



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:37 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

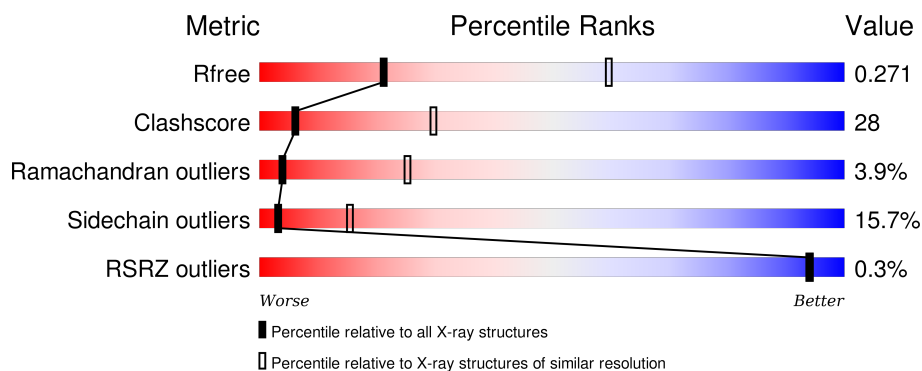
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	<div> <div>53%</div> <div>34%</div> <div>11%</div> <div>..</div> </div>
1	B	385	<div> <div>49%</div> <div>38%</div> <div>10%</div> <div>..</div> </div>
1	C	385	<div> <div>50%</div> <div>35%</div> <div>12%</div> <div>..</div> </div>
1	D	385	<div> <div>51%</div> <div>37%</div> <div>9%</div> <div>..</div> </div>
1	E	385	<div> <div>49%</div> <div>37%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	385	
1	G	385	
1	H	385	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRP	A	414	-	-	-	X
2	TRP	A	914	-	-	X	X
2	TRP	C	1414	-	-	X	X
2	TRP	D	1914	-	-	X	X
2	TRP	E	2414	-	-	-	X
2	TRP	E	2914	-	-	X	X
2	TRP	G	3414	-	-	X	X
2	TRP	H	3914	-	-	-	X
3	PLP	C	1413	-	X	-	-

## 2 Entry composition

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

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

- Molecule 1 is a protein called 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:

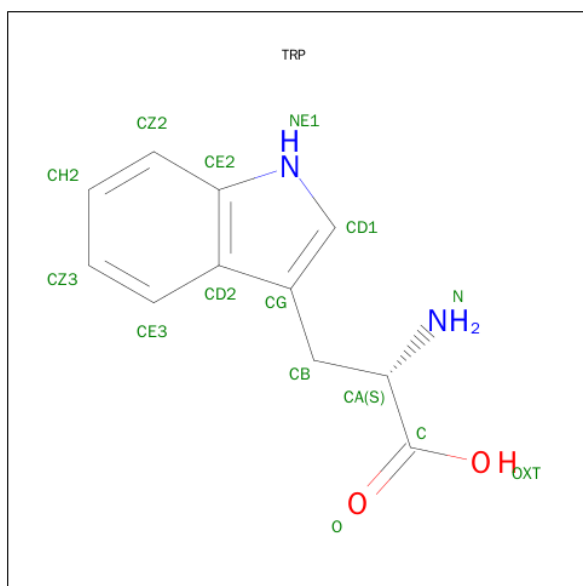
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	SER	ENGINEERED	UNP Q56232
A	16	VAL	THR	ENGINEERED	UNP Q56232
A	101	SER	LYS	ENGINEERED	UNP Q56232
A	261	ARG	SER	ENGINEERED	UNP Q56232
B	514	ASP	SER	ENGINEERED	UNP Q56232
B	516	VAL	THR	ENGINEERED	UNP Q56232
B	601	SER	LYS	ENGINEERED	UNP Q56232
B	761	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:  $C_{11}H_{12}N_2O_2$ ).



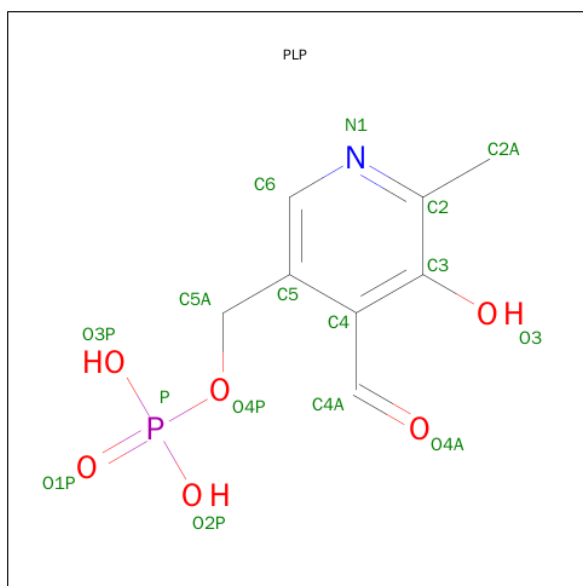
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	A	1	Total	C	N	O	0	0
			15	11	2	2		

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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: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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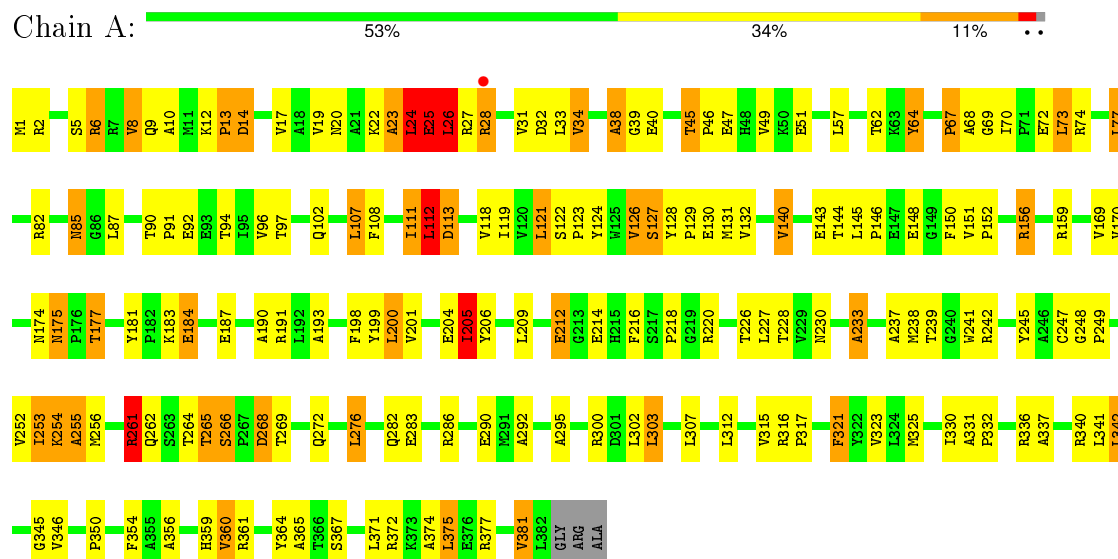
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

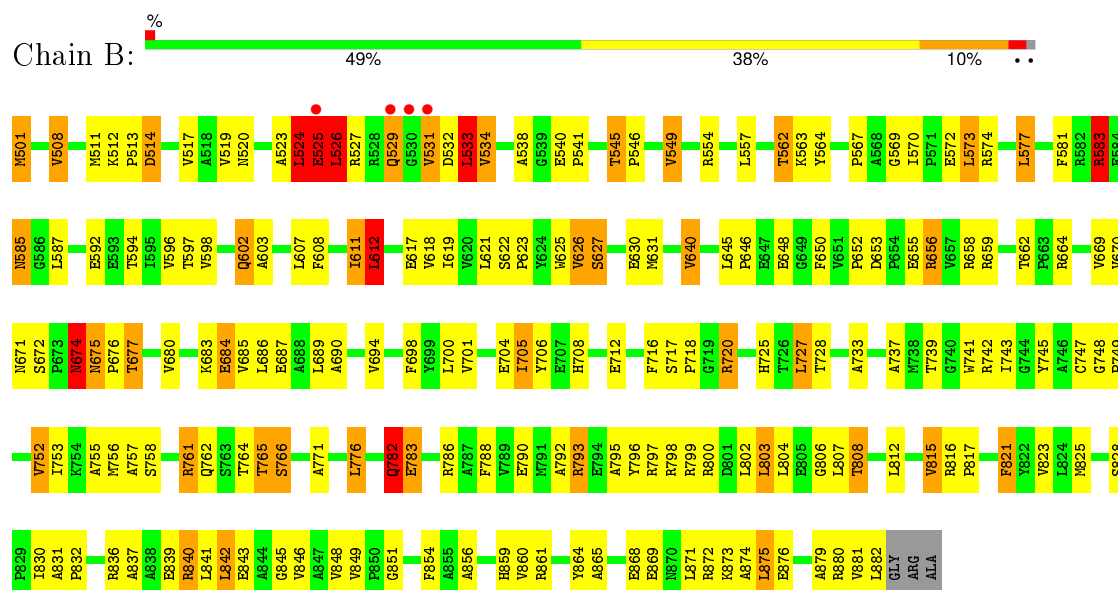
### 3 Residue-property plots

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

#### • Molecule 1: ASPARTATE AMINOTRANSFERASE



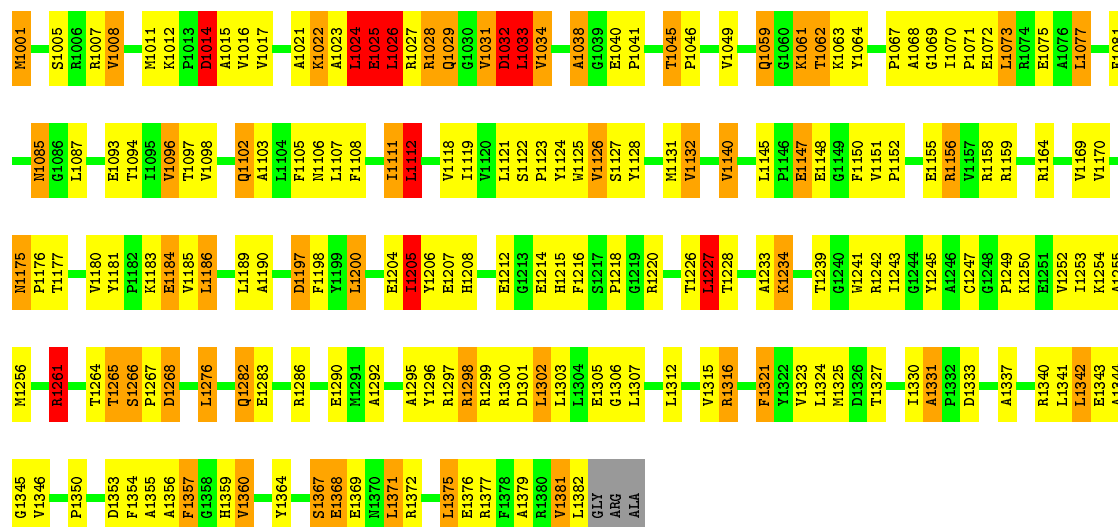
#### • Molecule 1: ASPARTATE AMINOTRANSFERASE



#### • Molecule 1: ASPARTATE AMINOTRANSFERASE

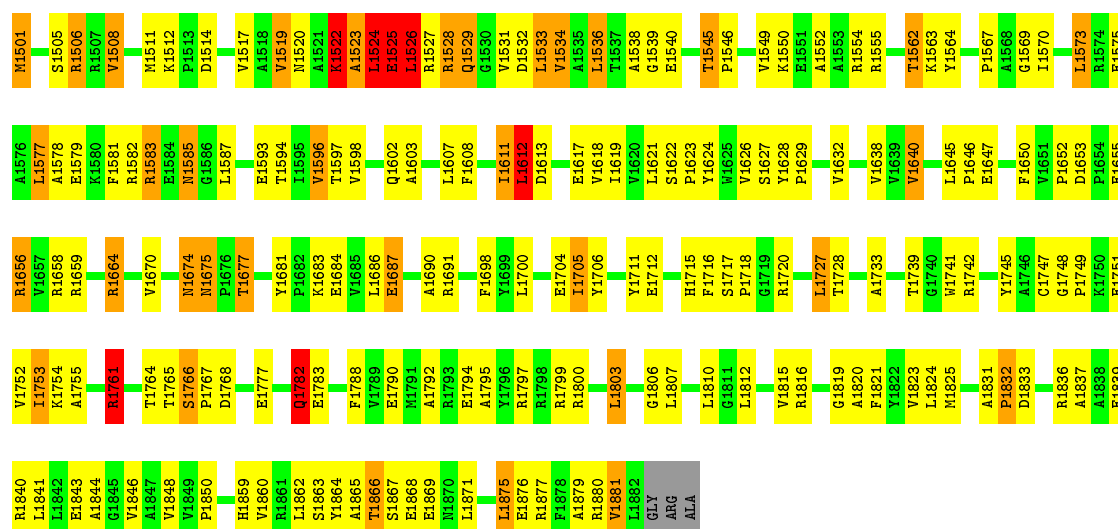


Chain C:



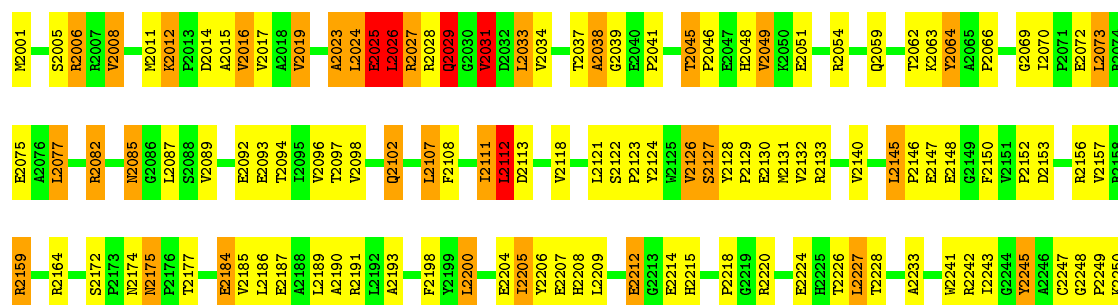
- Molecule 1: ASPARTATE AMINOTRANSFERASE

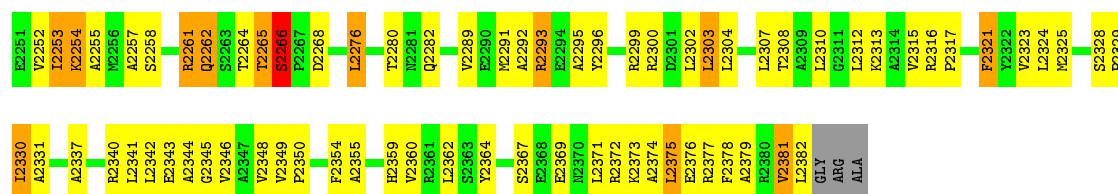
Chain D:



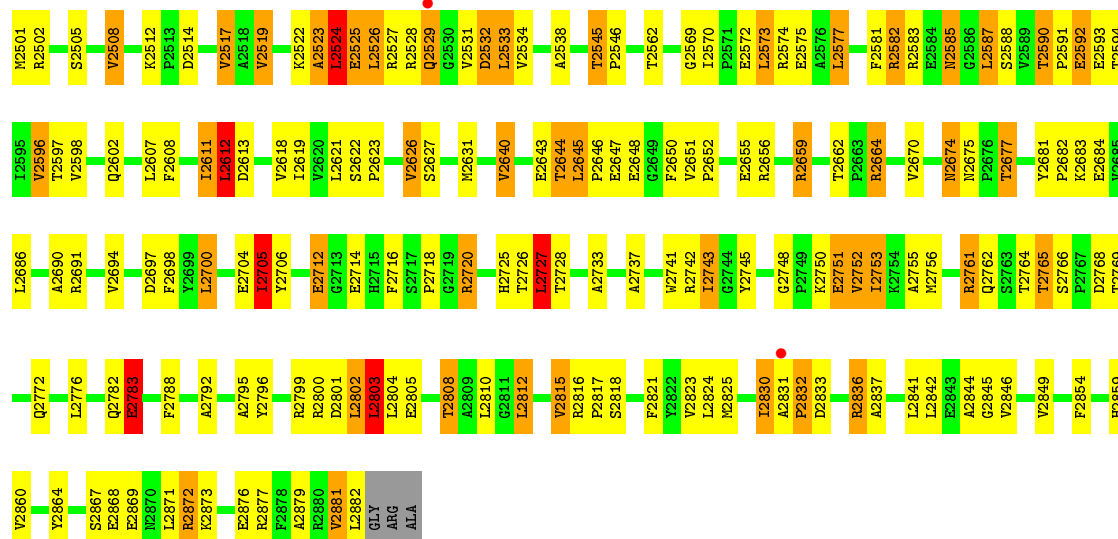
- Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain E:

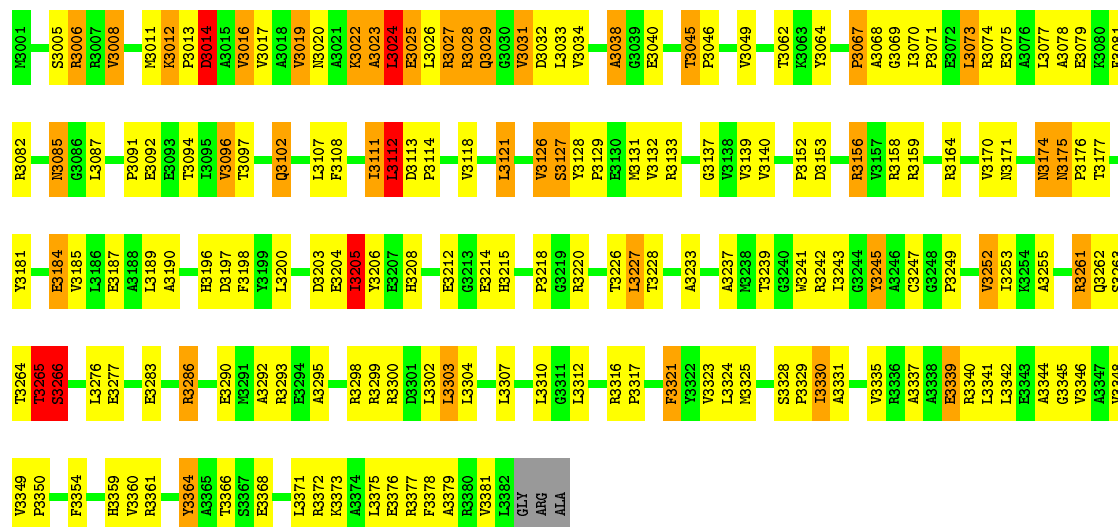




• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



GLY	A3838	C3747	R3656	L3873	M3601
	E3839	G3748	V3657	R3574	
	R3840	P3749	R3658		S3505
	L3841	K3750	R3659	L3577	R3506
	R3842	E3751			R3507
	E3843	V3752	R3664	F3581	V3508
	A3844	I3753		R3582	
	V3846	K3754	V3670	R3583	M3511
		A3755		E3584	P3513
				R3585	P3514
F3854	A3761	R3762	N3674	G3566	A3516
	S3763	I3764	P3675	L3587	V3517
	R3765	T3766	G3678	E3592	
	R3861	T3767	F3681	E3593	M3520
	L3862	P3767	P3682	T3594	A3521
	S3863	D3768	K3683	T3595	K3522
	V3864		E3684	V3596	A3523
	A3865	L3776	V3685	T3597	L3524
			L3686	V3598	E3525
	E3868	Q3782	E3687	Q3602	R3526
L3871	E3783		A3688	A3603	R3527
	R3872		L3689		R3528
	K3873	R3786	A3890	F3608	Q3529
	A3874		R3691		G3530
	L3875	E3790	L3692	I3611	V3531
	R3876	K3791	A3693	L3612	D3532
	R3877	A3792		D3613	L3533
			F3698		V3534
	F3878		V3699	E3617	A3535
	A3879	A3795	L3700	V3618	L3536
ALA	R3880	Y3796		I3619	T3537
	V3881			V3620	A3538
		R3799	E3704	L3621	G3539
	L3882	R3800	I3705	S3622	
		D3801	T3706	S3623	T3545
	L3802	L3802	E3707	P3622	P3546
	L3803	L3803	H3708	Y3624	
	L3804	L3804	L3709	A3625	V3549
				V3626	F3550
		L3807	E3714	S3627	R3551
ARG		L3812	H3715	Y3628	
			F3716	P3629	
		P3817	P3717	E3630	R3554
			P3718	M3631	R3555
			G3719	V3632	A3556
					L3557
				V3640	A3558
					Q3559
				E3643	T3562
				L3645	K3563
GLY			L3646	Y3564	
			A3733	E3647	
				E3648	P3567
			H3741	G3649	A3568
			R3742	F3650	G3569
			I3743		I3570
			K3744		
			Y3745	P3654	P3571
				P3655	P3572

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.50 Å 98.40 Å 187.00 Å 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) 94.8 (47.58-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.33 Å)	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 <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 70.3	EDS
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
3	D	15	0	6	2	0
3	E	15	0	7	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:SER:HA	1:B:761:ARG:HH11	1.46	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	5	31
1	B	380/385 (99%)	322 (85%)	42 (11%)	16 (4%)	3	23
1	C	380/385 (99%)	321 (84%)	41 (11%)	18 (5%)	3	20
1	D	380/385 (99%)	322 (85%)	41 (11%)	17 (4%)	3	21
1	E	380/385 (99%)	323 (85%)	42 (11%)	15 (4%)	4	25
1	F	380/385 (99%)	321 (84%)	45 (12%)	14 (4%)	4	27
1	G	380/385 (99%)	325 (86%)	41 (11%)	14 (4%)	4	27
1	H	380/385 (99%)	323 (85%)	43 (11%)	14 (4%)	4	27
All	All	3040/3080 (99%)	2589 (85%)	331 (11%)	120 (4%)	4	25

All (120) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	5	22
1	B	305/306 (100%)	263 (86%)	42 (14%)	4	20
1	C	305/306 (100%)	252 (83%)	53 (17%)	2	11
1	D	305/306 (100%)	259 (85%)	46 (15%)	3	16
1	E	305/306 (100%)	246 (81%)	59 (19%)	2	7
1	F	305/306 (100%)	250 (82%)	55 (18%)	2	10
1	G	305/306 (100%)	256 (84%)	49 (16%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	305/306 (100%)	269 (88%)	36 (12%)	6	27
All	All	2440/2448 (100%)	2060 (84%)	380 (16%)	3	16

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	15,15,16	2.62	4 (26%)	21,22,23	2.22	7 (33%)
2	TRP	A	414	3	12,16,16	0.92	0	7,22,22	0.94	0
2	TRP	A	914	3	12,16,16	0.87	0	7,22,22	1.52	1 (14%)
3	PLP	B	913	2	15,15,16	4.30	6 (40%)	21,22,23	2.50	10 (47%)
3	PLP	C	1413	2	15,15,16	2.30	7 (46%)	21,22,23	5.65	11 (52%)
2	TRP	C	1414	3	12,16,16	1.11	0	7,22,22	1.21	0
3	PLP	D	1913	2	15,15,16	3.62	7 (46%)	21,22,23	3.50	8 (38%)
2	TRP	D	1914	3	12,16,16	1.41	1 (8%)	7,22,22	1.25	0
3	PLP	E	2413	2	15,15,16	1.87	5 (33%)	21,22,23	5.47	9 (42%)
2	TRP	E	2414	3	12,16,16	1.11	1 (8%)	7,22,22	1.47	1 (14%)
2	TRP	E	2914	3	12,16,16	3.23	5 (41%)	7,22,22	1.35	1 (14%)
3	PLP	F	2913	2	15,15,16	3.50	6 (40%)	21,22,23	1.68	5 (23%)
3	PLP	G	3413	2	15,15,16	3.55	6 (40%)	21,22,23	3.15	11 (52%)
2	TRP	G	3414	3	12,16,16	1.13	1 (8%)	7,22,22	0.91	0
3	PLP	H	3913	2	15,15,16	4.25	8 (53%)	21,22,23	1.64	5 (23%)
2	TRP	H	3914	3	12,16,16	1.49	1 (8%)	7,22,22	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	413	2	-	0/6/6/8	0/1/1/1
2	TRP	A	414	3	-	0/3/8/8	0/2/2/2
2	TRP	A	914	3	-	0/3/8/8	0/2/2/2
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	-	0/3/8/8	0/2/2/2
3	PLP	D	1913	2	-	0/6/6/8	0/1/1/1
2	TRP	D	1914	3	-	0/3/8/8	0/2/2/2
3	PLP	E	2413	2	-	0/6/6/8	0/1/1/1
2	TRP	E	2414	3	-	0/3/8/8	0/2/2/2
2	TRP	E	2914	3	-	0/3/8/8	0/2/2/2
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	-	0/3/8/8	0/2/2/2
3	PLP	H	3913	2	-	0/6/6/8	0/1/1/1
2	TRP	H	3914	3	-	0/3/8/8	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2913	PLP	C3-C2	-7.52	1.35	1.40
2	E	2914	TRP	CD1-CG	-6.72	1.26	1.38
3	F	2913	PLP	C3-C4	-5.14	1.27	1.40
2	E	2914	TRP	CB-CG	-4.15	1.38	1.51
3	E	2413	PLP	C4A-C4	-3.51	1.44	1.51
3	G	3413	PLP	O3-C3	-2.87	1.30	1.37
3	F	2913	PLP	C5A-C5	-2.61	1.43	1.50
2	E	2414	TRP	CB-CG	-2.60	1.43	1.51
3	B	913	PLP	P-O3P	-2.48	1.45	1.54
3	H	3913	PLP	P-O3P	-2.47	1.45	1.54
3	A	413	PLP	P-O3P	-2.42	1.46	1.54
3	C	1413	PLP	O3-C3	-2.34	1.31	1.37
3	H	3913	PLP	C3-C4	-2.19	1.34	1.40
3	D	1913	PLP	P-O3P	-2.19	1.46	1.54
3	E	2413	PLP	C6-C5	-2.15	1.32	1.37
3	C	1413	PLP	P-O3P	-2.13	1.47	1.54
3	F	2913	PLP	P-O2P	2.02	1.62	1.54
3	C	1413	PLP	C3-C4	2.08	1.45	1.40
3	C	1413	PLP	C2-N1	2.08	1.38	1.34
3	B	913	PLP	O3-C3	2.18	1.42	1.37
3	H	3913	PLP	C2-N1	2.18	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3913	PLP	C2A-C2	2.23	1.54	1.50
3	G	3413	PLP	C6-C5	2.29	1.42	1.37
3	D	1913	PLP	P-O2P	2.32	1.63	1.54
3	D	1913	PLP	C2A-C2	2.32	1.55	1.50
3	H	3913	PLP	C6-C5	2.44	1.43	1.37
3	B	913	PLP	C6-C5	2.45	1.43	1.37
3	E	2413	PLP	O3-C3	2.49	1.42	1.37
2	G	3414	TRP	CZ3-CE3	2.61	1.42	1.36
3	G	3413	PLP	C5A-C5	2.63	1.58	1.50
2	E	2914	TRP	CD1-NE1	2.66	1.42	1.36
3	B	913	PLP	C2A-C2	2.71	1.55	1.50
3	E	2413	PLP	C3-C2	2.83	1.42	1.40
3	F	2913	PLP	C4A-C4	2.93	1.57	1.51
3	A	413	PLP	C5-C4	2.98	1.44	1.40
3	D	1913	PLP	C6-C5	3.03	1.44	1.37
3	E	2413	PLP	P-O2P	3.03	1.65	1.54
3	C	1413	PLP	C5A-C5	3.19	1.60	1.50
3	C	1413	PLP	C4A-C4	3.21	1.58	1.51
3	G	3413	PLP	C3-C2	3.25	1.43	1.40
2	D	1914	TRP	CB-CG	3.59	1.62	1.51
2	H	3914	TRP	CB-CG	4.52	1.64	1.51
3	D	1913	PLP	C4A-C4	4.81	1.61	1.51
2	E	2914	TRP	CH2-CZ2	5.06	1.48	1.36
2	E	2914	TRP	CZ2-CE2	5.10	1.51	1.41
3	H	3913	PLP	C3-C2	5.22	1.44	1.40
3	A	413	PLP	C3-C2	5.93	1.44	1.40
3	C	1413	PLP	C3-C2	5.94	1.44	1.40
3	D	1913	PLP	C3-C2	6.40	1.45	1.40
3	A	413	PLP	C4A-C4	6.51	1.65	1.51
3	G	3413	PLP	C4A-C4	7.30	1.66	1.51
3	B	913	PLP	C4A-C4	7.44	1.66	1.51
3	F	2913	PLP	C5-C4	8.44	1.50	1.40
3	G	3413	PLP	C5-C4	9.57	1.51	1.40
3	H	3913	PLP	C5-C4	9.97	1.52	1.40
3	D	1913	PLP	C5-C4	10.07	1.52	1.40
3	H	3913	PLP	C4A-C4	10.53	1.73	1.51
3	B	913	PLP	C5-C4	13.69	1.56	1.40

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2413	PLP	C4A-C4-C5	-23.48	96.42	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1413	PLP	C4A-C4-C5	-14.58	105.69	120.88
3	D	1913	PLP	C3-C4-C5	-10.06	107.81	118.78
3	B	913	PLP	C3-C4-C5	-7.26	110.86	118.78
3	C	1413	PLP	C3-C4-C5	-6.19	112.02	118.78
3	G	3413	PLP	C4A-C4-C5	-6.15	114.47	120.88
3	G	3413	PLP	C3-C4-C5	-5.65	112.62	118.78
3	C	1413	PLP	C5A-C5-C6	-5.24	109.37	119.28
3	C	1413	PLP	C5-C6-N1	-4.17	116.62	123.86
3	A	413	PLP	C4A-C4-C5	-3.72	117.00	120.88
3	H	3913	PLP	C3-C4-C5	-3.72	114.72	118.78
3	G	3413	PLP	C5A-C5-C6	-3.40	112.85	119.28
3	G	3413	PLP	O2P-P-O4P	-3.17	97.45	106.56
3	A	413	PLP	C3-C4-C5	-3.14	115.35	118.78
3	G	3413	PLP	C5-C6-N1	-3.12	118.44	123.86
3	B	913	PLP	C5A-C5-C6	-2.77	114.04	119.28
3	E	2413	PLP	O4P-C5A-C5	-2.56	104.76	108.99
3	C	1413	PLP	C4-C3-C2	-2.48	115.82	120.05
3	D	1913	PLP	O3-C3-C4	-2.48	111.16	118.12
2	A	914	TRP	CZ3-CE3-CD2	-2.42	117.46	120.88
3	B	913	PLP	C4A-C4-C3	-2.41	115.99	120.36
3	E	2413	PLP	C4A-C4-C3	-2.35	116.11	120.36
3	G	3413	PLP	O4P-C5A-C5	-2.28	105.22	108.99
3	E	2413	PLP	C5-C6-N1	-2.28	119.91	123.86
3	F	2913	PLP	C4A-C4-C3	-2.26	116.27	120.36
3	D	1913	PLP	O4P-P-O1P	-2.19	101.56	107.14
3	B	913	PLP	O3-C3-C4	-2.19	111.97	118.12
3	C	1413	PLP	C2A-C2-C3	-2.17	118.42	121.04
3	D	1913	PLP	C5A-C5-C6	-2.16	115.19	119.28
3	F	2913	PLP	C5-C6-N1	-2.14	120.15	123.86
3	E	2413	PLP	C4-C3-C2	-2.07	116.53	120.05
2	E	2914	TRP	CH2-CZ2-CE2	-2.06	116.77	120.06
3	B	913	PLP	C2A-C2-C3	-2.01	118.61	121.04
3	A	413	PLP	O3-C3-C2	2.08	121.27	117.66
3	H	3913	PLP	C4-C3-C2	2.08	123.60	120.05
3	D	1913	PLP	O3-C3-C2	2.09	121.29	117.66
3	G	3413	PLP	C3-C2-N1	2.18	123.63	120.61
3	B	913	PLP	C6-C5-C4	2.26	120.06	118.15
3	A	413	PLP	C2A-C2-C3	2.34	123.86	121.04
3	A	413	PLP	O3P-P-O1P	2.44	118.45	110.58
3	H	3913	PLP	C6-C5-C4	2.45	120.22	118.15
3	H	3913	PLP	O4P-C5A-C5	2.48	113.09	108.99
3	B	913	PLP	O3P-P-O1P	2.90	119.91	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2913	PLP	C4-C3-C2	2.91	125.01	120.05
3	H	3913	PLP	O3P-P-O1P	2.91	119.95	110.58
2	E	2414	TRP	CB-CG-CD1	2.93	131.59	127.97
3	G	3413	PLP	O3-C3-C2	2.93	122.76	117.66
3	E	2413	PLP	O3P-P-O1P	2.95	120.08	110.58
3	C	1413	PLP	O3P-P-O1P	3.01	120.28	110.58
3	E	2413	PLP	C2A-C2-C3	3.03	124.69	121.04
3	F	2913	PLP	C5A-C5-C4	3.10	125.76	121.65
3	B	913	PLP	C5A-C5-C4	3.15	125.82	121.65
3	G	3413	PLP	O3P-P-O1P	3.21	120.92	110.58
3	B	913	PLP	C4-C3-C2	3.29	125.66	120.05
3	C	1413	PLP	C3-C2-N1	3.30	125.17	120.61
3	C	1413	PLP	O3-C3-C2	3.37	123.52	117.66
3	E	2413	PLP	O3-C3-C2	3.42	123.61	117.66
3	E	2413	PLP	C6-C5-C4	3.46	121.08	118.15
3	B	913	PLP	O4P-C5A-C5	3.63	114.99	108.99
3	F	2913	PLP	O3P-P-O1P	3.70	122.48	110.58
3	D	1913	PLP	C4-C3-C2	3.85	126.61	120.05
3	A	413	PLP	C4A-C4-C3	3.90	127.42	120.36
3	G	3413	PLP	C4A-C4-C3	5.16	129.70	120.36
3	A	413	PLP	C6-C5-C4	5.63	122.92	118.15
3	G	3413	PLP	C6-C5-C4	6.37	123.55	118.15
3	D	1913	PLP	C4A-C4-C5	7.30	128.49	120.88
3	D	1913	PLP	C6-C5-C4	7.31	124.35	118.15
3	C	1413	PLP	C4A-C4-C3	9.78	138.06	120.36
3	C	1413	PLP	C6-C5-C4	15.06	130.91	118.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	413	PLP	2	0
2	A	414	TRP	2	0
2	A	914	TRP	8	0
3	B	913	PLP	3	0
3	C	1413	PLP	4	0
2	C	1414	TRP	8	0
3	D	1913	PLP	2	0
2	D	1914	TRP	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2413	PLP	2	0
2	E	2414	TRP	3	0
2	E	2914	TRP	11	0
3	G	3413	PLP	2	0
2	G	3414	TRP	6	0
3	H	3913	PLP	2	0
2	H	3914	TRP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	382/385 (99%)	-0.42	1 (0%) 94 94	3, 17, 38, 57	0
1	B	382/385 (99%)	-0.38	4 (1%) 84 80	3, 18, 40, 66	0
1	C	382/385 (99%)	-0.42	0 100 100	2, 17, 38, 50	0
1	D	382/385 (99%)	-0.46	0 100 100	2, 16, 33, 50	0
1	E	382/385 (99%)	-0.51	0 100 100	2, 16, 37, 53	0
1	F	382/385 (99%)	-0.51	2 (0%) 91 90	2, 15, 33, 56	0
1	G	382/385 (99%)	-0.52	0 100 100	3, 15, 34, 54	0
1	H	382/385 (99%)	-0.44	3 (0%) 87 84	3, 17, 37, 60	0
All	All	3056/3080 (99%)	-0.46	10 (0%) 94 94	2, 17, 37, 66	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	529	GLN	3.2
1	A	28	ARG	3.1
1	B	525	GLU	2.9
1	B	530	GLY	2.6
1	F	2529	GLN	2.4
1	H	3654	PRO	2.2
1	H	3528	ARG	2.2
1	B	531	VAL	2.1
1	H	3531	VAL	2.1
1	F	2831	ALA	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TRP	D	1914	15/15	0.78	0.50	13.25	32,43,59,61	0
2	TRP	G	3414	15/15	0.47	0.71	9.97	32,53,59,59	0
2	TRP	C	1414	15/15	0.58	0.73	9.07	41,64,68,70	0
2	TRP	E	2914	15/15	0.60	0.56	6.84	29,61,76,77	0
2	TRP	E	2414	15/15	0.68	0.48	6.78	21,50,56,57	0
2	TRP	A	414	15/15	0.76	0.56	6.39	35,41,47,49	0
2	TRP	A	914	15/15	0.71	0.47	6.27	26,59,74,75	0
2	TRP	H	3914	15/15	0.82	0.37	4.96	23,43,48,49	0
3	PLP	A	413	15/16	0.94	0.20	0.81	8,24,34,40	0
3	PLP	E	2413	15/16	0.94	0.17	0.78	2,7,23,33	0
3	PLP	C	1413	15/16	0.95	0.17	0.26	8,18,24,34	0
3	PLP	B	913	15/16	0.98	0.18	0.18	2,7,13,20	0
3	PLP	H	3913	15/16	0.96	0.17	0.06	7,17,27,30	0
3	PLP	D	1913	15/16	0.96	0.14	-0.29	2,14,19,26	0
3	PLP	G	3413	15/16	0.97	0.14	-0.58	2,5,17,27	0
3	PLP	F	2913	15/16	0.97	0.14	-0.75	2,5,16,21	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.