1	1:H:3562:THR:O	2.37	0.41
1:A:342:LEU:HA	1:A:342:LEU:HD23	1.84	0.41
1:D:1803:LEU:HD22	1:D:1807:LEU:CD1	2.51	0.41
1:C:1046:PRO:HB2	1:C:1049:VAL:CG2	2.45	0.41
1:F:2753:ILE:CG2	1:F:2753:ILE:O	2.63	0.41
1:F:2761:ARG:HG2	1:F:2761:ARG:O	2.17	0.41
1:G:3303:LEU:HD23	1:G:3375:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:3158:ARG:NH1	1:G:3196:HIS:CE1	2.89	0.41
1:D:1621:LEU:CD2	1:D:1652:PRO:HB3	2.51	0.41
1:F:2514:ASP:HB3	1:F:2517:VAL:HB	2.02	0.41
1:D:1506:ARG:CG	1:D:1506:ARG:HH11	2.33	0.41
1:F:2831:ALA:HB1	1:F:2832:PRO:CD	2.50	0.41
1:D:1782:GLN:O	1:D:1783:GLU:CB	2.68	0.41
1:B:554:ARG:HA	1:B:557:LEU:HD12	2.01	0.41
1:C:1067:PRO:HG2	1:C:1068:ALA:H	1.86	0.41
1:C:1067:PRO:HG2	1:C:1068:ALA:N	2.36	0.41
1:F:2529:GLN:HG3	1:F:2529:GLN:O	2.20	0.41
1:G:3025:GLU:O	1:G:3026:LEU:C	2.59	0.41
1:H:3622:SER:CB	1:H:3643:GLU:HA	2.51	0.41
1:G:3330:ILE:O	1:G:3331:ALA:HB2	2.20	0.41
1:E:2045:THR:HA	1:E:2046:PRO:HD3	1.91	0.41
1:F:2533:LEU:HD23	1:F:2533:LEU:C	2.41	0.41
1:A:57:LEU:HD21	1:B:741:TRP:CH2	2.56	0.41
1:C:1253:ILE:O	1:C:1253:ILE:CG2	2.67	0.41
1:B:581:PHE:O	1:B:585:ASN:HB2	2.21	0.41
1:C:1381:VAL:HG12	1:C:1382:LEU:N	2.35	0.41
1:E:2296:TYR:O	1:E:2300:ARG:HB2	2.20	0.41
1:E:2184:GLU:HA	1:E:2187:GLU:HB3	2.03	0.41
1:B:816:ARG:HA	1:B:817:PRO:HD2	1.98	0.41
1:B:804:LEU:CD1	1:B:816:ARG:HG3	2.51	0.41
1:D:1575:GLU:O	1:D:1579:GLU:HG3	2.21	0.41
1:F:2681:TYR:HA	1:F:2682:PRO:HD3	1.80	0.41
1:H:3683:LYS:HG3	1:H:3716:PHE:CG	2.56	0.41
1:H:3876:GLU:O	1:H:3879:ALA:HB3	2.21	0.41
1:D:1819:GLY:O	1:D:1820:ALA:HB3	2.21	0.41
1:H:3800:ARG:O	1:H:3804:LEU:HD23	2.20	0.41
1:A:107:LEU:HG	1:A:256:MET:CE	2.51	0.41
1:D:1741:TRP:O	1:D:1742:ARG:HB2	2.21	0.41
1:G:3025:GLU:O	1:G:3028:ARG:C	2.59	0.41
1:B:864:TYR:HA	1:B:871:LEU:HD21	2.02	0.41
1:G:3205:ILE:CG2	1:G:3206:TYR:N	2.84	0.41
1:C:1197:ASP:O	1:D:1501:MET:HA	2.21	0.41
1:D:1617:GLU:HG3	1:D:1664:ARG:HE	1.85	0.41
1:B:625:TRP:HB2	1:B:675:ASN:HB3	2.03	0.41
1:F:2621:LEU:HD22	1:F:2652:PRO:HB3	2.03	0.41
1:H:3693:ALA:HA	1:H:3698:PHE:CZ	2.56	0.41
1:B:574:ARG:NH2	1:B:592:GLU:HA	2.36	0.41
1:C:1017:VAL:CG1	1:D:1761:ARG:HH21	2.31	0.40
1:A:108:PHE:HB3	1:A:112:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:3008:VAL:O	1:G:3011:MET:HG2	2.21	0.40
1:G:3112:LEU:HD11	1:G:3118:VAL:HG23	2.04	0.40
1:C:1033:LEU:HD22	1:C:1033:LEU:N	2.35	0.40
1:A:45:THR:CG2	1:B:562:THR:OG1	2.69	0.40
1:D:1550:LYS:O	1:D:1554:ARG:HG3	2.22	0.40
1:H:3612:LEU:HD11	1:H:3618:VAL:HG23	2.04	0.40
1:F:2831:ALA:HB3	1:F:2837:ALA:CB	2.42	0.40
1:G:3127:SER:HB3	1:H:3762:GLN:OE1	2.21	0.40
1:E:2373:LYS:O	1:E:2376:GLU:HB3	2.21	0.40
1:B:646:PRO:HB3	1:B:650:PHE:CZ	2.57	0.40
1:B:672:SER:HA	1:B:674:ASN:N	2.37	0.40
1:B:686:LEU:HB2	1:B:716:PHE:CD2	2.56	0.40
1:B:572:GLU:HB3	1:B:776:LEU:HD11	2.03	0.40
1:F:2869:GLU:O	1:F:2873:LYS:HG3	2.21	0.40
1:G:3156:ARG:HA	1:G:3159:ARG:HG2	2.04	0.40
1:B:656:ARG:HA	1:B:659:ARG:HG2	2.02	0.40
1:B:680:VAL:HG13	1:B:680:VAL:O	2.21	0.40
1:F:2683:LYS:HG3	1:F:2716:PHE:CG	2.56	0.40
1:F:2612:LEU:HD21	1:F:2618:VAL:HG21	2.04	0.40
1:C:1005:SER:HB3	1:D:1611:ILE:O	2.21	0.40
1:D:1536:LEU:HB3	1:D:1863:SER:H	1.85	0.40
1:C:1298:ARG:HD3	1:C:1368:GLU:OE2	2.21	0.40
1:D:1705:ILE:HG23	1:D:1706:TYR:N	2.36	0.40
1:H:3845:GLY:HA3	1:H:3877:ARG:HH11	1.87	0.40
1:H:3539:GLY:O	1:H:3821:PHE:HZ	2.04	0.40
1:B:842:LEU:HD23	1:B:842:LEU:HA	1.81	0.40
1:A:122:SER:HB3	1:A:124:TYR:CD2	2.57	0.40
1:A:47:GLU:O	1:A:51:GLU:HB2	2.21	0.40
1:D:1810:LEU:HA	1:D:1810:LEU:HD23	1.95	0.40
1:C:1342:LEU:HA	1:C:1342:LEU:HD23	1.84	0.40
1:E:2312:LEU:HD21	1:E:2330:ILE:HD12	2.04	0.40
1:E:2248:GLY:C	1:E:2253:ILE:HD11	2.42	0.40
1:D:1742:ARG:NH2	3:D:1913:PLP:O3P	2.51	0.40
1:A:268:ASP:HA	1:B:742:ARG:HG2	2.04	0.40
1:B:823:VAL:HG23	1:B:864:TYR:CE2	2.55	0.40
1:D:1716:PHE:CE1	1:D:1720:ARG:HD3	2.56	0.40
1:E:2193:ALA:HA	1:E:2198:PHE:CZ	2.56	0.40
1:A:323:VAL:HG23	1:A:364:TYR:CE2	2.55	0.40
1:A:193:ALA:HA	1:A:198:PHE:CZ	2.56	0.40
1:B:848:VAL:HB	1:B:860:VAL:HG22	2.04	0.40
1:C:1207:GLU:HG3	1:C:1208:HIS:N	2.36	0.40
1:D:1552:ALA:HB2	1:D:1777:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:THR:HB	1:A:91:PRO:HD2	2.02	0.40
1:H:3828:SER:HB3	1:H:3829:PRO:HD3	2.04	0.40
1:H:3520:ASN:O	1:H:3523:ALA:HB3	2.21	0.40
1:D:1612:LEU:HD21	1:D:1618:VAL:HG21	2.02	0.40
1:C:1024:LEU:C	1:C:1028:ARG:HB2	2.42	0.40
1:D:1526:LEU:HA	1:D:1526:LEU:HD23	1.89	0.40
1:A:184:GLU:HA	1:A:187:GLU:HB3	2.03	0.40
1:A:40:GLU:H	1:A:40:GLU:HG2	1.73	0.40
1:F:2700:LEU:HD23	1:F:2700:LEU:HA	1.94	0.40
1:C:1180:VAL:O	1:C:1180:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/385 (99%)	332 (87%)	36 (10%)	12 (3%)	6	43
1	B	380/385 (99%)	322 (85%)	42 (11%)	16 (4%)	4	34
1	C	380/385 (99%)	321 (84%)	41 (11%)	18 (5%)	4	30
1	D	380/385 (99%)	322 (85%)	41 (11%)	17 (4%)	4	32
1	E	380/385 (99%)	323 (85%)	42 (11%)	15 (4%)	5	37
1	F	380/385 (99%)	321 (84%)	45 (12%)	14 (4%)	5	39
1	G	380/385 (99%)	325 (86%)	41 (11%)	14 (4%)	5	39
1	H	380/385 (99%)	323 (85%)	43 (11%)	14 (4%)	5	39
All	All	3040/3080 (99%)	2589 (85%)	331 (11%)	120 (4%)	5	37

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	25	GLU

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	205	ILE
1	A	266	SER
1	B	524	LEU
1	B	525	GLU
1	B	526	LEU
1	B	705	ILE
1	B	766	SER
1	C	1024	LEU
1	C	1025	GLU
1	C	1026	LEU
1	C	1029	GLN
1	C	1205	ILE
1	C	1266	SER
1	D	1524	LEU
1	D	1525	GLU
1	D	1526	LEU
1	D	1529	GLN
1	D	1531	VAL
1	D	1705	ILE
1	D	1766	SER
1	E	2025	GLU
1	E	2029	GLN
1	E	2205	ILE
1	E	2266	SER
1	F	2524	LEU
1	F	2525	GLU
1	F	2529	GLN
1	F	2531	VAL
1	F	2705	ILE
1	F	2766	SER
1	G	3024	LEU
1	G	3029	GLN
1	G	3031	VAL
1	G	3205	ILE
1	G	3266	SER
1	H	3525	GLU
1	H	3526	LEU
1	H	3529	GLN
1	H	3622	SER
1	H	3623	PRO
1	H	3705	ILE

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Mol	Chain	Res	Type
1	A	126	VAL
1	B	626	VAL
1	B	674	ASN
1	B	782	GLN
1	C	1031	VAL
1	C	1126	VAL
1	C	1283	GLU
1	C	1357	PHE
1	D	1626	VAL
1	E	2024	LEU
1	E	2126	VAL
1	F	2626	VAL
1	G	3126	VAL
1	H	3626	VAL
1	H	3783	GLU
1	A	38	ALA
1	A	112	LEU
1	A	233	ALA
1	B	529	GLN
1	B	612	LEU
1	B	783	GLU
1	B	793	ARG
1	C	1038	ALA
1	C	1112	LEU
1	D	1612	LEU
1	D	1790	GLU
1	E	2038	ALA
1	E	2112	LEU
1	E	2254	LYS
1	F	2612	LEU
1	F	2659	ARG
1	F	2783	GLU
1	G	3112	LEU
1	H	3612	LEU
1	A	13	PRO
1	B	733	ALA
1	C	1197	ASP
1	C	1233	ALA
1	C	1282	GLN
1	D	1522	LYS
1	D	1754	LYS
1	E	2026	LEU

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Mol	Chain	Res	Type
1	E	2159	ARG
1	E	2233	ALA
1	H	3733	ALA
1	H	3766	SER
1	C	1106	ASN
1	D	1583	ARG
1	D	1733	ALA
1	F	2733	ALA
1	F	2832	PRO
1	G	3197	ASP
1	G	3233	ALA
1	H	3782	GLN
1	A	111	ILE
1	A	253	ILE
1	B	611	ILE
1	C	1111	ILE
1	D	1611	ILE
1	E	2111	ILE
1	F	2611	ILE
1	G	3038	ALA
1	G	3111	ILE
1	G	3265	THR
1	G	3364	TYR
1	H	3611	ILE
1	C	1331	ALA
1	G	3091	PRO
1	B	513	PRO
1	E	2253	ILE
1	F	2753	ILE
1	B	531	VAL
1	D	1753	ILE
1	D	1832	PRO
1	H	3753	ILE
1	E	2031	VAL

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	305/306 (100%)	265 (87%)	40 (13%)	6	28
1	B	305/306 (100%)	263 (86%)	42 (14%)	5	25
1	C	305/306 (100%)	252 (83%)	53 (17%)	3	14
1	D	305/306 (100%)	259 (85%)	46 (15%)	4	21
1	E	305/306 (100%)	246 (81%)	59 (19%)	2	10
1	F	305/306 (100%)	250 (82%)	55 (18%)	2	13
1	G	305/306 (100%)	256 (84%)	49 (16%)	3	17
1	H	305/306 (100%)	269 (88%)	36 (12%)	8	34
All	All	2440/2448 (100%)	2060 (84%)	380 (16%)	4	19

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	VAL
1	A	19	VAL
1	A	24	LEU
1	A	25	GLU
1	A	28	ARG
1	A	32	ASP
1	A	33	LEU
1	A	45	THR
1	A	62	THR
1	A	73	LEU
1	A	77	LEU
1	A	94	THR
1	A	107	LEU
1	A	112	LEU
1	A	113	ASP
1	A	156	ARG
1	A	177	THR
1	A	184	GLU
1	A	200	LEU
1	A	212	GLU
1	A	214	GLU
1	A	226	THR
1	A	227	LEU
1	A	228	THR
1	A	245	TYR
1	A	265	THR

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Mol	Chain	Res	Type
1	A	268	ASP
1	A	276	LEU
1	A	282	GLN
1	A	302	LEU
1	A	303	LEU
1	A	315	VAL
1	A	321	PHE
1	A	342	LEU
1	A	360	VAL
1	A	367	SER
1	A	372	ARG
1	A	375	LEU
1	A	381	VAL
1	B	501	MET
1	B	508	VAL
1	B	512	LYS
1	B	524	LEU
1	B	532	ASP
1	B	533	LEU
1	B	545	THR
1	B	549	VAL
1	B	562	THR
1	B	563	LYS
1	B	573	LEU
1	B	577	LEU
1	B	583	ARG
1	B	594	THR
1	B	602	GLN
1	B	612	LEU
1	B	656	ARG
1	B	670	VAL
1	B	671	ASN
1	B	676	PRO
1	B	677	THR
1	B	684	GLU
1	B	700	LEU
1	B	712	GLU
1	B	727	LEU
1	B	728	THR
1	B	745	TYR
1	B	752	VAL
1	B	765	THR

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Mol	Chain	Res	Type
1	B	776	LEU
1	B	782	GLN
1	B	802	LEU
1	B	803	LEU
1	B	808	THR
1	B	812	LEU
1	B	815	VAL
1	B	821	PHE
1	B	828	SER
1	B	840	ARG
1	B	842	LEU
1	B	869	GLU
1	B	875	LEU
1	C	1001	MET
1	C	1008	VAL
1	C	1012	LYS
1	C	1014	ASP
1	C	1028	ARG
1	C	1032	ASP
1	C	1033	LEU
1	C	1045	THR
1	C	1059	GLN
1	C	1062	THR
1	C	1063	LYS
1	C	1073	LEU
1	C	1077	LEU
1	C	1094	THR
1	C	1096	VAL
1	C	1102	GLN
1	C	1112	LEU
1	C	1147	GLU
1	C	1156	ARG
1	C	1164	ARG
1	C	1169	VAL
1	C	1177	THR
1	C	1184	GLU
1	C	1186	LEU
1	C	1200	LEU
1	C	1214	GLU
1	C	1227	LEU
1	C	1228	THR
1	C	1234	LYS

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Mol	Chain	Res	Type
1	C	1243	ILE
1	C	1245	TYR
1	C	1254	LYS
1	C	1261	ARG
1	C	1265	THR
1	C	1268	ASP
1	C	1276	LEU
1	C	1282	GLN
1	C	1298	ARG
1	C	1302	LEU
1	C	1303	LEU
1	C	1316	ARG
1	C	1321	PHE
1	C	1330	ILE
1	C	1333	ASP
1	C	1342	LEU
1	C	1343	GLU
1	C	1360	VAL
1	C	1367	SER
1	C	1368	GLU
1	C	1369	GLU
1	C	1371	LEU
1	C	1375	LEU
1	C	1381	VAL
1	D	1501	MET
1	D	1506	ARG
1	D	1508	VAL
1	D	1512	LYS
1	D	1519	VAL
1	D	1522	LYS
1	D	1524	LEU
1	D	1525	GLU
1	D	1528	ARG
1	D	1532	ASP
1	D	1533	LEU
1	D	1536	LEU
1	D	1545	THR
1	D	1555	ARG
1	D	1562	THR
1	D	1563	LYS
1	D	1573	LEU
1	D	1577	LEU

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Mol	Chain	Res	Type
1	D	1594	THR
1	D	1596	VAL
1	D	1607	LEU
1	D	1612	LEU
1	D	1613	ASP
1	D	1645	LEU
1	D	1647	GLU
1	D	1656	ARG
1	D	1664	ARG
1	D	1677	THR
1	D	1687	GLU
1	D	1700	LEU
1	D	1727	LEU
1	D	1728	THR
1	D	1745	TYR
1	D	1751	GLU
1	D	1782	GLN
1	D	1794	GLU
1	D	1803	LEU
1	D	1815	VAL
1	D	1833	ASP
1	D	1836	ARG
1	D	1839	GLU
1	D	1866	THR
1	D	1868	GLU
1	D	1869	GLU
1	D	1875	LEU
1	D	1881	VAL
1	E	2006	ARG
1	E	2008	VAL
1	E	2012	LYS
1	E	2016	VAL
1	E	2019	VAL
1	E	2026	LEU
1	E	2027	ARG
1	E	2029	GLN
1	E	2031	VAL
1	E	2033	LEU
1	E	2037	THR
1	E	2045	THR
1	E	2049	VAL
1	E	2059	GLN

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Mol	Chain	Res	Type
1	E	2062	THR
1	E	2063	LYS
1	E	2073	LEU
1	E	2075	GLU
1	E	2077	LEU
1	E	2082	ARG
1	E	2094	THR
1	E	2102	GLN
1	E	2107	LEU
1	E	2112	LEU
1	E	2113	ASP
1	E	2127	SER
1	E	2145	LEU
1	E	2147	GLU
1	E	2164	ARG
1	E	2172	SER
1	E	2177	THR
1	E	2184	GLU
1	E	2200	LEU
1	E	2212	GLU
1	E	2214	GLU
1	E	2220	ARG
1	E	2226	THR
1	E	2227	LEU
1	E	2228	THR
1	E	2243	ILE
1	E	2245	TYR
1	E	2252	VAL
1	E	2262	GLN
1	E	2265	THR
1	E	2266	SER
1	E	2276	LEU
1	E	2282	GLN
1	E	2291	MET
1	E	2293	ARG
1	E	2303	LEU
1	E	2308	THR
1	E	2313	LYS
1	E	2321	PHE
1	E	2330	ILE
1	E	2342	LEU
1	E	2343	GLU

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Mol	Chain	Res	Type
1	E	2367	SER
1	E	2375	LEU
1	E	2381	VAL
1	F	2508	VAL
1	F	2512	LYS
1	F	2517	VAL
1	F	2519	VAL
1	F	2522	LYS
1	F	2524	LEU
1	F	2526	LEU
1	F	2532	ASP
1	F	2533	LEU
1	F	2545	THR
1	F	2562	THR
1	F	2573	LEU
1	F	2575	GLU
1	F	2577	LEU
1	F	2582	ARG
1	F	2587	LEU
1	F	2588	SER
1	F	2592	GLU
1	F	2594	THR
1	F	2596	VAL
1	F	2612	LEU
1	F	2613	ASP
1	F	2645	LEU
1	F	2647	GLU
1	F	2655	GLU
1	F	2664	ARG
1	F	2677	THR
1	F	2684	GLU
1	F	2686	LEU
1	F	2700	LEU
1	F	2712	GLU
1	F	2714	GLU
1	F	2720	ARG
1	F	2726	THR
1	F	2727	LEU
1	F	2728	THR
1	F	2743	ILE
1	F	2745	TYR
1	F	2751	GLU

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Mol	Chain	Res	Type
1	F	2752	VAL
1	F	2761	ARG
1	F	2765	THR
1	F	2768	ASP
1	F	2782	GLN
1	F	2783	GLU
1	F	2803	LEU
1	F	2808	THR
1	F	2812	LEU
1	F	2815	VAL
1	F	2830	ILE
1	F	2842	LEU
1	F	2860	VAL
1	F	2867	SER
1	F	2872	ARG
1	F	2881	VAL
1	G	3006	ARG
1	G	3008	VAL
1	G	3012	LYS
1	G	3014	ASP
1	G	3016	VAL
1	G	3019	VAL
1	G	3022	LYS
1	G	3027	ARG
1	G	3028	ARG
1	G	3032	ASP
1	G	3033	LEU
1	G	3045	THR
1	G	3062	THR
1	G	3067	PRO
1	G	3073	LEU
1	G	3094	THR
1	G	3096	VAL
1	G	3102	GLN
1	G	3112	LEU
1	G	3113	ASP
1	G	3114	PRO
1	G	3121	LEU
1	G	3156	ARG
1	G	3174	ASN
1	G	3176	PRO
1	G	3184	GLU

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Mol	Chain	Res	Type
1	G	3187	GLU
1	G	3200	LEU
1	G	3205	ILE
1	G	3214	GLU
1	G	3226	THR
1	G	3227	LEU
1	G	3228	THR
1	G	3243	ILE
1	G	3245	TYR
1	G	3252	VAL
1	G	3265	THR
1	G	3266	SER
1	G	3276	LEU
1	G	3277	GLU
1	G	3286	ARG
1	G	3298	ARG
1	G	3302	LEU
1	G	3303	LEU
1	G	3321	PHE
1	G	3330	ILE
1	G	3339	GLU
1	G	3342	LEU
1	G	3368	GLU
1	H	3508	VAL
1	H	3512	LYS
1	H	3517	VAL
1	H	3525	GLU
1	H	3531	VAL
1	H	3532	ASP
1	H	3533	LEU
1	H	3545	THR
1	H	3562	THR
1	H	3573	LEU
1	H	3594	THR
1	H	3602	GLN
1	H	3612	LEU
1	H	3613	ASP
1	H	3655	GLU
1	H	3656	ARG
1	H	3659	ARG
1	H	3664	ARG
1	H	3674	ASN

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Mol	Chain	Res	Type
1	H	3676	PRO
1	H	3677	THR
1	H	3684	GLU
1	H	3700	LEU
1	H	3714	GLU
1	H	3726	THR
1	H	3727	LEU
1	H	3728	THR
1	H	3743	ILE
1	H	3745	TYR
1	H	3765	THR
1	H	3800	ARG
1	H	3802	LEU
1	H	3842	LEU
1	H	3860	VAL
1	H	3875	LEU
1	H	3881	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	370	ASN
1	B	509	GLN
1	B	529	GLN
1	B	559	GLN
1	B	671	ASN
1	B	675	ASN
1	B	870	ASN
1	C	1171	ASN
1	D	1671	ASN
1	E	2106	ASN
1	E	2171	ASN
1	E	2175	ASN
1	F	2671	ASN
1	F	2870	ASN
1	G	3009	GLN
1	G	3171	ASN
1	G	3174	ASN
1	G	3196	HIS
1	H	3671	ASN
1	H	3674	ASN

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Mol	Chain	Res	Type
1	H	3782	GLN
1	H	3870	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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
3	PLP	A	413	2	14,15,16	2.02	3 (21%)	20,22,23	1.53	5 (25%)
2	TRP	A	414	3	16,16,16	1.07	1 (6%)	22,22,22	2.17	1 (4%)
2	TRP	A	914	3	16,16,16	1.37	2 (12%)	22,22,22	5.54	6 (27%)
3	PLP	B	913	2	14,15,16	3.03	5 (35%)	20,22,23	2.29	6 (30%)
3	PLP	C	1413	2	14,15,16	2.22	5 (35%)	20,22,23	2.76	9 (45%)
2	TRP	C	1414	3	16,16,16	1.52	3 (18%)	22,22,22	5.14	4 (18%)
3	PLP	D	1913	2	14,15,16	2.97	6 (42%)	20,22,23	2.53	6 (30%)
2	TRP	D	1914	3	16,16,16	2.17	3 (18%)	22,22,22	4.19	3 (13%)
3	PLP	E	2413	2	14,15,16	1.64	4 (28%)	20,22,23	1.83	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRP	E	2414	3	16,16,16	1.69	2 (12%)	22,22,22	2.33	5 (22%)
2	TRP	E	2914	3	16,16,16	3.53	5 (31%)	22,22,22	3.43	2 (9%)
3	PLP	F	2913	2	14,15,16	3.13	4 (28%)	20,22,23	1.76	5 (25%)
3	PLP	G	3413	2	14,15,16	2.59	5 (35%)	20,22,23	2.24	9 (45%)
2	TRP	G	3414	3	16,16,16	1.38	2 (12%)	22,22,22	4.28	5 (22%)
3	PLP	H	3913	2	14,15,16	2.85	7 (50%)	20,22,23	1.61	3 (15%)
2	TRP	H	3914	3	16,16,16	2.47	2 (12%)	22,22,22	5.09	4 (18%)

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
3	PLP	A	413	2	-	0/6/6/8	0/1/1/1
2	TRP	A	414	3	-	0/8/8/8	0/0/2/2
2	TRP	A	914	3	-	0/8/8/8	0/0/2/2
3	PLP	B	913	2	-	0/6/6/8	0/1/1/1
3	PLP	C	1413	2	-	0/6/6/8	0/1/1/1
2	TRP	C	1414	3	-	0/8/8/8	0/0/2/2
3	PLP	D	1913	2	-	0/6/6/8	0/1/1/1
2	TRP	D	1914	3	-	0/8/8/8	0/0/2/2
3	PLP	E	2413	2	-	0/6/6/8	0/1/1/1
2	TRP	E	2414	3	-	0/8/8/8	0/0/2/2
2	TRP	E	2914	3	-	0/8/8/8	0/0/2/2
3	PLP	F	2913	2	-	0/6/6/8	0/1/1/1
3	PLP	G	3413	2	-	0/6/6/8	0/1/1/1
2	TRP	G	3414	3	-	0/8/8/8	0/0/2/2
3	PLP	H	3913	2	-	0/6/6/8	0/1/1/1
2	TRP	H	3914	3	-	0/8/8/8	0/0/2/2

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	913	PLP	C4-C5	9.76	1.56	1.39
2	H	3914	TRP	CB-CG	9.17	1.64	1.51
2	E	2914	TRP	CB-CG	-9.00	1.38	1.51
3	D	1913	PLP	C4-C5	7.40	1.52	1.39
3	H	3913	PLP	C4-C5	7.33	1.52	1.39
2	E	2914	TRP	CD1-CG	-7.33	1.26	1.37
3	F	2913	PLP	C3-C2	-7.26	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1914	TRP	CB-CG	7.23	1.62	1.51
3	G	3413	PLP	C4-C5	7.07	1.51	1.39
3	F	2913	PLP	C4-C5	6.33	1.50	1.39
3	D	1913	PLP	C3-C2	6.19	1.45	1.40
2	E	2414	TRP	CB-CG	-5.75	1.43	1.51
3	C	1413	PLP	C3-C2	5.74	1.44	1.40
3	A	413	PLP	C3-C2	5.73	1.44	1.40
2	E	2914	TRP	CH2-CZ2	5.05	1.48	1.36
3	H	3913	PLP	C3-C2	5.04	1.44	1.40
2	E	2914	TRP	CZ2-CE2	4.82	1.51	1.40
3	F	2913	PLP	C4-C3	-4.81	1.27	1.40
2	A	914	TRP	O-C	3.85	1.35	1.22
2	G	3414	TRP	CB-CG	3.65	1.56	1.51
2	C	1414	TRP	O-C	3.45	1.34	1.22
3	C	1413	PLP	C5A-C5	3.31	1.60	1.51
3	G	3413	PLP	C3-C2	3.14	1.43	1.40
3	E	2413	PLP	P-O2P	2.98	1.65	1.54
2	A	414	TRP	CB-CG	2.96	1.55	1.51
3	D	1913	PLP	C6-C5	2.88	1.44	1.37
2	D	1914	TRP	CA-C	-2.81	1.42	1.53
3	G	3413	PLP	O3-C3	-2.78	1.30	1.37
3	A	413	PLP	C4-C5	2.77	1.44	1.39
2	C	1414	TRP	CA-C	2.74	1.63	1.53
3	E	2413	PLP	C3-C2	2.74	1.42	1.40
3	G	3413	PLP	C5A-C5	2.73	1.58	1.51
3	F	2913	PLP	C5A-C5	-2.72	1.43	1.51
2	A	914	TRP	CD1-CG	2.72	1.42	1.37
3	B	913	PLP	C2A-C2	2.70	1.55	1.50
2	E	2914	TRP	CD1-NE1	2.65	1.42	1.37
2	G	3414	TRP	CZ3-CE3	2.62	1.42	1.36
3	H	3913	PLP	C2-N1	2.60	1.38	1.33
3	C	1413	PLP	C2-N1	2.49	1.38	1.33
3	B	913	PLP	P-O3P	-2.44	1.45	1.54
3	H	3913	PLP	P-O3P	-2.43	1.45	1.54
3	E	2413	PLP	O3-C3	2.40	1.42	1.37
3	A	413	PLP	P-O3P	-2.38	1.46	1.54
2	H	3914	TRP	CA-C	2.34	1.61	1.53
3	B	913	PLP	C6-C5	2.33	1.43	1.37
2	C	1414	TRP	CB-CG	-2.33	1.48	1.51
3	H	3913	PLP	C6-C5	2.33	1.43	1.37
3	D	1913	PLP	C2A-C2	2.31	1.55	1.50
3	D	1913	PLP	P-O2P	2.27	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1413	PLP	O3-C3	-2.27	1.31	1.37
2	E	2414	TRP	OXT-C	-2.26	1.22	1.30
3	H	3913	PLP	C2A-C2	2.22	1.54	1.50
2	D	1914	TRP	O-C	2.19	1.29	1.22
3	G	3413	PLP	C6-C5	2.19	1.42	1.37
3	D	1913	PLP	P-O3P	-2.15	1.46	1.54
3	B	913	PLP	O3-C3	2.10	1.42	1.37
3	C	1413	PLP	P-O3P	-2.10	1.47	1.54
3	H	3913	PLP	C4-C3	-2.08	1.34	1.40
3	E	2413	PLP	C6-C5	-2.01	1.32	1.37

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	914	TRP	C-CA-N	24.38	149.72	109.36
2	H	3914	TRP	C-CA-N	23.10	147.61	109.36
2	C	1414	TRP	C-CA-N	22.34	146.35	109.36
2	D	1914	TRP	C-CA-N	18.89	140.64	109.36
2	G	3414	TRP	C-CA-N	18.38	139.78	109.36
2	E	2914	TRP	C-CA-N	15.32	134.73	109.36
2	A	414	TRP	C-CA-N	9.55	125.17	109.36
2	C	1414	TRP	CG-CB-CA	7.14	130.09	113.87
3	D	1913	PLP	C3-C4-C5	-7.12	107.81	121.29
2	E	2414	TRP	C-CA-N	6.82	120.66	109.36
2	E	2414	TRP	CG-CB-CA	6.62	128.89	113.87
3	D	1913	PLP	C4-C3-C2	6.05	126.61	119.67
3	B	913	PLP	C3-C4-C5	-5.51	110.86	121.29
3	C	1413	PLP	C6-C5-C4	5.48	130.91	118.18
2	G	3414	TRP	CG-CB-CA	5.47	126.29	113.87
3	C	1413	PLP	C5A-C5-C6	-5.23	109.37	119.28
3	B	913	PLP	C4-C3-C2	5.22	125.66	119.67
3	C	1413	PLP	C3-C4-C5	-4.90	112.02	121.29
2	A	914	TRP	CG-CB-CA	-4.78	103.02	113.87
2	A	914	TRP	CB-CA-C	-4.71	96.86	111.20
3	F	2913	PLP	C4-C3-C2	4.65	125.01	119.67
3	G	3413	PLP	C3-C4-C5	-4.58	112.62	121.29
3	C	1413	PLP	C5-C6-N1	-4.01	116.62	123.86
2	G	3414	TRP	CB-CA-N	-3.77	94.46	111.60
3	F	2913	PLP	O3P-P-O1P	3.68	122.48	110.44
2	A	914	TRP	OXT-C-O	-3.61	115.90	124.07
3	H	3913	PLP	C3-C4-C5	-3.47	114.72	121.29
3	H	3913	PLP	C4-C3-C2	3.42	123.60	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3413	PLP	C5A-C5-C6	-3.40	112.85	119.28
3	E	2413	PLP	O3-C3-C2	3.38	123.61	117.61
3	C	1413	PLP	C4-C3-C2	-3.36	115.82	119.67
2	H	3914	TRP	CB-CA-C	-3.36	100.98	111.20
3	G	3413	PLP	O2P-P-O4P	-3.33	97.45	106.65
3	C	1413	PLP	O3-C3-C2	3.33	123.52	117.61
3	C	1413	PLP	C3-C2-N1	3.28	125.17	120.66
3	G	3413	PLP	O3P-P-O1P	3.20	120.92	110.44
3	A	413	PLP	C3-C4-C5	-3.14	115.35	121.29
3	E	2413	PLP	C2A-C2-C3	3.02	124.69	121.02
2	E	2414	TRP	CB-CA-N	-3.02	97.86	111.60
3	C	1413	PLP	O3P-P-O1P	3.01	120.28	110.44
3	G	3413	PLP	C5-C6-N1	-3.00	118.44	123.86
3	E	2413	PLP	O3P-P-O1P	2.95	120.08	110.44
3	H	3913	PLP	O3P-P-O1P	2.91	119.95	110.44
3	G	3413	PLP	O3-C3-C2	2.90	122.76	117.61
3	B	913	PLP	O3P-P-O1P	2.90	119.91	110.44
3	B	913	PLP	O4P-C5A-C5	2.82	114.99	109.26
3	B	913	PLP	C5A-C5-C6	-2.77	114.04	119.28
3	D	1913	PLP	O3-C3-C4	-2.75	111.16	120.61
3	E	2413	PLP	C4-C3-C2	-2.74	116.53	119.67
2	E	2914	TRP	OXT-C-O	-2.73	117.90	124.07
3	D	1913	PLP	C6-C5-C4	2.66	124.35	118.18
2	C	1414	TRP	OXT-C-O	-2.58	118.23	124.07
3	B	913	PLP	O3-C3-C4	-2.51	111.97	120.61
2	E	2414	TRP	CB-CG-CD2	-2.47	121.43	126.56
3	A	413	PLP	O3P-P-O1P	2.45	118.45	110.44
2	D	1914	TRP	OXT-C-O	-2.38	118.68	124.07
3	F	2913	PLP	O3-C3-C4	-2.35	112.53	120.61
2	A	914	TRP	CZ3-CE3-CD2	-2.35	117.46	120.88
2	G	3414	TRP	OXT-C-O	-2.35	118.77	124.07
3	A	413	PLP	C2A-C2-C3	2.34	123.86	121.02
3	G	3413	PLP	C6-C5-C4	2.31	123.55	118.18
2	H	3914	TRP	O-C-CA	-2.26	111.85	118.36
3	E	2413	PLP	P-O4P-C5A	2.25	129.34	121.22
3	E	2413	PLP	O4P-C5A-C5	-2.21	104.76	109.26
3	E	2413	PLP	C5-C6-N1	-2.19	119.91	123.86
3	G	3413	PLP	C3-C2-N1	2.16	123.63	120.66
3	D	1913	PLP	C5A-C5-C6	-2.16	115.19	119.28
2	C	1414	TRP	CB-CA-N	-2.16	101.80	111.60
2	G	3414	TRP	CB-CA-C	-2.15	104.66	111.20
3	F	2913	PLP	C3-C4-C5	-2.15	117.23	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1413	PLP	C2A-C2-C3	-2.14	118.42	121.02
2	D	1914	TRP	CB-CA-C	-2.11	104.78	111.20
3	D	1913	PLP	O3-C3-C2	2.07	121.29	117.61
3	A	413	PLP	O3-C3-C2	2.06	121.27	117.61
3	F	2913	PLP	C5-C6-N1	-2.06	120.15	123.86
3	A	413	PLP	C6-C5-C4	2.04	122.92	118.18
2	H	3914	TRP	OXT-C-CA	2.03	121.45	116.88
2	E	2414	TRP	CB-CG-CD1	2.03	131.59	128.12
3	G	3413	PLP	C4-C3-C2	2.03	122.00	119.67
2	A	914	TRP	OXT-C-CA	2.02	121.42	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	382/385 (99%)	-0.31	1 (0%) 91 63	3, 17, 38, 57	0
1	B	382/385 (99%)	-0.30	1 (0%) 91 63	3, 18, 40, 66	0
1	C	382/385 (99%)	-0.31	0 100 100	2, 17, 38, 50	0
1	D	382/385 (99%)	-0.33	0 100 100	2, 16, 33, 50	0
1	E	382/385 (99%)	-0.36	0 100 100	2, 16, 37, 53	0
1	F	382/385 (99%)	-0.36	0 100 100	2, 15, 33, 56	0
1	G	382/385 (99%)	-0.37	0 100 100	3, 15, 34, 54	0
1	H	382/385 (99%)	-0.32	0 100 100	3, 17, 37, 60	0
All	All	3056/3080 (99%)	-0.33	2 (0%) 93 77	2, 17, 37, 66	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	ARG	2.1
1	B	525	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TRP	D	1914	15/15	0.50	11.58	32,43,59,61	0
2	TRP	G	3414	15/15	0.69	9.35	32,53,59,59	0
2	TRP	C	1414	15/15	0.73	9.20	41,64,68,70	0
2	TRP	E	2414	15/15	0.47	6.83	21,50,56,57	0
2	TRP	E	2914	15/15	0.56	6.70	29,61,76,77	0
2	TRP	A	914	15/15	0.48	6.32	26,59,74,75	0
2	TRP	A	414	15/15	0.53	5.49	35,41,47,49	0
2	TRP	H	3914	15/15	0.37	4.93	23,43,48,49	0
3	PLP	A	413	15/16	0.19	0.98	8,24,34,40	0
3	PLP	C	1413	15/16	0.19	0.90	8,18,24,34	0
3	PLP	E	2413	15/16	0.16	0.62	2,7,23,33	0
3	PLP	H	3913	15/16	0.17	0.13	7,17,27,30	0
3	PLP	D	1913	15/16	0.14	-0.44	2,14,19,26	0
3	PLP	B	913	15/16	0.15	-0.48	2,7,13,20	0
3	PLP	G	3413	15/16	0.14	-0.78	2,5,17,27	0
3	PLP	F	2913	15/16	0.13	-1.05	2,5,16,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.