



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:38 PM UTC

PDB ID : 1GC3 / pdb_00001gc3
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

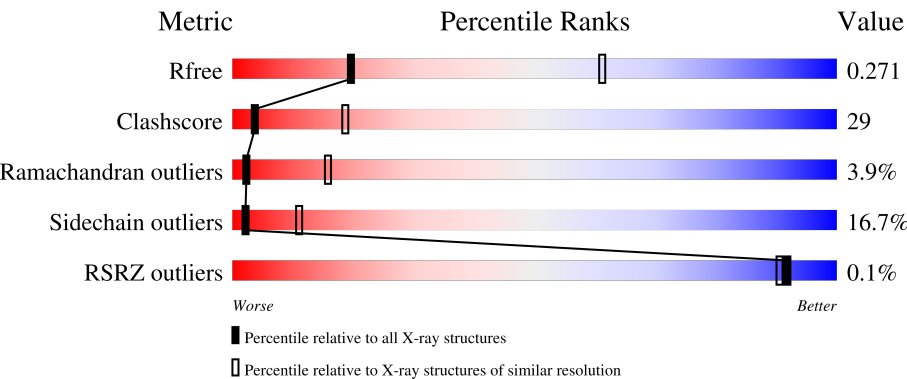
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	42%35%18%. .
1	B	385	41%39%15%. .
1	C	385	40%37%16%5%. .
1	D	385	40%41%15%. .
1	E	385	40%37%19%. .

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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	914	-	-	X	-
2	TRP	C	1414	-	-	X	-
2	TRP	D	1914	-	-	X	-
2	TRP	E	2914	-	-	X	-
2	TRP	G	3414	-	-	X	-
3	PLP	C	1413	-	X	-	-
3	PLP	G	3413	-	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:

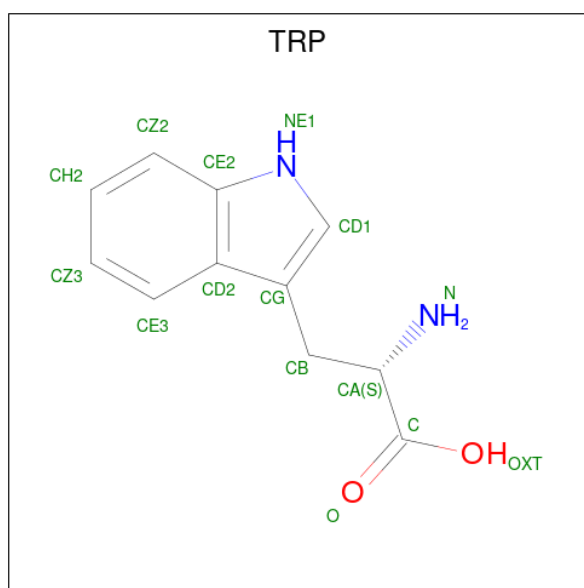
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	SER	engineered mutation	UNP Q56232
A	16	VAL	THR	engineered mutation	UNP Q56232
A	101	SER	LYS	engineered mutation	UNP Q56232
A	261	ARG	SER	engineered mutation	UNP Q56232
B	514	ASP	SER	engineered mutation	UNP Q56232
B	516	VAL	THR	engineered mutation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

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

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



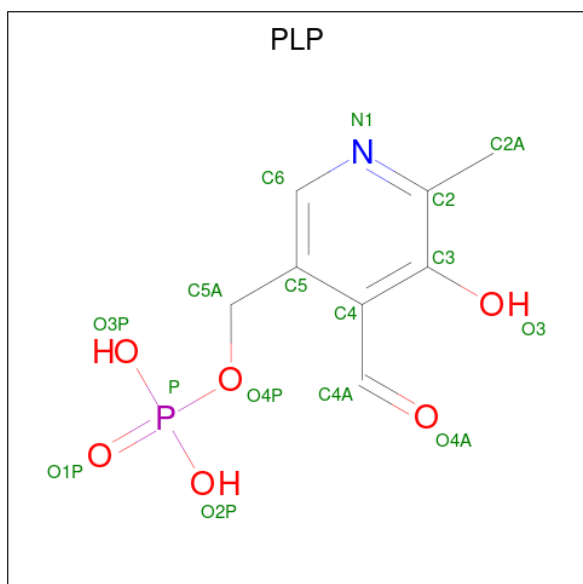
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	A	1	Total	C	N	O	0	0
			15	11	2	2		

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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 (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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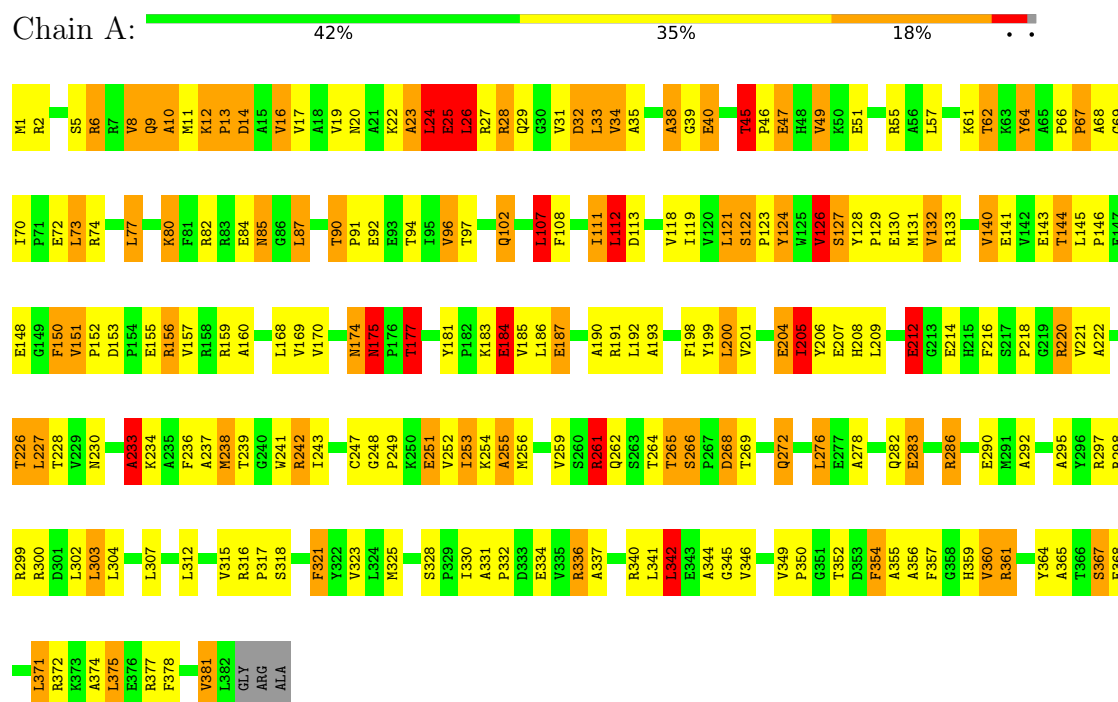
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

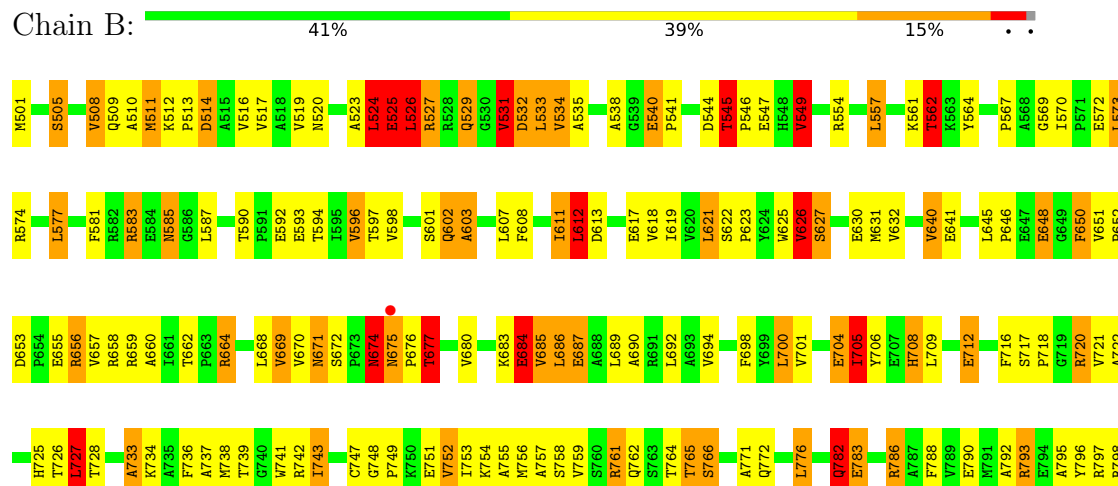
3 Residue-property plots

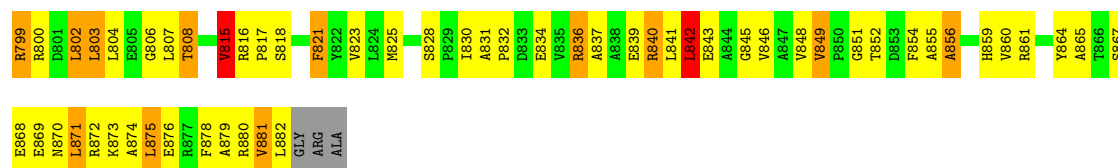
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ASPARTATE AMINOTRANSFERASE



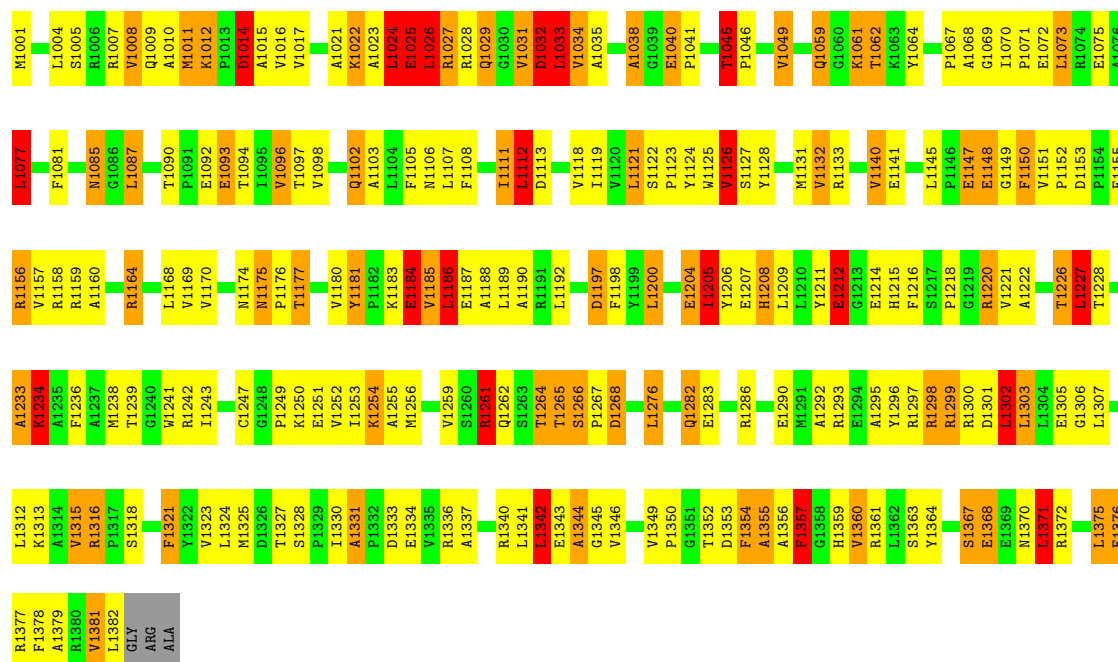
• Molecule 1: ASPARTATE AMINOTRANSFERASE





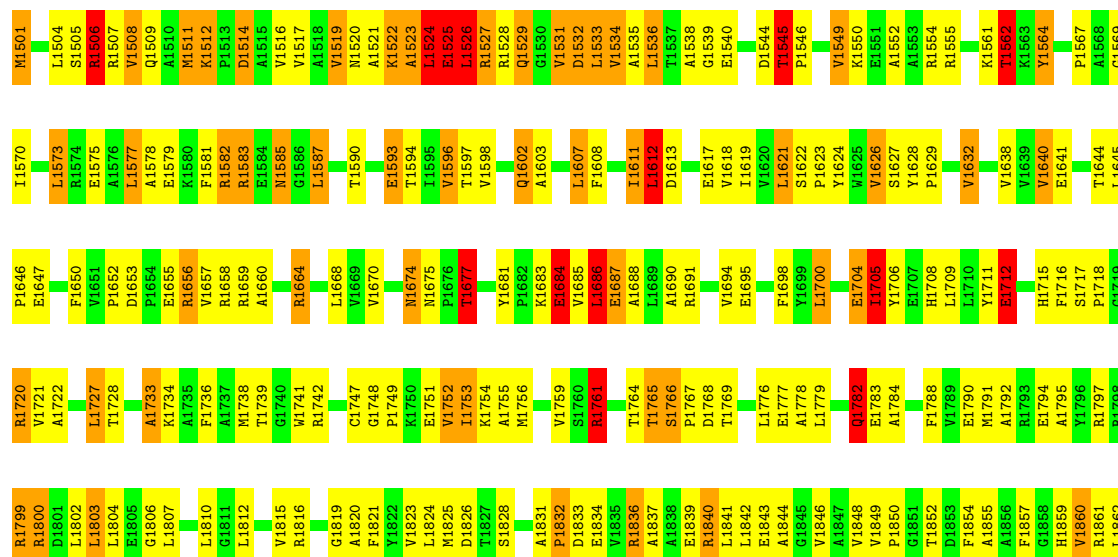
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain C: 40% 37% 16% 5%



• Molecule 1: ASPARTATE AMINOTRANSFERASE

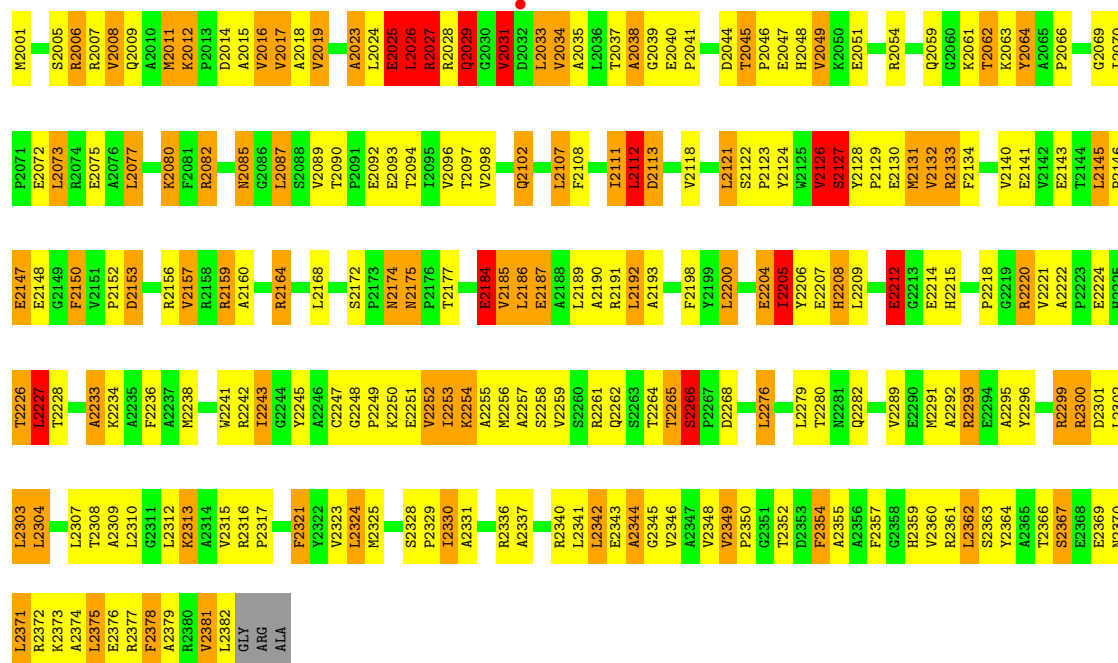
Chain D: 40% 41% 15%





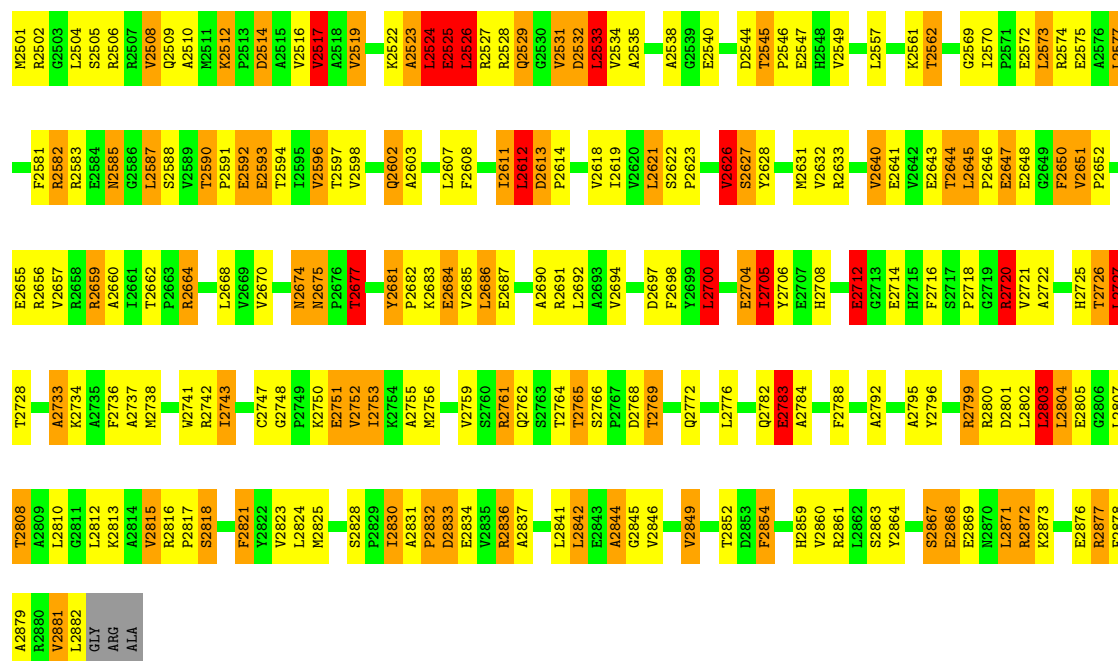
● Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain E: 



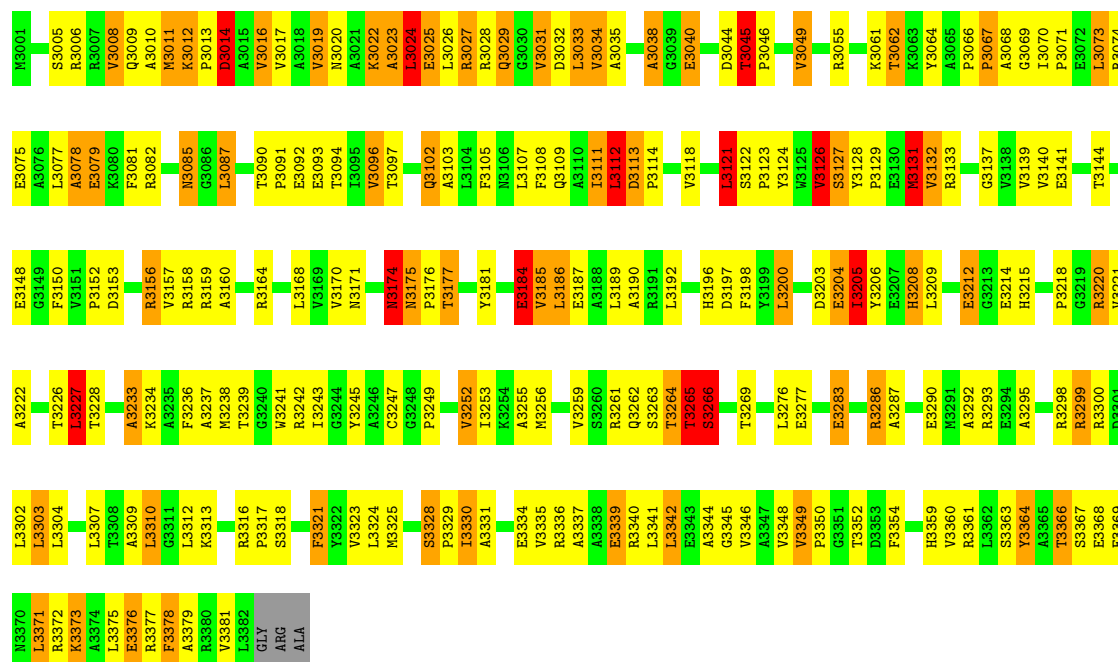
● Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain F: 

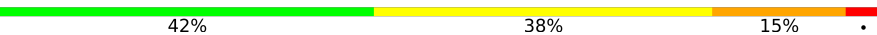


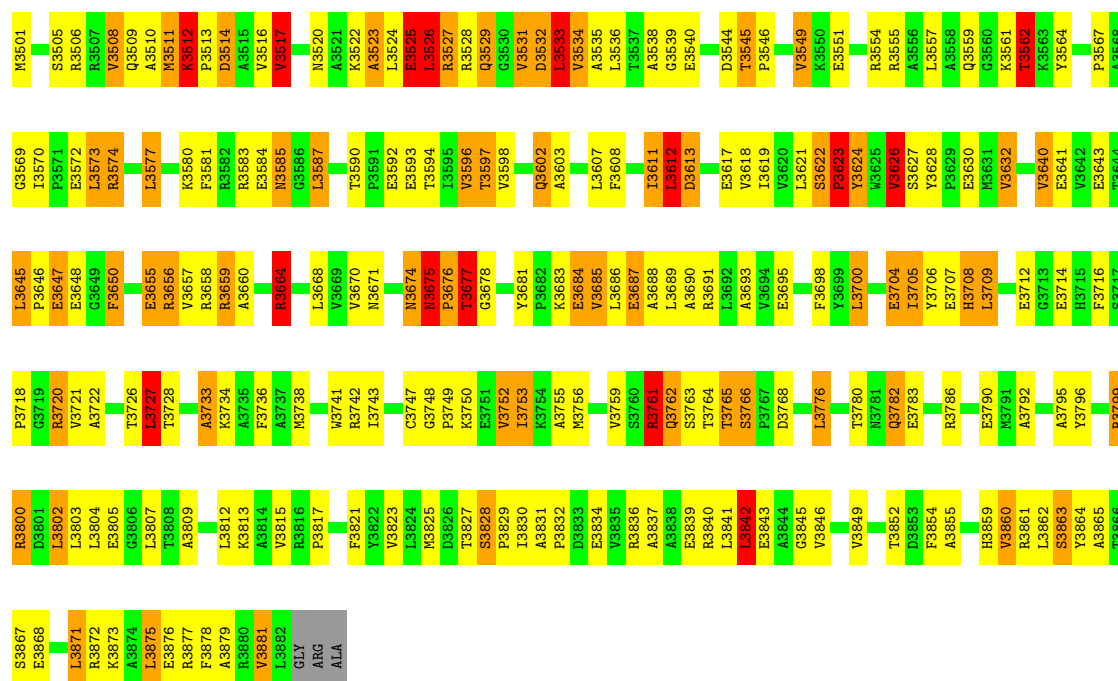
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain G: 



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.50Å 98.40Å 187.00Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30 8.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (8.00-3.30) 88.1 (8.00-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.33Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.203 , 0.282 0.196 , 0.271	Depositor DCC
R_{free} test set	4282 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23824	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	3/3009 (0.1%)	1.63	107/4092 (2.6%)
1	B	0.54	1/3009 (0.0%)	1.67	92/4092 (2.2%)
1	C	0.59	3/3009 (0.1%)	1.67	106/4092 (2.6%)
1	D	0.56	2/3009 (0.1%)	1.63	100/4092 (2.4%)
1	E	0.57	0/3009	1.59	90/4092 (2.2%)
1	F	0.53	0/3009	1.61	97/4092 (2.4%)
1	G	0.54	0/3009	1.56	98/4092 (2.4%)
1	H	0.56	2/3009 (0.1%)	1.56	92/4092 (2.2%)
All	All	0.56	11/24072 (0.0%)	1.62	782/32736 (2.4%)

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	A	261	ARG	NE-CZ	8.59	1.42	1.33
1	C	1261	ARG	CG-CD	-8.52	1.26	1.52
1	A	67	PRO	CA-CB	-8.17	1.41	1.53
1	C	1023	ALA	CA-C	8.16	1.56	1.52
1	D	1761	ARG	NE-CZ	6.56	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1564	TYR	CA-CB	-6.43	1.43	1.53
1	A	67	PRO	CG-CD	-6.23	1.29	1.50
1	B	761	ARG	NE-CZ	6.14	1.39	1.33
1	H	3761	ARG	CZ-NH2	6.08	1.41	1.33
1	C	1261	ARG	NE-CZ	6.03	1.39	1.33
1	H	3761	ARG	CG-CD	5.47	1.68	1.52

All (782) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	675	ASN	CA-C-N	-25.16	93.55	120.47
1	B	675	ASN	C-N-CA	-25.16	93.55	120.47
1	F	2526	LEU	N-CA-C	-22.98	81.33	112.12
1	E	2255	ALA	N-CA-C	-21.91	84.67	111.40
1	B	755	ALA	N-CA-C	-20.04	86.95	111.40
1	E	2023	ALA	N-CA-C	-19.12	78.47	108.30
1	C	1023	ALA	N-CA-C	-18.54	78.64	108.12
1	D	1755	ALA	N-CA-C	-17.52	90.02	111.40
1	A	255	ALA	N-CA-C	-17.46	90.10	111.40
1	H	3755	ALA	N-CA-C	-16.93	90.75	111.40
1	G	3255	ALA	N-CA-C	-16.47	93.35	111.14
1	F	2755	ALA	N-CA-C	-15.56	89.63	112.04
1	C	1185	VAL	N-CA-C	-14.59	100.08	111.90
1	C	1255	ALA	N-CA-C	-14.49	95.50	111.14
1	C	1132	VAL	N-CA-C	-14.28	97.00	110.42
1	H	3685	VAL	N-CA-C	-14.28	100.34	111.90
1	A	185	VAL	N-CA-C	-14.06	100.51	111.90
1	C	1026	LEU	N-CA-C	-13.97	81.04	110.80
1	C	1261	ARG	NE-CZ-NH2	13.89	131.70	119.20
1	F	2836	ARG	N-CA-C	-13.85	96.18	111.14
1	G	3185	VAL	N-CA-C	-13.53	100.17	111.81
1	D	1761	ARG	NE-CZ-NH2	13.40	131.26	119.20
1	B	720	ARG	N-CA-C	-13.31	96.77	111.14
1	F	2685	VAL	N-CA-C	-13.18	101.23	111.90
1	A	23	ALA	N-CA-C	-13.10	82.89	110.80
1	E	2025	GLU	N-CA-C	-12.91	83.31	110.80
1	C	1221	VAL	N-CA-C	12.87	123.72	110.72
1	A	26	LEU	N-CA-C	-12.85	83.43	110.80
1	C	1261	ARG	NH1-CZ-NH2	-12.83	102.62	119.30
1	D	1538	ALA	N-CA-C	12.82	129.62	110.64
1	D	1685	VAL	N-CA-C	-12.81	101.53	111.90
1	F	2632	VAL	N-CA-C	-12.78	98.52	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	721	VAL	N-CA-C	12.72	123.56	110.72
1	B	526	LEU	N-CA-C	-12.69	83.78	110.80
1	B	523	ALA	N-CA-C	-12.66	83.83	110.80
1	G	3023	ALA	N-CA-C	-12.65	83.85	110.80
1	C	1014	ASP	N-CA-C	12.65	128.77	108.41
1	H	3721	VAL	N-CA-C	12.57	123.42	110.72
1	F	2523	ALA	N-CA-C	-12.54	84.09	110.80
1	F	2803	LEU	N-CA-C	-12.43	96.15	112.68
1	D	1523	ALA	N-CA-C	-12.42	84.35	110.80
1	D	1526	LEU	N-CA-C	-12.38	84.44	110.80
1	B	685	VAL	N-CA-C	-12.34	101.20	111.81
1	E	2185	VAL	N-CA-C	-12.31	101.22	111.81
1	C	1220	ARG	N-CA-C	-12.31	97.85	111.14
1	D	1721	VAL	N-CA-C	12.25	123.10	110.72
1	H	3525	GLU	N-CA-C	-12.21	84.80	110.80
1	A	66	PRO	CA-C-N	12.14	132.53	119.05
1	A	66	PRO	C-N-CA	12.14	132.53	119.05
1	D	1761	ARG	NH1-CZ-NH2	-12.01	103.69	119.30
1	C	1049	VAL	N-CA-C	-11.82	99.99	110.74
1	B	870	ASN	N-CA-C	-11.77	98.60	113.43
1	G	3127	SER	N-CA-C	11.77	127.64	113.28
1	D	1525	GLU	N-CA-C	-11.66	85.96	110.80
1	D	1674	ASN	N-CA-C	11.66	126.68	110.24
1	B	761	ARG	NE-CZ-NH2	11.62	129.66	119.20
1	G	3221	VAL	N-CA-C	11.57	122.41	110.72
1	F	2704	GLU	N-CA-C	11.53	123.85	111.28
1	H	3720	ARG	N-CA-C	-11.52	96.38	111.24
1	D	1627	SER	N-CA-C	11.51	127.10	113.18
1	H	3627	SER	N-CA-C	11.48	127.07	113.18
1	G	3014	ASP	N-CA-C	11.38	127.67	108.20
1	D	1527	ARG	N-CA-C	-11.26	99.02	111.07
1	A	204	GLU	N-CA-C	11.22	123.51	111.28
1	A	127	SER	N-CA-C	11.19	126.77	112.89
1	H	3704	GLU	N-CA-C	11.18	123.03	111.07
1	A	132	VAL	N-CA-C	-11.08	100.00	110.42
1	D	1720	ARG	N-CA-C	-11.06	97.91	111.40
1	C	1025	GLU	N-CA-C	-11.02	87.33	110.80
1	H	3523	ALA	N-CA-C	-10.94	87.50	110.80
1	B	627	SER	N-CA-C	10.88	126.39	112.89
1	D	1782	GLN	N-CA-C	-10.84	94.43	110.48
1	G	3024	LEU	N-CA-C	10.81	133.82	110.80
1	E	2221	VAL	N-CA-C	10.77	122.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1127	SER	N-CA-C	10.76	126.23	112.89
1	F	2721	VAL	N-CA-C	10.72	122.69	111.00
1	H	3527	ARG	N-CA-C	-10.69	99.42	111.82
1	B	525	GLU	N-CA-C	-10.67	88.07	110.80
1	G	3220	ARG	N-CA-C	-10.66	98.40	111.40
1	B	632	VAL	N-CA-C	-10.63	100.54	110.53
1	A	220	ARG	N-CA-C	-10.54	98.73	111.69
1	H	3836	ARG	N-CA-C	-10.48	99.86	111.07
1	E	2220	ARG	N-CA-C	-10.43	98.68	111.40
1	C	1085	ASN	N-CA-C	10.38	127.26	113.97
1	B	514	ASP	N-CA-C	10.21	125.16	108.52
1	A	121	LEU	N-CA-C	10.18	126.69	107.75
1	F	2878	PHE	N-CA-C	-10.16	100.17	111.14
1	E	2204	GLU	N-CA-C	10.12	121.90	111.07
1	A	367	SER	N-CA-C	10.10	123.66	110.43
1	A	259	VAL	N-CA-C	-10.08	101.04	110.82
1	D	1585	ASN	N-CA-C	10.07	127.30	114.31
1	F	2674	ASN	N-CA-C	10.04	124.78	110.23
1	A	14	ASP	N-CA-C	10.03	124.76	108.41
1	A	261	ARG	NE-CZ-NH1	9.84	131.34	121.50
1	A	221	VAL	N-CA-C	9.82	121.71	111.00
1	C	1254	LYS	N-CA-C	-9.81	103.44	114.62
1	A	85	ASN	N-CA-C	9.78	126.93	114.31
1	G	3361	ARG	N-CA-C	9.72	124.95	108.23
1	D	1686	LEU	N-CA-C	-9.64	100.64	111.82
1	E	2085	ASN	N-CA-C	9.63	126.73	114.31
1	E	2027	ARG	N-CA-C	-9.62	99.28	111.02
1	G	3025	GLU	N-CA-C	-9.62	90.30	110.80
1	D	1779	LEU	N-CA-C	9.60	121.82	111.36
1	H	3514	ASP	N-CA-C	9.60	124.61	108.20
1	H	3585	ASN	N-CA-C	9.57	126.65	114.31
1	G	3378	PHE	N-CA-C	-9.57	100.83	111.07
1	F	2720	ARG	N-CA-C	-9.56	99.74	111.40
1	B	836	ARG	N-CA-C	-9.54	99.95	111.69
1	B	738	MET	N-CA-C	9.52	123.33	112.57
1	C	1024	LEU	N-CA-C	9.50	131.04	110.80
1	F	2585	ASN	N-CA-C	9.50	126.56	114.31
1	C	1093	GLU	N-CA-C	-9.49	100.07	112.41
1	F	2621	LEU	N-CA-C	9.49	123.69	108.41
1	B	878	PHE	N-CA-C	-9.46	100.92	111.14
1	D	1836	ARG	N-CA-C	-9.46	101.05	111.36
1	A	336	ARG	N-CA-C	-9.44	100.34	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	867	SER	N-CA-C	9.38	122.72	110.43
1	C	1378	PHE	N-CA-C	-9.38	101.01	111.14
1	H	3878	PHE	N-CA-C	-9.38	101.04	111.07
1	E	2132	VAL	N-CA-C	-9.37	101.21	110.30
1	F	2867	SER	N-CA-C	9.34	122.85	110.53
1	A	175	ASN	N-CA-C	-9.33	90.44	108.45
1	E	2367	SER	N-CA-C	9.33	122.65	110.43
1	F	2627	SER	N-CA-C	9.29	124.41	112.89
1	G	3085	ASN	N-CA-C	9.28	126.28	114.31
1	A	361	ARG	N-CA-C	9.26	124.16	108.23
1	F	2532	ASP	N-CA-C	-9.24	94.12	109.46
1	G	3234	LYS	N-CA-C	9.22	121.33	111.28
1	H	3534	VAL	N-CA-C	-9.21	94.31	107.75
1	C	1336	ARG	N-CA-C	-9.20	100.37	111.69
1	C	1034	VAL	N-CA-C	-9.20	95.29	108.17
1	D	1871	LEU	N-CA-C	-9.19	100.39	111.69
1	G	3038	ALA	N-CA-C	9.19	130.37	110.80
1	H	3675	ASN	N-CA-C	-9.19	89.08	107.91
1	H	3861	ARG	N-CA-C	9.18	125.15	108.17
1	E	2017	VAL	N-CA-C	-9.15	99.23	112.04
1	E	2150	PHE	N-CA-C	9.14	123.81	112.47
1	C	1303	LEU	N-CA-C	-9.14	100.52	112.68
1	G	3263	SER	N-CA-C	-9.14	97.13	111.02
1	B	871	LEU	N-CA-C	-9.11	101.43	111.36
1	E	2038	ALA	N-CA-C	9.10	130.18	110.80
1	F	2738	MET	N-CA-C	9.09	123.11	112.93
1	A	38	ALA	N-CA-C	9.07	130.12	110.80
1	A	113	ASP	N-CA-C	-9.07	96.23	110.10
1	F	2647	GLU	N-CA-C	-9.06	99.86	112.45
1	E	2279	LEU	N-CA-C	-9.03	102.17	113.55
1	B	538	ALA	N-CA-C	9.02	130.00	110.80
1	D	1878	PHE	N-CA-C	-9.02	101.40	111.14
1	G	3336	ARG	N-CA-C	-9.01	101.54	111.36
1	D	1514	ASP	N-CA-C	9.01	123.41	108.73
1	B	641	GLU	N-CA-C	9.00	124.09	109.59
1	F	2538	ALA	N-CA-C	9.00	129.97	110.80
1	B	861	ARG	N-CA-C	8.99	123.81	107.99
1	C	1204	GLU	N-CA-C	8.97	120.83	111.14
1	A	45	THR	CA-C-N	8.96	129.04	119.90
1	A	45	THR	C-N-CA	8.96	129.04	119.90
1	D	1759	VAL	N-CA-C	-8.96	102.13	110.82
1	C	1022	LYS	N-CA-C	8.95	124.70	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	3526	LEU	N-CA-C	-8.94	91.75	110.80
1	D	1524	LEU	N-CA-C	8.94	129.83	110.80
1	A	67	PRO	CA-CB-CG	-8.93	87.53	104.50
1	F	2549	VAL	N-CA-C	-8.93	102.13	110.53
1	A	342	LEU	N-CA-C	-8.91	101.48	111.82
1	C	1032	ASP	N-CA-C	-8.90	96.14	110.20
1	H	3705	ILE	N-CA-C	8.88	127.81	109.34
1	A	34	VAL	N-CA-C	-8.87	95.67	108.53
1	B	585	ASN	N-CA-C	8.87	125.75	114.31
1	H	3759	VAL	N-CA-C	-8.85	102.24	110.82
1	C	1259	VAL	N-CA-C	-8.80	102.25	110.53
1	G	3174	ASN	N-CA-C	8.81	122.66	110.24
1	B	534	VAL	N-CA-C	-8.75	94.82	107.77
1	A	49	VAL	N-CA-C	-8.75	102.33	110.82
1	C	1175	ASN	N-CA-C	-8.74	91.59	108.45
1	C	1186	LEU	N-CA-C	-8.73	101.67	111.71
1	D	1734	LYS	N-CA-C	8.73	120.87	111.36
1	H	3538	ALA	N-CA-C	8.72	129.38	110.80
1	A	174	ASN	N-CA-C	8.71	122.86	110.23
1	A	186	LEU	N-CA-C	-8.67	101.74	111.71
1	E	2378	PHE	N-CA-C	-8.62	101.46	111.03
1	E	2361	ARG	N-CA-C	8.62	122.29	108.41
1	C	1238	MET	N-CA-C	8.62	122.10	112.97
1	B	684	GLU	N-CA-C	8.59	123.41	113.19
1	B	734	LYS	N-CA-C	8.58	120.63	111.28
1	C	1038	ALA	N-CA-C	8.57	129.06	110.80
1	E	2127	SER	N-CA-C	8.57	123.51	112.89
1	G	3121	LEU	N-CA-C	8.56	122.20	108.41
1	D	1712	GLU	N-CA-C	8.50	121.43	107.23
1	E	2035	ALA	N-CA-C	8.50	123.57	107.75
1	D	1752	VAL	N-CA-C	8.48	122.88	111.17
1	A	234	LYS	N-CA-C	8.45	120.48	111.28
1	D	1587	LEU	N-CA-C	-8.44	98.00	110.48
1	F	2686	LEU	N-CA-C	-8.43	102.09	111.28
1	G	3141	GLU	N-CA-C	8.43	123.17	109.59
1	B	761	ARG	NH1-CZ-NH2	-8.43	108.34	119.30
1	G	3113	ASP	N-CA-C	-8.42	98.36	110.40
1	A	67	PRO	N-CD-CG	-8.41	90.58	103.20
1	A	378	PHE	N-CA-C	-8.41	101.69	111.03
1	C	1141	GLU	N-CA-C	8.41	123.56	109.76
1	E	2259	VAL	N-CA-C	-8.41	101.84	111.00
1	E	2234	LYS	N-CA-C	8.40	120.06	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2187	GLU	N-CA-C	-8.40	101.82	110.97
1	F	2759	VAL	N-CA-C	-8.35	102.68	110.53
1	B	759	VAL	N-CA-C	-8.35	102.72	110.82
1	A	25	GLU	N-CA-C	-8.33	93.06	110.80
1	F	2641	GLU	N-CA-C	8.31	122.97	109.59
1	E	2134	PHE	N-CA-C	-8.30	102.23	111.28
1	G	3150	PHE	N-CA-C	8.28	122.96	112.86
1	D	1861	ARG	N-CA-C	8.28	122.47	108.23
1	E	2141	GLU	N-CA-C	8.27	122.90	109.59
1	F	2534	VAL	N-CA-C	-8.27	96.10	108.17
1	C	1264	THR	N-CA-C	8.25	123.65	113.50
1	F	2612	LEU	N-CA-C	8.23	128.33	110.80
1	C	1234	LYS	N-CA-C	8.22	121.36	111.82
1	H	3509	GLN	N-CA-C	-8.19	102.30	111.14
1	A	205	ILE	N-CA-C	8.15	126.29	109.34
1	H	3674	ASN	N-CA-C	8.13	122.02	110.23
1	C	1112	LEU	N-CA-C	8.10	128.04	110.80
1	B	612	LEU	N-CA-C	8.09	128.02	110.80
1	G	3112	LEU	N-CA-C	8.07	128.00	110.80
1	H	3708	HIS	N-CA-C	8.05	122.67	113.01
1	A	87	LEU	N-CA-C	-8.04	98.58	110.48
1	H	3734	LYS	N-CA-C	8.04	119.67	111.07
1	F	2844	ALA	N-CA-C	-8.03	103.57	112.72
1	B	712	GLU	N-CA-C	8.02	120.56	107.32
1	G	3093	GLU	N-CA-C	-8.02	101.39	112.30
1	H	3512	LYS	N-CA-C	8.02	119.88	109.93
1	B	802	LEU	N-CA-C	-8.02	102.23	110.97
1	F	2512	LYS	N-CA-C	8.02	121.36	110.29
1	F	2524	LEU	N-CA-C	8.02	127.87	110.80
1	G	3204	GLU	N-CA-C	8.02	120.02	111.28
1	D	1612	LEU	N-CA-C	8.01	127.87	110.80
1	G	3238	MET	N-CA-C	8.01	121.90	112.93
1	D	1632	VAL	N-CA-C	-7.98	102.56	110.30
1	E	2184	GLU	N-CA-C	7.98	122.69	113.19
1	H	3612	LEU	N-CA-C	7.98	127.80	110.80
1	F	2640	VAL	N-CA-C	-7.94	93.91	107.24
1	C	1157	VAL	N-CA-C	-7.93	101.18	111.09
1	H	3632	VAL	N-CA-C	-7.93	102.97	110.42
1	H	3809	ALA	N-CA-C	-7.91	102.73	111.36
1	E	2112	LEU	N-CA-C	7.91	127.65	110.80
1	G	3140	VAL	N-CA-C	-7.91	93.95	107.24
1	F	2651	VAL	N-CA-C	-7.90	91.83	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1675	ASN	N-CA-C	-7.86	93.28	108.45
1	B	524	LEU	N-CA-C	7.85	127.51	110.80
1	G	3066	PRO	CA-C-N	7.84	127.75	119.05
1	G	3066	PRO	C-N-CA	7.84	127.75	119.05
1	D	1509	GLN	N-CA-C	-7.82	102.69	111.14
1	E	2299	ARG	N-CA-C	-7.82	102.84	111.36
1	H	3587	LEU	N-CA-C	-7.82	98.91	110.48
1	C	1208	HIS	N-CA-C	7.81	122.38	113.01
1	E	2011	MET	N-CA-C	7.80	122.41	109.46
1	H	3535	ALA	N-CA-C	7.80	122.26	107.75
1	E	2186	LEU	N-CA-C	-7.78	102.80	111.82
1	A	238	MET	N-CA-C	7.77	121.35	112.57
1	A	84	GLU	N-CA-C	7.77	120.83	111.82
1	B	590	THR	N-CA-C	-7.75	98.24	110.10
1	D	1534	VAL	N-CA-C	-7.74	97.33	108.17
1	C	1205	ILE	N-CA-C	7.72	125.39	109.34
1	A	141	GLU	N-CA-C	7.71	122.40	109.76
1	F	2813	LYS	N-CA-C	7.70	122.38	109.76
1	H	3590	THR	N-CA-C	-7.70	98.80	110.50
1	D	1544	ASP	N-CA-C	-7.69	99.13	110.52
1	F	2544	ASP	N-CA-C	-7.69	98.50	110.42
1	A	11	MET	N-CA-C	7.68	122.20	109.46
1	C	1299	ARG	N-CA-C	-7.67	103.00	111.36
1	H	3687	GLU	N-CA-C	-7.66	101.36	111.24
1	B	686	LEU	N-CA-C	-7.66	102.93	111.28
1	F	2644	THR	N-CA-C	-7.65	95.94	108.41
1	E	2212	GLU	N-CA-C	7.65	120.01	107.23
1	D	1854	PHE	N-CA-C	-7.64	102.15	113.61
1	F	2734	LYS	N-CA-C	7.64	119.24	111.07
1	F	2784	ALA	N-CA-C	-7.64	102.77	112.93
1	C	1371	LEU	N-CA-C	-7.63	102.96	111.28
1	D	1778	ALA	N-CA-C	-7.62	103.05	111.36
1	E	2147	GLU	N-CA-C	-7.62	102.91	111.07
1	D	1641	GLU	N-CA-C	7.61	121.85	109.59
1	E	2121	LEU	N-CA-C	7.60	121.05	108.96
1	D	1660	ALA	N-CA-C	-7.60	103.09	114.64
1	D	1535	ALA	N-CA-C	7.60	122.59	107.62
1	H	3650	PHE	N-CA-C	7.57	121.84	111.54
1	E	2174	ASN	N-CA-C	7.57	120.64	110.35
1	D	1695	GLU	N-CA-C	7.55	119.15	111.07
1	E	2160	ALA	N-CA-C	-7.55	103.62	114.12
1	F	2593	GLU	N-CA-C	-7.55	104.04	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3205	ILE	N-CA-C	7.55	125.05	109.34
1	C	1342	LEU	N-CA-C	-7.55	103.33	112.54
1	B	852	THR	N-CA-C	7.55	120.17	111.11
1	F	2712	GLU	N-CA-C	7.54	121.99	107.44
1	E	2047	GLU	N-CA-C	7.53	119.56	111.36
1	G	3160	ALA	N-CA-C	-7.51	103.50	114.39
1	H	3657	VAL	N-CA-C	-7.51	101.38	111.44
1	A	251	GLU	N-CA-C	7.48	119.51	111.36
1	H	3511	MET	N-CA-C	7.46	122.50	109.96
1	G	3367	SER	N-CA-C	7.45	120.14	110.53
1	E	2309	ALA	N-CA-C	-7.44	102.53	111.69
1	F	2705	ILE	N-CA-C	7.44	124.82	109.34
1	H	3660	ALA	N-CA-C	-7.44	103.61	114.39
1	A	12	LYS	N-CA-C	7.44	119.27	109.83
1	C	1187	GLU	N-CA-C	-7.43	102.87	110.97
1	H	3763	SER	N-CA-C	-7.42	102.17	112.12
1	E	2208	HIS	N-CA-C	7.42	122.15	113.18
1	A	9	GLN	N-CA-C	-7.42	103.13	111.14
1	H	3852	THR	N-CA-C	7.41	120.00	111.11
1	D	1824	LEU	N-CA-C	-7.38	97.20	109.46
1	A	112	LEU	N-CA-C	7.38	126.51	110.80
1	B	613	ASP	N-CA-C	-7.38	99.85	110.40
1	H	3641	GLU	N-CA-C	7.38	122.05	110.17
1	A	208	HIS	N-CA-C	7.36	122.08	113.18
1	D	1640	VAL	N-CA-C	-7.35	95.59	107.28
1	H	3664	ARG	N-CA-C	-7.35	104.46	113.50
1	B	799	ARG	N-CA-C	-7.32	103.38	111.36
1	H	3762	GLN	N-CA-C	7.32	121.92	112.92
1	H	3549	VAL	N-CA-C	-7.32	103.65	110.53
1	B	675	ASN	C-N-CD	7.32	155.00	125.00
1	D	1549	VAL	N-CA-C	-7.30	103.67	110.53
1	D	1799	ARG	N-CA-C	-7.30	103.40	111.36
1	F	2736	PHE	N-CA-C	7.29	121.10	112.93
1	H	3640	VAL	N-CA-C	-7.26	95.03	107.24
1	B	540	GLU	N-CA-C	7.26	120.33	110.31
1	F	2871	LEU	N-CA-C	-7.26	103.45	111.36
1	F	2783	GLU	N-CA-C	7.25	126.24	110.80
1	B	640	VAL	N-CA-C	-7.25	95.07	107.24
1	G	3034	VAL	N-CA-C	-7.25	98.03	108.17
1	H	3842	LEU	N-CA-C	-7.25	103.41	111.82
1	A	140	VAL	N-CA-C	-7.23	95.09	107.24
1	F	2657	VAL	N-CA-C	-7.22	101.77	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3236	PHE	N-CA-C	7.22	121.01	112.93
1	C	1212	GLU	N-CA-C	7.20	119.44	107.20
1	F	2533	LEU	N-CA-C	-7.20	97.57	109.80
1	C	1236	PHE	N-CA-C	7.19	120.98	112.93
1	C	1090	THR	N-CA-C	-7.18	99.38	110.58
1	B	842	LEU	N-CA-C	-7.17	103.79	112.54
1	G	3049	VAL	N-CA-C	-7.16	103.80	110.53
1	G	3212	GLU	N-CA-C	7.14	122.16	107.37
1	D	1736	PHE	N-CA-C	7.13	120.91	112.93
1	H	3736	PHE	N-CA-C	7.13	120.91	112.93
1	B	708	HIS	N-CA-C	7.12	121.80	113.18
1	A	236	PHE	N-CA-C	7.11	120.89	112.93
1	D	1738	MET	N-CA-C	7.11	121.92	112.25
1	G	3035	ALA	N-CA-C	7.11	121.36	107.57
1	B	660	ALA	N-CA-C	-7.10	104.09	114.39
1	E	2157	VAL	N-CA-C	-7.10	102.22	111.09
1	H	3813	LYS	N-CA-C	7.10	120.81	109.24
1	A	160	ALA	N-CA-C	-7.10	103.85	114.64
1	B	736	PHE	N-CA-C	7.09	120.88	112.93
1	G	3148	GLU	N-CA-C	-7.09	102.60	112.45
1	D	1705	ILE	N-CA-C	7.08	124.07	109.34
1	A	352	THR	N-CA-C	7.08	119.61	111.11
1	D	1562	THR	N-CA-C	7.08	121.93	112.30
1	G	3157	VAL	N-CA-C	-7.06	102.26	111.09
1	F	2681	TYR	CA-C-N	7.05	127.02	119.76
1	F	2681	TYR	C-N-CA	7.05	127.02	119.76
1	A	29	GLN	N-CA-C	7.05	118.90	110.44
1	F	2675	ASN	N-CA-C	-7.03	93.49	107.91
1	G	3299	ARG	N-CA-C	-7.03	103.69	111.36
1	E	2354	PHE	N-CA-C	-7.03	103.07	113.61
1	D	1653	ASP	N-CA-C	-7.01	95.70	109.10
1	D	1708	HIS	N-CA-C	7.01	121.42	113.01
1	H	3799	ARG	N-CA-C	-7.01	103.72	111.36
1	F	2660	ALA	N-CA-C	-7.01	104.23	114.39
1	C	1150	PHE	N-CA-C	6.99	121.56	113.38
1	D	1842	LEU	N-CA-C	-6.98	103.43	112.23
1	B	549	VAL	N-CA-C	-6.96	103.42	111.00
1	E	2034	VAL	N-CA-C	-6.96	97.59	107.75
1	B	657	VAL	N-CA-C	-6.95	102.12	111.44
1	G	3062	THR	N-CA-C	6.94	121.44	112.41
1	G	3342	LEU	N-CA-C	-6.94	103.77	111.82
1	E	2192	LEU	N-CA-C	-6.93	103.80	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	705	ILE	N-CA-C	6.93	123.76	109.34
1	D	1852	THR	N-CA-C	6.93	119.42	111.11
1	E	2342	LEU	N-CA-C	-6.92	104.09	112.54
1	G	3371	LEU	N-CA-C	-6.92	103.67	111.14
1	A	261	ARG	NE-CZ-NH2	-6.91	112.98	119.20
1	D	1802	LEU	N-CA-C	-6.91	102.98	111.40
1	H	3780	THR	N-CA-C	6.91	120.96	112.54
1	F	2650	PHE	N-CA-C	6.90	119.65	111.02
1	E	2090	THR	N-CA-C	-6.90	99.55	110.10
1	C	1168	LEU	N-CA-C	-6.89	98.61	109.50
1	E	2113	ASP	N-CA-C	-6.89	99.55	110.10
1	C	1033	LEU	N-CA-C	-6.88	98.95	109.41
1	C	1140	VAL	N-CA-C	-6.88	95.69	107.24
1	E	2140	VAL	N-CA-C	-6.88	96.35	107.28
1	C	1160	ALA	N-CA-C	-6.87	104.19	114.64
1	D	1504	LEU	N-CA-C	6.87	119.39	110.53
1	E	2087	LEU	N-CA-C	-6.87	100.32	110.48
1	B	509	GLN	N-CA-C	-6.85	103.74	111.14
1	F	2833	ASP	N-CA-C	-6.85	99.14	109.96
1	A	299	ARG	N-CA-C	-6.83	103.91	111.36
1	E	2080	LYS	N-CA-C	-6.83	103.07	111.40
1	G	3208	HIS	N-CA-C	6.82	121.43	113.18
1	F	2852	THR	N-CA-C	6.82	119.29	111.11
1	E	2164	ARG	N-CA-C	-6.81	103.97	112.90
1	B	650	PHE	N-CA-C	6.79	120.93	112.24
1	A	212	GLU	N-CA-C	6.79	121.42	107.37
1	A	200	LEU	N-CA-C	-6.78	97.22	108.34
1	C	1200	LEU	N-CA-C	-6.77	97.31	108.76
1	A	209	LEU	N-CA-C	-6.77	95.99	108.24
1	G	3109	GLN	N-CA-C	-6.76	104.84	113.23
1	C	1227	LEU	N-CA-C	-6.76	96.10	107.80
1	C	1148	GLU	N-CA-C	-6.76	105.81	112.97
1	E	2200	LEU	N-CA-C	-6.75	97.41	108.41
1	E	2371	LEU	N-CA-C	-6.74	104.01	111.36
1	A	168	LEU	N-CA-C	-6.74	97.98	109.24
1	C	1262	GLN	N-CA-C	6.74	121.67	113.38
1	E	2236	PHE	N-CA-C	6.73	120.47	112.93
1	C	1184	GLU	N-CA-C	6.72	122.64	113.37
1	A	304	LEU	N-CA-C	6.71	119.43	111.71
1	D	1545	THR	CA-C-N	6.71	126.67	119.76
1	D	1545	THR	C-N-CA	6.71	126.67	119.76
1	H	3727	LEU	N-CA-C	-6.71	97.34	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3168	LEU	N-CA-C	-6.71	98.04	109.24
1	A	33	LEU	N-CA-C	-6.69	100.05	109.69
1	H	3695	GLU	N-CA-C	6.67	119.40	111.33
1	D	1657	VAL	N-CA-C	-6.66	102.51	111.44
1	H	3738	MET	N-CA-C	6.66	121.31	112.25
1	B	532	ASP	N-CA-C	-6.66	98.83	109.76
1	A	157	VAL	N-CA-C	-6.65	102.78	111.09
1	F	2514	ASP	N-CA-C	6.65	119.12	108.41
1	C	1009	GLN	N-CA-C	-6.65	103.96	111.14
1	G	3186	LEU	N-CA-C	-6.64	104.04	111.28
1	C	1061	LYS	N-CA-C	-6.64	97.01	108.56
1	F	2700	LEU	N-CA-C	-6.64	98.08	108.90
1	A	80	LYS	N-CA-C	-6.63	104.14	111.36
1	B	527	ARG	N-CA-C	-6.62	104.00	111.14
1	C	1352	THR	N-CA-C	6.62	119.05	111.11
1	A	272	GLN	N-CA-C	-6.60	103.70	111.03
1	C	1164	ARG	N-CA-C	-6.60	105.38	113.50
1	G	3078	ALA	N-CA-C	-6.60	104.12	111.71
1	H	3645	LEU	N-CA-C	6.60	118.02	109.64
1	C	1087	LEU	N-CA-C	-6.59	99.79	110.20
1	H	3700	LEU	N-CA-C	-6.59	98.16	108.90
1	E	2044	ASP	N-CA-C	-6.59	99.56	110.17
1	D	1512	LYS	N-CA-C	6.58	119.85	110.24
1	F	2726	THR	N-CA-C	6.57	120.59	110.20
1	C	1363	SER	N-CA-C	6.54	122.46	107.48
1	D	1532	ASP	N-CA-C	-6.54	99.36	109.76
1	G	3177	THR	N-CA-C	6.53	120.99	112.89
1	B	700	LEU	N-CA-C	-6.53	97.63	108.34
1	F	2804	LEU	N-CA-C	6.52	118.39	111.28
1	B	674	ASN	N-CA-C	6.50	124.65	110.80
1	G	3227	LEU	N-CA-C	-6.50	97.68	108.34
1	H	3761	ARG	CG-CD-NE	-6.50	97.70	112.00
1	A	226	THR	N-CA-C	6.48	119.87	110.28
1	D	1533	LEU	N-CA-C	-6.47	100.37	109.69
1	F	2861	ARG	N-CA-C	6.47	118.83	108.41
1	F	2799	ARG	N-CA-C	-6.47	104.23	111.28
1	C	1035	ALA	N-CA-C	6.46	120.36	107.62
1	G	3309	ALA	N-CA-C	-6.46	103.74	111.69
1	B	709	LEU	N-CA-C	-6.46	100.60	109.71
1	E	2251	GLU	N-CA-C	6.46	118.90	111.02
1	B	544	ASP	N-CA-C	-6.44	100.99	110.52
1	D	1709	LEU	N-CA-C	-6.44	100.63	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3144	THR	N-CA-C	-6.44	97.58	108.26
1	C	1153	ASP	CA-C-N	6.43	125.92	119.24
1	C	1153	ASP	C-N-CA	6.43	125.92	119.24
1	F	2708	HIS	N-CA-C	6.40	120.92	113.18
1	F	2517	VAL	N-CA-C	-6.39	102.88	111.44
1	G	3259	VAL	N-CA-C	-6.39	104.53	110.53
1	E	2131	MET	N-CA-C	6.38	121.26	112.90
1	G	3033	LEU	N-CA-C	-6.38	100.05	109.81
1	H	3855	ALA	N-CA-C	-6.38	104.80	112.58
1	B	510	ALA	N-CA-C	6.38	120.16	112.38
1	F	2547	GLU	N-CA-C	6.38	118.31	111.36
1	B	653	ASP	N-CA-C	-6.38	96.92	109.10
1	C	1040	GLU	N-CA-C	6.38	118.68	110.39
1	D	1834	GLU	N-CA-C	6.36	120.71	113.15
1	E	2205	ILE	N-CA-C	6.36	122.56	109.34
1	G	3352	THR	N-CA-C	6.36	118.74	111.11
1	D	1531	VAL	N-CA-C	6.35	122.55	109.34
1	F	2854	PHE	N-CA-C	-6.35	104.09	113.61
1	G	3044	ASP	N-CA-C	-6.34	100.24	110.32
1	F	2668	LEU	N-CA-C	-6.33	98.66	109.24
1	G	3200	LEU	N-CA-C	-6.32	98.59	108.90
1	B	751	GLU	N-CA-C	6.32	117.97	111.14
1	G	3090	THR	N-CA-C	-6.32	100.44	110.10
1	A	357	PHE	N-CA-C	6.30	119.50	110.10
1	D	1784	ALA	N-CA-C	-6.30	104.30	112.68
1	E	2227	LEU	N-CA-C	-6.30	98.14	108.41
1	C	1126	VAL	N-CA-C	6.30	122.44	109.34
1	D	1769	THR	N-CA-C	6.30	118.67	111.11
1	H	3668	LEU	N-CA-C	-6.30	98.72	109.24
1	B	535	ALA	N-CA-C	6.29	119.78	107.57
1	C	1233	ALA	N-CA-C	6.29	124.20	110.80
1	E	2133	ARG	N-CA-C	6.29	119.12	111.82
1	A	133	ARG	N-CA-C	6.28	118.12	111.28
1	G	3363	SER	N-CA-C	6.28	120.37	107.37
1	G	3192	LEU	N-CA-C	-6.27	104.52	111.36
1	B	505	SER	N-CA-C	6.27	118.81	110.53
1	D	1561	LYS	N-CA-C	-6.27	101.97	110.68
1	D	1704	GLU	N-CA-C	6.26	118.66	111.02
1	H	3712	GLU	N-CA-C	6.24	119.49	107.44
1	H	3626	VAL	N-CA-C	6.24	122.32	109.34
1	H	3561	LYS	N-CA-C	-6.24	100.27	109.62
1	E	2209	LEU	N-CA-C	-6.22	96.98	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2357	PHE	N-CA-C	6.22	119.25	110.23
1	A	155	GLU	N-CA-C	6.22	118.85	111.33
1	C	1113	ASP	N-CA-C	-6.22	101.51	110.40
1	B	557	LEU	N-CA-C	-6.21	104.42	111.07
1	B	545	THR	CA-C-N	6.21	126.24	119.90
1	B	545	THR	C-N-CA	6.21	126.24	119.90
1	G	3132	VAL	N-CA-C	-6.21	104.28	110.62
1	D	1700	LEU	N-CA-C	-6.20	98.17	108.34
1	H	3580	LYS	N-CA-C	-6.20	104.21	110.97
1	D	1687	GLU	N-CA-C	-6.19	104.22	110.97
1	F	2509	GLN	N-CA-C	-6.18	104.47	111.14
1	B	626	VAL	N-CA-C	6.17	122.17	109.34
1	F	2727	LEU	N-CA-C	-6.17	97.22	108.02
1	B	668	LEU	N-CA-C	-6.16	98.95	109.24
1	C	1293	ARG	N-CA-C	6.14	117.64	111.07
1	G	3153	ASP	N-CA-C	-6.14	97.37	109.10
1	G	3184	GLU	N-CA-C	6.14	123.88	110.80
1	C	1370	ASN	N-CA-C	-6.14	104.86	112.90
1	F	2540	GLU	N-CA-C	6.14	118.44	110.40
1	H	3686	LEU	N-CA-C	-6.14	105.05	112.54
1	D	1626	VAL	N-CA-C	6.13	122.09	109.34
1	B	733	ALA	N-CA-C	6.11	123.82	110.80
1	E	2301	ASP	N-CA-C	6.11	117.61	111.07
1	D	1664	ARG	N-CA-C	-6.11	104.89	112.90
1	G	3011	MET	N-CA-C	6.10	119.59	109.46
1	E	2126	VAL	N-CA-C	6.10	122.03	109.34
1	H	3623	PRO	CA-N-CD	-6.10	103.46	112.00
1	F	2590	THR	N-CA-C	-6.10	96.34	109.81
1	E	2007	ARG	N-CA-C	-6.09	97.82	110.80
1	A	126	VAL	N-CA-C	6.08	121.98	109.34
1	A	233	ALA	N-CA-C	6.04	123.67	110.80
1	E	2222	ALA	CA-C-N	6.04	125.72	119.56
1	E	2222	ALA	C-N-CA	6.04	125.72	119.56
1	C	1027	ARG	N-CA-C	-6.03	104.63	111.14
1	A	47	GLU	N-CA-C	6.02	119.72	112.38
1	B	562	THR	N-CA-C	6.01	120.48	112.30
1	E	2009	GLN	N-CA-C	-6.01	104.65	111.14
1	H	3647	GLU	N-CA-C	-6.01	104.85	111.82
1	E	2143	GLU	N-CA-C	6.00	119.69	110.20
1	E	2352	THR	N-CA-C	6.00	118.32	111.11
1	G	3126	VAL	N-CA-C	6.00	121.83	109.34
1	H	3688	ALA	N-CA-C	6.00	118.31	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	687	GLU	N-CA-C	-5.99	104.44	110.97
1	E	2300	ARG	N-CA-C	-5.99	103.92	111.11
1	C	1355	ALA	N-CA-C	-5.99	104.58	112.24
1	D	1733	ALA	N-CA-C	5.97	123.51	110.80
1	A	122	SER	N-CA-C	5.97	118.95	110.24
1	E	2313	LYS	N-CA-C	5.97	119.36	109.46
1	G	3103	ALA	N-CA-C	-5.97	104.41	111.03
1	A	318	SER	N-CA-C	-5.96	106.34	113.97
1	A	150	PHE	N-CA-C	5.96	119.87	112.24
1	E	2336	ARG	N-CA-C	-5.96	104.72	112.23
1	E	2040	GLU	N-CA-C	5.94	118.11	110.39
1	F	2633	ARG	N-CA-C	5.93	117.75	111.28
1	D	1791	MET	N-CA-C	-5.93	98.17	110.80
1	A	328	SER	N-CA-C	5.93	122.91	109.81
1	G	3328	SER	N-CA-C	5.93	121.59	113.77
1	C	1222	ALA	CA-C-N	5.92	125.60	119.56
1	C	1222	ALA	C-N-CA	5.92	125.60	119.56
1	F	2733	ALA	N-CA-C	5.92	123.41	110.80
1	E	2226	THR	N-CA-C	5.92	119.55	110.20
1	F	2677	THR	N-CA-C	5.92	120.22	112.89
1	E	2304	LEU	N-CA-C	5.91	119.32	111.75
1	C	1209	LEU	N-CA-C	-5.91	97.54	108.24
1	H	3510	ALA	N-CA-C	5.91	120.02	112.34
1	G	3131	MET	N-CA-C	5.90	119.67	112.23
1	B	722	ALA	CA-C-N	5.90	125.58	119.56
1	B	722	ALA	C-N-CA	5.90	125.58	119.56
1	D	1840	ARG	N-CA-C	-5.89	104.86	111.28
1	G	3045	THR	CA-C-N	5.89	125.90	119.89
1	G	3045	THR	C-N-CA	5.89	125.90	119.89
1	C	1181	TYR	CA-C-N	5.89	125.84	119.78
1	C	1181	TYR	C-N-CA	5.89	125.84	119.78
1	F	2603	ALA	N-CA-C	-5.88	103.65	111.24
1	F	2842	LEU	N-CA-C	-5.88	104.99	111.82
1	F	2863	SER	N-CA-C	5.88	119.55	107.37
1	A	334	GLU	N-CA-C	5.88	120.07	113.02
1	D	1722	ALA	CA-C-N	5.88	125.74	119.28
1	D	1722	ALA	C-N-CA	5.88	125.74	119.28
1	H	3517	VAL	CA-CB-CG2	-5.87	100.41	110.40
1	G	3269	THR	N-CA-C	5.87	118.16	111.11
1	C	1121	LEU	N-CA-C	5.87	118.28	108.96
1	D	1613	ASP	N-CA-C	-5.87	101.13	110.10
1	F	2561	LYS	N-CA-C	-5.86	100.83	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1644	THR	N-CA-C	-5.86	97.66	107.80
1	B	849	VAL	CA-C-N	5.86	125.80	119.76
1	B	849	VAL	C-N-CA	5.86	125.80	119.76
1	F	2626	VAL	N-CA-C	5.86	121.53	109.34
1	F	2722	ALA	CA-C-N	5.86	125.53	119.56
1	F	2722	ALA	C-N-CA	5.86	125.53	119.56
1	F	2562	THR	N-CA-C	5.85	120.26	112.30
1	H	3709	LEU	N-CA-C	-5.85	97.65	108.24
1	F	2613	ASP	N-CA-C	-5.85	101.61	110.50
1	B	704	GLU	N-CA-C	5.84	117.34	110.97
1	E	2062	THR	N-CA-C	5.84	120.24	112.30
1	G	3061	LYS	N-CA-C	-5.84	102.57	110.68
1	B	531	VAL	N-CA-C	5.82	121.44	109.34
1	H	3533	LEU	N-CA-C	-5.81	101.32	109.69
1	H	3733	ALA	N-CA-C	5.81	123.17	110.80
1	A	222	ALA	CA-C-N	5.81	125.48	119.56
1	A	222	ALA	C-N-CA	5.81	125.48	119.56
1	A	24	LEU	N-CA-C	5.80	123.16	110.80
1	H	3540	GLU	N-CA-C	5.78	117.91	110.39
1	H	3677	THR	N-CA-C	5.78	120.06	112.89
1	G	3318	SER	N-CA-C	-5.78	106.86	114.31
1	B	593	GLU	N-CA-C	-5.78	106.85	112.97
1	E	2363	SER	N-CA-C	5.77	119.96	107.49
1	G	3233	ALA	N-CA-C	5.77	123.09	110.80
1	A	67	PRO	CA-N-CD	-5.76	103.94	112.00
1	G	3040	GLU	CA-C-N	5.76	125.52	119.76
1	G	3040	GLU	C-N-CA	5.76	125.52	119.76
1	C	1012	LYS	N-CA-C	5.75	117.31	110.07
1	G	3366	THR	N-CA-C	-5.75	101.15	109.31
1	B	561	LYS	N-CA-C	-5.74	101.00	109.62
1	D	1668	LEU	N-CA-C	-5.74	99.66	109.24
1	F	2828	SER	N-CA-C	5.74	122.49	109.81
1	G	3313	LYS	N-CA-C	5.73	119.16	109.76
1	A	10	ALA	N-CA-C	5.73	119.37	112.38
1	G	3222	ALA	CA-C-N	5.73	125.58	119.28
1	G	3222	ALA	C-N-CA	5.73	125.58	119.28
1	C	1012	LYS	CA-C-N	5.72	126.52	120.11
1	C	1012	LYS	C-N-CA	5.72	126.52	120.11
1	D	1684	GLU	N-CA-C	5.72	119.99	113.19
1	E	2344	ALA	N-CA-C	-5.70	106.22	112.72
1	E	2175	ASN	N-CA-C	-5.70	90.51	107.37
1	A	151	VAL	CA-C-N	5.69	125.70	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	VAL	C-N-CA	5.69	125.70	119.89
1	A	90	THR	N-CA-C	-5.69	101.70	110.58
1	H	3593	GLU	N-CA-C	-5.69	106.14	112.57
1	G	3321	PHE	N-CA-C	5.67	117.31	109.54
1	E	2153	ASP	N-CA-C	-5.67	98.28	109.10
1	A	177	THR	N-CA-C	5.66	119.91	112.89
1	H	3517	VAL	CG1-CB-CG2	-5.66	98.36	110.80
1	A	61	LYS	N-CA-C	-5.65	101.14	109.62
1	C	1261	ARG	CD-NE-CZ	-5.65	116.50	124.40
1	B	648	GLU	N-CA-C	-5.64	104.58	112.25
1	D	1511	MET	N-CA-C	5.64	119.43	109.96
1	D	1677	THR	N-CA-C	5.64	119.88	112.89
1	G	3209	LEU	N-CA-C	-5.63	98.05	108.24
1	F	2535	ALA	N-CA-C	5.63	118.78	107.41
1	B	511	MET	N-CA-C	5.62	119.08	110.20
1	C	1011	MET	N-CA-C	5.62	119.08	110.20
1	C	1251	GLU	N-CA-C	5.61	118.17	111.71
1	F	2510	ALA	N-CA-C	5.61	119.23	112.38
1	H	3562	THR	N-CA-C	5.61	119.94	112.30
1	F	2664	ARG	N-CA-C	-5.61	105.55	112.90
1	C	1062	THR	N-CA-C	5.60	119.92	112.30
1	E	2233	ALA	N-CA-C	5.60	122.73	110.80
1	C	1177	THR	N-CA-C	5.60	120.11	113.28
1	B	664	ARG	N-CA-C	-5.60	104.67	112.45
1	A	16	VAL	N-CA-C	5.60	120.24	112.35
1	D	1863	SER	N-CA-C	5.59	118.23	107.44
1	C	1354	PHE	N-CA-C	-5.59	105.23	113.61
1	H	3849	VAL	CA-C-N	5.59	125.86	119.83
1	H	3849	VAL	C-N-CA	5.59	125.86	119.83
1	E	2370	ASN	N-CA-C	-5.57	106.61	113.41
1	F	2821	PHE	N-CA-C	5.56	119.25	111.30
1	H	3834	GLU	N-CA-C	5.56	119.69	113.02
1	B	772	GLN	N-CA-C	-5.55	104.86	111.03
1	E	2243	ILE	N-CA-C	5.55	116.78	107.18
1	G	3369	GLU	N-CA-C	5.54	117.40	111.36
1	E	2349	VAL	CA-C-N	5.54	125.81	119.83
1	E	2349	VAL	C-N-CA	5.54	125.81	119.83
1	E	2168	LEU	N-CA-C	-5.53	100.00	109.24
1	H	3584	GLU	N-CA-C	5.53	119.28	112.54
1	A	278	ALA	N-CA-C	-5.53	105.35	111.71
1	B	727	LEU	N-CA-C	-5.53	98.24	107.80
1	D	1688	ALA	N-CA-C	5.53	117.74	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	855	ALA	N-CA-C	-5.53	104.52	111.92
1	G	3349	VAL	CA-C-N	5.53	125.80	119.83
1	G	3349	VAL	C-N-CA	5.53	125.80	119.83
1	G	3376	GLU	N-CA-C	-5.53	104.66	111.40
1	H	3574	ARG	N-CA-C	-5.53	104.95	110.97
1	H	3828	SER	N-CA-C	5.52	121.06	113.77
1	B	677	THR	N-CA-C	5.52	119.18	112.23
1	C	1188	ALA	N-CA-C	5.51	117.72	111.11
1	D	1860	VAL	N-CA-C	-5.51	101.08	108.35
1	F	2818	SER	N-CA-C	-5.49	106.95	113.97
1	A	62	THR	N-CA-C	5.48	119.76	112.30
1	C	1349	VAL	CA-C-N	5.48	125.75	119.83
1	C	1349	VAL	C-N-CA	5.48	125.75	119.83
1	A	349	VAL	CA-C-N	5.47	125.73	119.83
1	A	349	VAL	C-N-CA	5.47	125.73	119.83
1	G	3027	ARG	N-CA-C	-5.46	105.02	110.97
1	H	3722	ALA	CA-C-N	5.46	125.13	119.56
1	H	3722	ALA	C-N-CA	5.46	125.13	119.56
1	D	1857	PHE	N-CA-C	5.46	118.23	110.10
1	B	547	GLU	N-CA-C	5.46	119.03	112.38
1	D	1800	ARG	N-CA-C	-5.45	105.24	111.07
1	A	32	ASP	N-CA-C	-5.42	100.46	109.46
1	B	601	SER	N-CA-C	-5.42	105.01	111.03
1	B	603	ALA	N-CA-C	-5.41	105.03	111.03
1	F	2557	LEU	N-CA-C	-5.41	105.29	111.07
1	D	1855	ALA	N-CA-C	-5.40	105.33	112.24
1	A	321	PHE	N-CA-C	5.40	119.02	111.30
1	G	3187	GLU	N-CA-C	-5.39	105.30	111.07
1	A	207	GLU	N-CA-C	5.39	117.86	111.33
1	D	1849	VAL	CA-C-N	5.39	125.65	119.83
1	D	1849	VAL	C-N-CA	5.39	125.65	119.83
1	H	3867	SER	N-CA-C	5.39	117.64	110.53
1	H	3597	THR	N-CA-C	5.38	117.77	110.35
1	G	3087	LEU	N-CA-C	-5.37	101.71	110.20
1	G	3264	THR	N-CA-C	5.37	120.10	113.50
1	F	2849	VAL	CA-C-N	5.35	125.61	119.83
1	F	2849	VAL	C-N-CA	5.35	125.61	119.83
1	H	3871	LEU	N-CA-C	-5.35	105.61	111.82
1	B	834	GLU	N-CA-C	5.35	119.80	113.16
1	E	2061	LYS	N-CA-C	-5.35	101.59	109.62
1	F	2525	GLU	N-CA-C	-5.34	99.42	110.80
1	G	3124	TYR	N-CA-C	5.34	117.94	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLU	N-CA-C	-5.34	105.15	110.97
1	A	371	LEU	N-CA-C	-5.34	105.50	112.23
1	C	1334	GLU	N-CA-C	5.33	119.65	113.20
1	D	1653	ASP	CA-C-N	5.33	124.79	119.24
1	D	1653	ASP	C-N-CA	5.33	124.79	119.24
1	B	675	ASN	N-CA-C	5.33	121.58	109.81
1	H	3613	ASP	N-CA-C	-5.33	102.10	110.14
1	F	2834	GLU	N-CA-C	5.32	119.47	112.92
1	G	3175	ASN	N-CA-C	-5.31	91.65	107.37
1	A	40	GLU	N-CA-C	5.30	117.28	110.39
1	D	1507	ARG	N-CA-C	5.30	117.74	111.33
1	C	1313	LYS	N-CA-C	5.30	117.87	109.24
1	F	2504	LEU	N-CA-C	5.28	117.68	110.55
1	E	2238	MET	N-CA-C	5.28	119.43	112.25
1	C	1174	ASN	N-CA-C	5.28	117.88	109.96
1	G	3373	LYS	N-CA-C	-5.27	104.97	111.40
1	C	1133	ARG	N-CA-C	5.27	117.02	111.28
1	B	818	SER	N-CA-C	-5.27	107.23	113.97
1	C	1357	PHE	N-CA-C	5.26	122.01	110.80
1	H	3532	ASP	N-CA-C	-5.26	101.13	109.76
1	H	3671	ASN	N-CA-C	5.26	116.01	107.23
1	D	1506	ARG	N-CA-C	-5.25	105.56	111.28
1	F	2877	ARG	N-CA-C	5.25	118.79	112.38
1	A	354	PHE	N-CA-C	-5.25	106.27	113.30
1	A	283	GLU	N-CA-C	5.24	121.96	110.80
1	G	3009	GLN	N-CA-C	-5.24	105.65	111.36
1	C	1361	ARG	N-CA-C	5.24	117.28	108.96
1	C	1010	ALA	N-CA-C	5.23	118.77	112.38
1	E	2113	ASP	CA-C-N	5.23	126.38	119.84
1	E	2113	ASP	C-N-CA	5.23	126.38	119.84
1	F	2769	THR	N-CA-C	5.23	120.00	111.37
1	C	1344	ALA	N-CA-C	-5.22	107.08	112.93
1	A	355	ALA	N-CA-C	-5.22	105.56	112.24
1	C	1004	LEU	N-CA-C	5.22	117.26	110.53
1	E	2031	VAL	N-CA-C	5.21	120.18	109.34
1	C	1321	PHE	N-CA-C	5.21	116.69	110.44
1	H	3863	SER	N-CA-C	5.20	117.48	107.44
1	B	856	ALA	N-CA-C	-5.20	97.83	107.71
1	C	1045	THR	CA-C-N	5.19	126.32	119.84
1	C	1045	THR	C-N-CA	5.19	126.32	119.84
1	H	3624	TYR	N-CA-C	5.18	118.51	110.17
1	D	1621	LEU	N-CA-C	5.18	117.17	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3287	ALA	N-CA-C	5.17	117.00	111.36
1	H	3544	ASP	N-CA-C	-5.17	102.10	110.32
1	A	107	LEU	N-CA-C	-5.16	105.31	111.03
1	C	1077	LEU	N-CA-C	-5.16	105.31	111.03
1	C	1092	GLU	N-CA-C	5.16	119.28	113.15
1	D	1582	ARG	N-CA-C	-5.15	103.05	111.04
1	D	1593	GLU	N-CA-C	-5.13	105.28	112.25
1	G	3079	GLU	N-CA-C	5.13	116.72	111.03
1	A	144	THR	N-CA-C	-5.12	98.90	108.02
1	F	2655	GLU	N-CA-C	5.12	117.60	111.71
1	A	242	ARG	N-CA-C	5.12	118.19	111.28
1	G	3010	ALA	N-CA-C	5.12	118.62	112.38
1	C	1302	LEU	N-CA-C	-5.11	107.01	113.20
1	E	2324	LEU	N-CA-C	-5.11	100.84	108.96
1	A	35	ALA	N-CA-C	5.10	118.50	107.49
1	A	124	TYR	N-CA-C	5.10	117.56	109.50
1	C	1328	SER	N-CA-C	5.10	121.08	109.81
1	D	1804	LEU	N-CA-C	5.09	117.22	111.11
1	F	2684	GLU	N-CA-C	5.08	119.20	113.15
1	A	184	GLU	N-CA-C	5.08	120.38	113.37
1	F	2687	GLU	N-CA-C	-5.08	105.44	110.97
1	F	2692	LEU	N-CA-C	-5.08	105.83	111.36
1	A	153	ASP	CA-C-N	5.07	124.52	119.24
1	A	153	ASP	C-N-CA	5.07	124.52	119.24
1	F	2807	LEU	N-CA-C	-5.07	105.67	111.14
1	G	3164	ARG	N-CA-C	-5.07	106.26	112.90
1	B	815	VAL	N-CA-C	5.06	115.62	107.73
1	H	3802	LEU	N-CA-C	-5.06	105.46	110.97
1	A	344	ALA	N-CA-C	-5.04	106.87	112.57
1	B	621	LEU	N-CA-C	5.04	117.46	109.24
1	G	3334	GLU	N-CA-C	5.04	119.52	113.17
1	C	1318	SER	N-CA-C	-5.03	107.82	114.31
1	C	1376	GLU	N-CA-C	-5.03	105.71	111.14
1	D	1516	VAL	N-CA-C	5.02	118.17	111.44
1	D	1590	THR	N-CA-C	-5.02	98.72	109.81
1	A	297	ARG	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ARG	Sidechain

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Mol	Chain	Res	Type	Group
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	168	0
1	B	2948	0	2962	210	0
1	C	2948	0	2962	192	0
1	D	2948	0	2962	176	0
1	E	2948	0	2962	200	0
1	F	2948	0	2962	147	0
1	G	2948	0	2962	184	0
1	H	2948	0	2962	184	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	1	0
3	B	15	0	7	3	0
3	C	15	0	6	5	0
3	D	15	0	6	1	0
3	E	15	0	7	1	0
3	F	15	0	7	0	0
3	G	15	0	6	1	0
3	H	15	0	6	1	0
All	All	23824	0	23822	1381	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 29.

All (1381) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2293:ARG:HH11	1:E:2293:ARG:HB2	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:A:312:LEU:HD22	1:A:325:MET:SD	2.18	0.84
1:H:3611:ILE:HG13	1:H:3612:LEU:H	1.42	0.84
2:C:1414:TRP:CZ3	1:D:1564:TYR:CB	2.61	0.83
1:F:2611:ILE:HG13	1:F:2612:LEU:H	1.43	0.83
1:G:3111:ILE:HG13	1:G:3112: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:D:1611:ILE:HG13	1:D:1612:LEU:H	1.43	0.81
1:E:2064:TYR:CG	2:E:2914:TRP:CZ3	2.68	0.81
1:C:1111:ILE:HG13	1:C:1112:LEU:H	1.44	0.81
1:C:1025:GLU:O	1:C:1026:LEU:HG	1.81	0.81
1:A:248:GLY:N	1:A:253:ILE:HD11	1.96	0.81
1:A:67:PRO:HG3	1:A:261:ARG:NH1	1.95	0.80
1:F:2802:LEU:HD21	1:F:2872:ARG:NH1	1.96	0.80
1:C:1067:PRO:HB3	1:C:1261:ARG:CD	2.12	0.80
1:H:3674:ASN:HD22	1:H:3675:ASN:N	1.79	0.80
1:A:25:GLU:O	1:A:26:LEU:HG	1.81	0.80
1:D:1522:LYS:O	1:D:1526:LEU:HD12	1.82	0.80
1:G:3016:VAL:HG21	2:G:3414:TRP:CD1	2.17	0.79
1:A:22:LYS:O	1:A:26:LEU:HD12	1.82	0.79
1:A:67:PRO:HD3	1:A:261:ARG:NH2	1.98	0.79
1:B:758:SER:HA	1:B:761:ARG:HH11	1.46	0.79
1:D:1567:PRO:HB3	1:D:1761:ARG:CG	2.14	0.78
1:D:1831:ALA:HB3	1:D:1837:ALA:HB2	1.65	0.78
1:G:3261:ARG:CZ	1:H:3517:VAL:CG2	2.60	0.78
1:D:1628:TYR:O	1:D:1632:VAL:HG23	1.84	0.78
1:C:1097:THR:HB	1:C:1102:GLN:HG2	1.66	0.78
1:D:1524:LEU:O	1:D:1525:GLU:HG3	1.84	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:708:HIS:O	1:B:793:ARG:HD3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:SER:HA	1:B:761:ARG:HD2	1.66	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:G:3331:ALA:HB3	1:G:3337:ALA:HB2	1.67	0.76
1:H:3597:THR:HB	1:H:3602:GLN:HG2	1.68	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:E:2025:GLU:O	1:E:2027:ARG:N	2.20	0.74
1:H:3622:SER:OG	1:H:3643:GLU:HA	1.86	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:D:1812:LEU:HD22	1:D:1825:MET:SD	2.27	0.74
1:G:3261:ARG:NH2	1:H:3517:VAL:HG23	2.02	0.74
1:H:3622:SER:OG	1:H:3623:PRO:HD2	1.87	0.74
1:C:1145:LEU:HB2	1:C:1148:GLU:HG2	1.68	0.73
1:E:2045:THR:HG21	1:E:2241:TRP:HE1	1.53	0.73
1:A:331:ALA:HB3	1:A:337:ALA:HB2	1.70	0.73
1:E:2023:ALA:O	1:E:2025:GLU:O	2.06	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:A:23:ALA:HB1	1:A:27:ARG:HH21	1.54	0.73
1:G:3067:PRO:HD3	1:G:3261:ARG:CZ	2.18	0.73
1:A:45:THR:HG21	1:A:241:TRP:HE1	1.52	0.73
1:A:108:PHE:O	1:A:112:LEU:HB2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1205:ILE:HD11	1:C:1234:LYS:HD3	1.71	0.72
1:F:2742:ARG:O	1:F:2743:ILE:HD12	1.88	0.72
1:G:3014:ASP:HB3	1:G:3017:VAL:HG22	1.69	0.72
1:G:3242:ARG:HH12	1:H:3564:TYR:HE2	1.37	0.72
1:C:1298:ARG:HB3	1:C:1298:ARG:NH1	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:C:1087:LEU:HD23	1:C:1247:CYS:SG	2.30	0.71
1:H:3674:ASN:HD22	1:H:3675:ASN:H	1.36	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:C:1107:LEU:HG	1:C:1256:MET:HE2	1.72	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:HB3	1:E:2082:ARG:NH1	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:C:1128:TYR:O	1:C:1132:VAL:HG23	1.91	0.70
1:D:1528:ARG:O	1:D:1529:GLN:HB2	1.91	0.70
1:F:2607:LEU:HG	1:F:2756:MET:HE2	1.71	0.70
1:E:2258:SER:HA	1:E:2261:ARG:CD	2.16	0.70
1:C:1344:ALA:O	1:C:1377:ARG:HD2	1.92	0.70
1:C:1265:THR:O	1:C:1266:SER:HB3	1.92	0.70
1:G:3017:VAL:HG11	1:H:3761:ARG:HD2	1.74	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:B:607:LEU:HG	1:B:756:MET:HE2	1.75	0.69
1:E:2293:ARG:HB2	1:E:2293:ARG:NH1	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2064:TYR:CD1	2:E:2914:TRP:CZ3	2.80	0.69
1:B:807:LEU:HD21	1:B:825:MET:SD	2.33	0.69
1:C:1069:GLY:HA3	1:C:1096:VAL:HG13	1.74	0.69
1:C:1155:GLU:O	1:C:1158:ARG:HB3	1.93	0.69
1:C:1181:TYR:HB2	1:C:1186:LEU:HD21	1.72	0.69
1:E:2039:GLY:HA3	2:E:2414:TRP:CD1	2.27	0.69
1:F:2753:ILE:HG22	1:F:2753:ILE:O	1.92	0.69
1:G:3205:ILE:HG22	1:G:3206:TYR:CD2	2.27	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:E:2025:GLU:H	1:E:2028:ARG:H	1.41	0.68
1:G:3025:GLU:O	1:G:3029:GLN:HG2	1.93	0.68
1:G:3067:PRO:HG2	1:G:3068:ALA:N	2.09	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:B:803:LEU:HG	1:B:871:LEU:HD22	1.76	0.68
1:E:2191:ARG:HD2	1:H:3528:ARG:HH22	1.56	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:B:782:GLN:C	1:B:786:ARG:HD3	2.19	0.68
1:D:1717:SER:H	1:D:1720:ARG:HH11	1.42	0.68
1:A:1:MET:O	1:B:698:PHE:HA	1.94	0.67
1:G:3045:THR:HG21	1:G:3241:TRP:HE1	1.59	0.67
1:B:524:LEU:H	1:B:524:LEU:HD23	1.58	0.67
2:C:1414:TRP:CH2	1:D:1564:TYR:HB3	2.28	0.67
1:B:545:THR:HG21	1:B:741:TRP:HE1	1.60	0.67
1:G:3127:SER:O	1:G:3131:MET:HG2	1.94	0.67
1:A:371:LEU:O	1:A:375:LEU:HB2	1.95	0.67
1:C:1212:GLU:HG3	1:C:1316:ARG:HH22	1.58	0.67
1:C:1286:ARG:HG3	1:C:1286:ARG:HH11	1.59	0.67
1:C:1212:GLU:CG	1:C:1316:ARG:HH22	2.07	0.67
1:A:64:TYR:HB3	2:A:914:TRP:HH2	1.60	0.67
1:C:1005:SER:OG	1:C:1008:VAL:HB	1.94	0.67
1:H:3569:GLY:HA3	1:H:3596:VAL:CG1	2.25	0.67
1:G:3045:THR:HG22	1:G:3237:ALA:O	1.95	0.67
1:G:3242:ARG:NH1	1:H:3564:TYR:HE2	1.92	0.67
1:B:831:ALA:HB3	1:B:837:ALA:HB2	1.77	0.67
1:E:2026:LEU:HA	1:E:2031:VAL:HG13	1.77	0.67
1:A:261:ARG:NE	1:B:517:VAL:HG21	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2340:ARG:HE	1:E:2381:VAL:HG22	1.58	0.67
1:H:3752:VAL:HG22	1:H:3756:MET:HE3	1.77	0.67
1:C:1021:ALA:O	1:C:1024:LEU:HG	1.95	0.66
1:C:1234:LYS:H	1:C:1234:LYS:HD2	1.61	0.66
1:E:2069:GLY:HA3	1:E:2096:VAL:CG1	2.25	0.66
1:A:97:THR:HB	1:A:102:GLN:HG2	1.77	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: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:B:840:ARG:HH11	1:B:881:VAL:HG13	1.61	0.66
1:C:1085:ASN:HB3	1:C:1087:LEU:HD13	1.78	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:G:3107:LEU:HG	1:G:3256:MET:HE2	1.77	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:H:3608:PHE:HD2	1:H:3612:LEU:CD2	2.08	0.66
1:G:3017:VAL:HG21	1:H:3761:ARG:HH11	1.62	0.65
1:G:3067:PRO:HD3	1:G:3261:ARG:NH2	2.11	0.65
1:A:332:PRO:HB2	1:A:336:ARG:NH2	2.11	0.65
1:H:3587:LEU:HD23	1:H:3747:CYS:SG	2.36	0.65
1:B:655:GLU:O	1:B:658:ARG:HB3	1.96	0.65
1:B:758:SER:O	1:B:761:ARG:HG3	1.96	0.65
1:A:6:ARG:HH21	1:A:10:ALA:HB2	1.61	0.65
1:G:3024:LEU:HA	1:G:3027:ARG:HB3	1.77	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:D:1704:GLU:HG2	1:D:1715:HIS:CE1	2.32	0.65
1:F:2533:LEU:HD22	1:F:2533:LEU:H	1.60	0.65
1:H:3525:GLU:N	1:H:3528:ARG:HB3	2.11	0.65
1:F:2720:ARG:HG2	1:F:2720:ARG:HH11	1.61	0.65
1:G:3064:TYR:HE2	1:H:3742:ARG:NH1	1.94	0.65
1:F:2748:GLY:N	1:F:2753:ILE:HD11	2.11	0.65
1:G:3132:VAL:HG11	1:G:3139:VAL:HG22	1.77	0.65
1:C:1067:PRO:HG3	1:C:1261:ARG:CZ	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:2227:LEU:HD21	1:E:2256:MET:HE1	1.78	0.64
1:E:2289:VAL:HG12	1:E:2293:ARG:HH12	1.62	0.64
1:A:111:ILE:HG13	1:A:112:LEU:N	2.11	0.64
1:E:2204:GLU:HG2	1:E:2215:HIS:CE1	2.32	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: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:D:1569:GLY:HA3	1:D:1596:VAL:CG1	2.28	0.64
1:F:2646:PRO:HB3	1:F:2650:PHE:CZ	2.33	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:C:1212:GLU:CD	1:C:1316:ARG:HH22	2.05	0.63
1:A:24:LEU:O	1:A:25:GLU:HB3	1.97	0.63
1:A:69:GLY:HA3	1:A:96:VAL:CG1	2.29	0.63
1:F:2720:ARG:HH11	1:F:2720:ARG:CG	2.11	0.63
1:G:3330:ILE:HD11	1:G:3381:VAL:HG21	1.79	0.63
1:A:212:GLU:HG3	1:A:316:ARG:HH22	1.63	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:D:1752:VAL:HG22	1:D:1756:MET:HE3	1.79	0.63
1:A:156:ARG:HA	1:A:159:ARG:HG2	1.80	0.62
1:C:1017:VAL:CG1	1:D:1761:ARG:NH2	2.60	0.62
1:D:1611:ILE:HG13	1:D:1612:LEU:N	2.13	0.62
1:A:350:PRO:HA	1:A:360:VAL:HG23	1.81	0.62
1:D:1670:VAL:HG23	1:D:1681:TYR:HE1	1.63	0.62
1:C:1028:ARG:O	1:C:1029:GLN:HB2	1.99	0.62
1:H:3512:LYS:HG2	1:H:3513:PRO:CD	2.29	0.62
1:A:67:PRO:HB3	1:A:261:ARG:CG	2.18	0.62
1:B:608:PHE:O	1:B:612:LEU:HB2	1.99	0.62
1:D:1597:THR:HB	1:D:1602:GLN:HG2	1.82	0.62
1:G:3078:ALA:O	1:G:3082:ARG:HG3	2.00	0.62
1:G:3111:ILE:HG13	1:G:3112:LEU:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3628:TYR:O	1:H:3632:VAL:HG23	1.99	0.62
1:A:146:PRO:HB3	1:A:150:PHE:CZ	2.35	0.62
1:B:527:ARG:HA	1:B:531:VAL:O	2.00	0.62
1:G:3252:VAL:HG22	1:G:3256:MET:HE3	1.82	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:2008:VAL:O	1:E:2011:MET:HG2	2.00	0.61
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:C:1064:TYR:HB3	2:D:1914:TRP:CZ3	2.35	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:F:2674:ASN:CG	1:F:2677:THR:HG23	2.25	0.61
1:H:3545:THR:HG21	1:H:3741:TRP:NE1	2.10	0.61
1:D:1585:ASN:HB3	1:D:1587:LEU:HD13	1.81	0.61
1:G:3025:GLU:OE1	1:G:3025:GLU:HA	2.00	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:H:3753:ILE:O	1:H:3753:ILE:HG22	2.01	0.61
1:A:67:PRO:CG	1:A:261:ARG:NH1	2.63	0.61
1:F:2502:ARG:HH12	1:G:3082:ARG:HH22	1.48	0.61
1:F:2611:ILE:HG13	1:F:2612:LEU:N	2.14	0.61
1:A:87:LEU:HD23	1:A:247:CYS:SG	2.40	0.61
1:A:269:THR:HA	1:A:272:GLN:HG3	1.82	0.61
1:C:1234:LYS:HD2	1:C:1234:LYS:N	2.16	0.61
1:G:3265:THR:O	1:G:3266:SER:HB3	1.99	0.61
1:B:871:LEU:O	1:B:875:LEU:HB2	2.00	0.61
2:G:3414:TRP:HZ3	1:H:3564:TYR:CB	2.13	0.61
1:G:3300:ARG:O	1:G:3304:LEU:HD23	2.01	0.60
1:H:3611:ILE:HG13	1:H:3612:LEU:N	2.13	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:E:2108:PHE:HD2	1:E:2112:LEU:CD2	2.14	0.60
1:C:1022:LYS:HG3	1:C:1025:GLU:HG3	1.82	0.60
1:F:2524:LEU:H	1:F:2524:LEU:HD22	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:A:107:LEU:HG	1:A:256:MET:HE2	1.83	0.60
1:B:806:GLY:HA3	1:B:875:LEU:HD11	1.83	0.60
1:C:1064:TYR:CB	2:D:1914:TRP:CZ3	2.84	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:E:2127:SER:O	1:E:2131:MET:HG2	2.01	0.60
1:D:1508:VAL:O	1:D:1511:MET:HG2	2.02	0.60
1:E:2145:LEU:HD22	1:E:2156:ARG:NH2	2.15	0.60
1:F:2622:SER:HA	1:F:2623:PRO:C	2.26	0.60
1:G:3227:LEU:HD22	1:G:3256:MET:HE1	1.84	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:C:1350:PRO:HA	1:C:1360:VAL:HG23	1.84	0.59
1:E:2150:PHE:CE1	1:E:2315:VAL:HG21	2.37	0.59
1:H:3526:LEU:O	1:H:3531:VAL:HG22	2.02	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:B:622:SER:HA	1:B:623:PRO:C	2.28	0.59
1:B:717:SER:HB2	1:B:720:ARG:HH11	1.67	0.59
1:D:1871:LEU:O	1:D:1875:LEU:HB2	2.03	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:2027:ARG:HG3	1:E:2027:ARG:HH11	1.67	0.59
1:E:2248:GLY:H	1:E:2253:ILE:HD11	1.66	0.59
1:F:2761:ARG:HD3	1:F:2762:GLN:HE21	1.68	0.59
1:A:262:GLN:OE1	1:B:630:GLU:HB3	2.03	0.59
1:E:2111:ILE:HG13	1:E:2112:LEU:N	2.14	0.59
1:E:2156:ARG:HA	1:E:2159:ARG:HG2	1.83	0.59
1:A:25:GLU:O	1:A:25:GLU:HG2	2.03	0.59
1:B:533:LEU:H	1:B:533:LEU:HD22	1.68	0.59
1:D:1524:LEU:HA	1:D:1527:ARG:HB3	1.85	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: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:3607:LEU:HG	1:H:3756:MET:HE2	1.84	0.59
1:F:2830:ILE:HD11	1:F:2881:VAL:HG11	1.84	0.58
1:H:3868:GLU:O	1:H:3872:ARG:HG3	2.03	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:E:2145:LEU:HB2	1:E:2148:GLU:CG	2.33	0.58
1:E:2191:ARG:HH11	1:H:3528:ARG:NH2	2.01	0.58
1:D:1656:ARG:HA	1:D:1659:ARG:HG2	1.85	0.58
1:H:3684:GLU:CD	1:H:3684:GLU:H	2.09	0.58
1:C:1014:ASP:HB3	1:C:1017:VAL:HB	1.84	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:B:727:LEU:HD22	1:B:756:MET:HE1	1.84	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:E:2122:SER:HA	1:E:2123:PRO:C	2.28	0.58
1:F:2694:VAL:HG23	1:F:2725:HIS:CE1	2.39	0.58
1:C:1064:TYR:HB2	2:D:1914:TRP:CH2	2.38	0.58
1:C:1045:THR:HG21	1:C:1241:TRP:NE1	2.16	0.58
1:E:2264:THR:O	1:E:2265:THR:HB	2.03	0.58
1:G:3121:LEU:CD2	1:G:3152:PRO:HB3	2.34	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:F:2727:LEU:HD22	1:F:2756:MET:HE1	1.84	0.58
1:G:3067:PRO:HG2	1:G:3068:ALA:H	1.68	0.58
1:B:799:ARG:HG2	1:B:868:GLU:HG3	1.86	0.58
1:E:2145:LEU:HB2	1:E:2148:GLU:HG2	1.85	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: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:C:1340:ARG:NH2	1:C:1381:VAL:O	2.37	0.58
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:C:1205:ILE:HG23	1:C:1206:TYR:CD2	2.38	0.57
1:A:72:GLU:HB3	1:A:276:LEU:HD11	1.86	0.57
1:D:1748:GLY:H	1:D:1753:ILE:HD11	1.70	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:F:2712:GLU:CD	1:F:2816:ARG:HH12	2.11	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
1:A:283:GLU:OE1	1:A:286:ARG:NH1	2.38	0.57
2:C:1414:TRP:CZ3	1:D:1564:TYR:CG	2.92	0.57
1:F:2752:VAL:HG23	1:F:2756:MET:HE3	1.87	0.57
1:H:3525:GLU:O	1:H:3526:LEU:HG	2.05	0.57
1:A:67:PRO:CD	1:A:261:ARG:NH2	2.66	0.57
1:A:216:PHE:HE1	1:A:220:ARG:HH11	1.53	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:G:3303:LEU:HG	1:G:3371:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3749:PRO:HB2	1:H:3752:VAL:HG12	1.87	0.57
1:A:73:LEU:O	1:A:77:LEU:HB2	2.05	0.57
1:C:1312:LEU:HD11	1:C:1382:LEU:HD11	1.86	0.57
1:G:3378:PHE:O	1:G:3381:VAL:HG22	2.05	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:B:705:ILE:HG23	1:B:706:TYR:CD2	2.39	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:B:752:VAL:HG22	1:B:756:MET:HE3	1.87	0.57
1:H:3821:PHE:CD1	1:H:3865:ALA:HB2	2.39	0.57
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:1025:GLU:N	1:C:1028:ARG:H	2.03	0.56
1:C:1121:LEU:CD2	1:C:1152:PRO:HB3	2.34	0.56
1:E:2026:LEU:CA	1:E:2031:VAL:HG13	2.35	0.56
1:E:2128:TYR:O	1:E:2132:VAL:HG23	2.05	0.56
1:H:3525:GLU:H	1:H:3528:ARG:H	1.53	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:A:64:TYR:HE2	1:B:742:ARG:NH1	2.02	0.56
1:A:145:LEU:HB2	1:A:148:GLU:HG2	1.88	0.56
1:A:238:MET:HG2	1:A:241:TRP:CD1	2.40	0.56
1:C:1356:ALA:O	1:C:1359:HIS:HB2	2.05	0.56
1:E:2005:SER:HB3	1:F:2611:ILE:O	2.04	0.56
1:E:2064:TYR:CE1	2:E:2914:TRP:CE3	2.94	0.56
1:E:2198:PHE:HA	1:F:2501:MET:O	2.06	0.56
1:F:2803:LEU:HG	1:F:2871:LEU:HD22	1.87	0.56
1:G:3073:LEU:O	1:G:3077:LEU:HB2	2.05	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:H:3527:ARG:HA	1:H:3531:VAL:O	2.04	0.56
1:E:2184:GLU:HA	1:E:2187:GLU:HB2	1.88	0.56
1:F:2833:ASP:HB3	1:F:2836:ARG:NH2	2.19	0.56
1:B:674:ASN:CG	1:B:677:THR:HG23	2.29	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:B:546:PRO:HB2	1:B:549:VAL:CG1	2.35	0.56
1:B:799:ARG:HB3	1:B:871:LEU:CD1	2.35	0.56
1:D:1712:GLU:CG	1:D:1816:ARG:HH22	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2227:LEU:CD2	1:E:2256:MET:HE1	2.36	0.56
1:F:2825:MET:O	1:F:2859:HIS:HA	2.06	0.56
1:G:3006:ARG:HG3	1:G:3006:ARG:NH1	2.21	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: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:D:1539:GLY:HA3	2:D:1914:TRP:CA	2.35	0.56
1:H:3534:VAL:HG22	1:H:3873:LYS:HD2	1.88	0.56
1:H:3727:LEU:HD11	1:H:3752:VAL:HG21	1.88	0.56
1:B:797:ARG:O	1:B:800:ARG:HB3	2.06	0.56
1:E:2184:GLU:HA	1:E:2187:GLU:CB	2.36	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:D:1597:THR:HG21	1:D:1603:ALA:HA	1.88	0.55
1:G:3330:ILE:O	1:G:3340:ARG:HD3	2.06	0.55
1:H:3674:ASN:CG	1:H:3677:THR:HG23	2.32	0.55
1:A:303:LEU:O	1:A:307:LEU:HB2	2.06	0.55
1:E:2303:LEU:HD22	1:E:2307:LEU:CD1	2.36	0.55
1:F:2810:LEU:HD22	1:F:2882:LEU:HD12	1.87	0.55
1:H:3685:VAL:O	1:H:3689:LEU:HG	2.07	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:2064:TYR:HE2	1:F:2742:ARG:NH1	2.04	0.55
1:E:2310:LEU:HD11	1:E:2379:ALA:HB2	1.87	0.55
1:H:3803:LEU:HD13	1:H:3871:LEU:HD22	1.88	0.55
1:A:64:TYR:HB3	2:A:914:TRP:CH2	2.41	0.55
1:B:685:VAL:O	1:B:689:LEU:HG	2.07	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:C:1206:TYR:HE2	3:C:1413:PLP:H2A3	1.70	0.55
1:D:1764:THR:O	1:D:1765:THR:HB	2.06	0.55
1:E:2330:ILE:HG13	1:E:2382:LEU:HD21	1.87	0.55
1:G:3022:LYS:HD2	1:G:3022:LYS:O	2.05	0.55
1:H:3645:LEU:HB3	1:H:3647:GLU:OE2	2.06	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:A:169:VAL:HG22	1:A:201:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1331:ALA:HB3	1:C:1337:ALA:HB2	1.88	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:39:GLY:HA3	2:A:414:TRP:HA	1.88	0.55
1:A:321:PHE:HA	1:A:364:TYR:CZ	2.41	0.55
1:C:1069:GLY:HA3	1:C:1096:VAL:CG1	2.37	0.55
1:D:1823:VAL:HG23	1:D:1864:TYR:HE2	1.71	0.55
1:E:2129:PRO:O	1:E:2133:ARG:HD2	2.06	0.55
1:H:3572:GLU:HB3	1:H:3776:LEU:HD11	1.88	0.55
1:B:650:PHE:HE1	1:B:815:VAL:HG21	1.71	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:717:SER:CB	1:B:720:ARG:NH1	2.70	0.55
1:H:3748:GLY:N	1:H:3753:ILE:CD1	2.66	0.55
1:D:1523:ALA:O	1:D:1526:LEU:HB2	2.07	0.54
1:G:3064:TYR:HE2	1:H:3742:ARG:HH12	1.56	0.54
1:A:127:SER:O	1:A:131:MET:HG2	2.06	0.54
1:H:3812:LEU:HD13	1:H:3825:MET:SD	2.47	0.54
1:A:28:ARG:HD2	1:A:28:ARG:O	2.07	0.54
1:A:121:LEU:CD2	1:A:152:PRO:HB3	2.37	0.54
1:C:1205:ILE:HD11	1:C:1234:LYS:CD	2.36	0.54
1:H:3526:LEU:C	1:H:3531:VAL:HG22	2.33	0.54
1:H:3868:GLU:HG3	1:H:3872:ARG:HE	1.73	0.54
1:B:585:ASN:HB3	1:B:587:LEU:CD1	2.38	0.54
1:C:1150:PHE:CE1	1:C:1315:VAL:HG21	2.42	0.54
1:D:1704:GLU:O	1:D:1706:TYR:N	2.41	0.54
1:F:2812:LEU:HD11	1:F:2882:LEU:HD11	1.89	0.54
1:G:3323:VAL:HG23	1:G:3364:TYR:HE2	1.73	0.54
1:A:126:VAL:HG23	1:A:354:PHE:CE2	2.42	0.54
1:C:1107:LEU:HD21	1:C:1227:LEU:HD13	1.90	0.54
1:D:1850:PRO:HA	1:D:1860:VAL:HG23	1.89	0.54
1:G:3286:ARG:HH11	1:G:3286:ARG:CG	2.20	0.54
1:H:3622:SER:O	1:H:3623:PRO:C	2.51	0.54
1:B:534:VAL:O	1:B:846:VAL:HA	2.07	0.54
1:C:1108:PHE:HB3	1:C:1112:LEU:HD23	1.89	0.54
1:D:1638:VAL:HG21	1:D:1664:ARG:NH2	2.22	0.54
1:E:2064:TYR:CE1	2:E:2914:TRP:HE3	2.26	0.54
1:H:3747:CYS:C	1:H:3753:ILE:HD11	2.33	0.54
1:D:1536:LEU:CD1	1:D:1866:THR:HG21	2.34	0.54
1:A:286:ARG:O	1:A:290:GLU:HG2	2.08	0.54
1:C:1298:ARG:HB3	1:C:1298:ARG:HH11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1371:LEU:O	1:C:1375:LEU:HB2	2.07	0.54
1:D:1582:ARG:HA	1:D:1587:LEU:O	2.08	0.54
1:D:1821:PHE:HA	1:D:1864:TYR:CZ	2.43	0.54
1:B:684:GLU:HA	1:B:687:GLU:HB2	1.89	0.54
1:B:717:SER:CB	1:B:720:ARG:HH11	2.21	0.54
1:E:2048:HIS:CD2	1:E:2049:VAL:HG12	2.43	0.54
1:B:747:CYS:C	1:B:753:ILE:HD11	2.32	0.54
1:G:3132:VAL:HG13	1:G:3133:ARG:N	2.23	0.54
1:G:3253:ILE:O	1:G:3253:ILE:HG22	2.08	0.54
1:C:1108:PHE:O	1:C:1112:LEU:HB2	2.07	0.53
1:F:2761:ARG:HD2	1:F:2762:GLN:HG2	1.89	0.53
1:G:3204:GLU:O	1:G:3206:TYR:N	2.41	0.53
1:E:2242:ARG:HH22	3:E:2413:PLP:P	2.31	0.53
1:G:3064:TYR:CE2	1:H:3742:ARG:NH1	2.75	0.53
1:B:597:THR:HG21	1:B:603:ALA:HA	1.90	0.53
1:E:2014:ASP:HB3	1:E:2017:VAL:HB	1.89	0.53
1:F:2573:LEU:HD22	1:F:2577:LEU:HD22	1.90	0.53
1:G:3087:LEU:HD23	1:G:3247:CYS:SG	2.47	0.53
1:C:1064:TYR:HE2	1:D:1742:ARG:NH1	2.06	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:G:3005:SER:OG	1:G:3008:VAL:HB	2.08	0.53
1:A:212:GLU:CG	1:A:316:ARG:HH22	2.21	0.53
1:G:3264:THR:O	1:G:3265:THR:HB	2.08	0.53
1:B:567:PRO:CG	1:B:761:ARG:NH2	2.70	0.53
1:C:1323:VAL:HG23	1:C:1364:TYR:HE2	1.74	0.53
1:E:2026:LEU:HD23	1:E:2026:LEU:N	2.22	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:C:1024:LEU:O	1:C:1024:LEU:HD12	2.08	0.53
1:E:2033:LEU:H	1:E:2033:LEU:HD22	1.74	0.53
1:E:2064:TYR:HB3	2:E:2914:TRP:CZ3	2.43	0.53
1:E:2323:VAL:HG23	1:E:2364:TYR:HE2	1.72	0.53
1:F:2704:GLU:O	1:F:2706:TYR:N	2.42	0.53
1:G:3249:PRO:HB2	1:G:3252:VAL:HG12	1.91	0.53
1:H:3799:ARG:HB3	1:H:3871:LEU:CD1	2.38	0.53
1:H:3817:PRO:HG2	1:H:3823:VAL:HG22	1.91	0.53
1:H:3821:PHE:HA	1:H:3864:TYR:CZ	2.43	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:HH11	1:B:583:ARG:CG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:VAL:HG23	1:B:864:TYR:HE2	1.74	0.53
1:C:1299:ARG:HA	1:C:1302:LEU:HD23	1.91	0.53
1:E:2344:ALA:O	1:E:2377:ARG:HD2	2.09	0.53
1:F:2602:GLN:HG3	1:F:2602:GLN:O	2.08	0.53
1:H:3645:LEU:O	1:H:3648:GLU:HG2	2.09	0.53
1:B:704:GLU:O	1:B:706:TYR:N	2.42	0.53
1:B:782:GLN:HB3	1:B:786:ARG:CD	2.38	0.53
1:B:782:GLN:HB3	1:B:786:ARG:HD2	1.90	0.53
1:D:1525:GLU:HA	1:D:1528:ARG:HB3	1.89	0.53
1:E:2098:VAL:HG12	1:E:2098:VAL:O	2.08	0.53
1:F:2581:PHE:O	1:F:2585:ASN:HB2	2.09	0.53
1:F:2627:SER:O	1:F:2631:MET:HG2	2.08	0.53
1:H:3545:THR:CG2	1:H:3741:TRP:HE1	2.16	0.53
1:H:3646:PRO:HB3	1:H:3650:PHE:CZ	2.44	0.53
1:A:323:VAL:HG23	1:A:364:TYR:HE2	1.74	0.52
1:B:608:PHE:HD2	1:B:612:LEU:CD2	2.22	0.52
1:B:758:SER:HA	1:B:761:ARG:CG	2.39	0.52
1:C:1032:ASP:OD1	1:C:1032:ASP:C	2.52	0.52
1:E:2085:ASN:HB3	1:E:2087:LEU:CD1	2.39	0.52
1:F:2525:GLU:CA	1:F:2528:ARG:HB3	2.35	0.52
1:H:3523:ALA:O	1:H:3526:LEU:HB2	2.09	0.52
1:H:3551:GLU:HG2	1:H:3554:ARG:NH1	2.23	0.52
1:C:1296:TYR:O	1:C:1300:ARG:HB2	2.09	0.52
1:D:1622:SER:HA	1:D:1623:PRO:C	2.34	0.52
1:D:1717:SER:H	1:D:1720:ARG:NH1	2.07	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:H:3546:PRO:HB2	1:H:3549:VAL:HG23	1.91	0.52
1:H:3626:VAL:HG23	1:H:3854:PHE:CZ	2.45	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:D:1539:GLY:CA	2:D:1914:TRP:HA	2.39	0.52
1:A:128:TYR:N	1:A:129:PRO:HD2	2.24	0.52
1:G:3376:GLU:O	1:G:3379:ALA:HB3	2.08	0.52
1:H:3581:PHE:O	1:H:3585:ASN:HB2	2.10	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:2369:GLU:HG2	1:E:2369:GLU:O	2.10	0.52
1:A:174:ASN:CG	1:A:177:THR:HG23	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2026:LEU:H	1:E:2029:GLN:CD	2.17	0.52
1:E:2064:TYR:CE2	1:F:2742:ARG:NH1	2.78	0.52
1:E:2108:PHE:CD2	1:E:2112:LEU:CD2	2.92	0.52
1:F:2751:GLU:HG2	1:F:2752:VAL:N	2.24	0.52
1:C:1364:TYR:HA	1:C:1371:LEU:HD11	1.92	0.52
1:E:2026:LEU:HA	1:E:2031:VAL:CG1	2.40	0.52
1:H:3522:LYS:O	1:H:3526:LEU:HD12	2.09	0.52
1:C:1212:GLU:HG3	1:C:1316:ARG:NH2	2.25	0.52
1:E:2207:GLU:HG3	1:E:2208:HIS:N	2.25	0.52
1:E:2261:ARG:O	1:E:2265:THR:HA	2.09	0.52
1:E:2299:ARG:HB3	1:E:2371:LEU:CD1	2.39	0.52
1:F:2505:SER:OG	1:F:2508:VAL:HB	2.09	0.52
1:F:2572:GLU:HB3	1:F:2776:LEU:HD11	1.92	0.52
1:G:3303:LEU:HD22	1:G:3307:LEU:CD1	2.40	0.52
1:H:3506:ARG:O	1:H:3506:ARG:HG2	2.10	0.52
1:C:1073:LEU:O	1:C:1077:LEU:HB2	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:B:585:ASN:O	1:B:720:ARG:CZ	2.58	0.51
1:C:1264:THR:O	1:C:1265:THR:HB	2.10	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:B:669:VAL:HG22	1:B:701:VAL:HB	1.91	0.51
1:G:3040:GLU:HB3	1:G:3239:THR:HG21	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:B:675:ASN:ND2	3:B:913:PLP:O3	2.44	0.51
1:C:1072:GLU:CB	1:C:1276:LEU:HD11	2.40	0.51
1:E:2249:PRO:O	1:E:2253:ILE:HG13	2.10	0.51
1:C:1183:LYS:HG3	1:C:1216:PHE:CD1	2.46	0.51
1:B:684:GLU:H	1:B:684:GLU:CD	2.18	0.51
1:C:1064:TYR:HB3	2:D:1914:TRP:CH2	2.46	0.51
1:D:1519:VAL:HG11	1:D:1848:VAL:O	2.11	0.51
1:E:2064:TYR:CD1	2:E:2914:TRP:CE3	2.99	0.51
1:G:3158:ARG:HH12	1:G:3196:HIS:HE1	1.59	0.51
1:G:3344:ALA:O	1:G:3377:ARG:HD3	2.09	0.51
1:F:2582:ARG:HD2	1:F:2582:ARG:C	2.35	0.51
1:G:3171:ASN:ND2	1:G:3203:ASP:O	2.44	0.51
1:A:2:ARG:HH21	1:B:725:HIS:CE1	2.29	0.51
1:A:122:SER:HA	1:A:123:PRO:C	2.36	0.51
1:B:608:PHE:CD2	1:B:612:LEU:CD2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:GLU:O	1:B:843:GLU:HG3	2.10	0.51
1:E:2001:MET:HA	1:F:2697:ASP:O	2.10	0.51
1:F:2764:THR:O	1:F:2765:THR:HB	2.10	0.51
1:G:3026:LEU:HD12	1:G:3031:VAL:HG21	1.93	0.51
1:G:3303:LEU:HD22	1:G:3307:LEU:HD12	1.93	0.51
1:G:3345:GLY:HA3	1:G:3377:ARG:HH11	1.76	0.51
1:H:3506:ARG:HB3	1:H:3506:ARG:CZ	2.41	0.51
1:H:3516:VAL:HG21	2:H:3914:TRP:CD1	2.46	0.51
1:A:361:ARG:HH22	2:A:414:TRP:HD1	1.58	0.51
1:E:2376:GLU:O	1:E:2379:ALA:HB3	2.11	0.51
1:G:3069:GLY:HA3	1:G:3096:VAL:CG1	2.39	0.51
1:G:3299:ARG:NH1	1:G:3366:THR:O	2.44	0.51
1:A:85:ASN:HB3	1:A:87:LEU:HD13	1.93	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:H:3608:PHE:CD2	1:H:3612:LEU:CD2	2.92	0.50
1:A:183:LYS:HG3	1:A:216:PHE:CD1	2.46	0.50
1:D:1514:ASP:HB3	1:D:1517:VAL:CG1	2.40	0.50
1:G:3085:ASN:O	1:G:3220:ARG:NE	2.39	0.50
1:H:3764:THR:O	1:H:3765:THR:HB	2.11	0.50
1:A:265:THR:O	1:A:266:SER:HB2	2.11	0.50
1:B:520:ASN:O	1:B:524:LEU:HG	2.12	0.50
1:E:2046:PRO:CB	1:E:2048:HIS:CE1	2.94	0.50
1:E:2121:LEU:HD22	1:E:2152:PRO:HB3	1.93	0.50
1:G:3105:PHE:HA	1:G:3131:MET:HE2	1.92	0.50
1:G:3121:LEU:HD22	1:G:3152:PRO:HB3	1.92	0.50
1:H:3807:LEU:HD21	1:H:3825:MET:SD	2.50	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: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:E:2108:PHE:O	1:E:2112:LEU:HB2	2.12	0.50
1:E:2254:LYS:HA	1:E:2257:ALA:HB3	1.92	0.50
1:F:2574:ARG:NH2	1:F:2592:GLU:HA	2.26	0.50
1:F:2621:LEU:CD2	1:F:2652:PRO:HB3	2.42	0.50
1:G:3118:VAL:HG21	1:G:3132:VAL:HG23	1.93	0.50
1:G:3175:ASN:ND2	3:G:3413:PLP:O3	2.44	0.50
1:H:3709:LEU:HD22	1:H:3796:TYR:CE1	2.46	0.50
1:C:1122:SER:HB3	1:C:1124:TYR:CD2	2.47	0.50
1:D:1807:LEU:HD11	1:D:1862:LEU:CD1	2.41	0.50
1:G:3185:VAL:O	1:G:3189:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:2720:ARG:NH1	1:F:2720:ARG:HB3	2.27	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:C:1292:ALA:O	1:C:1295:ALA:HB3	2.12	0.50
1:E:2184:GLU:H	1:E:2184:GLU:CD	2.18	0.50
1:H:3567:PRO:HG3	1:H:3761:ARG:HD3	1.94	0.50
1:A:249:PRO:HB2	1:A:252:VAL:CG1	2.39	0.50
1:B:743:ILE:HD12	1:B:771:ALA:O	2.12	0.50
1:C:1184:GLU:CD	1:C:1184:GLU:H	2.20	0.50
1:F:2800:ARG:NH1	1:F:2817:PRO:O	2.45	0.50
1:D:1607:LEU:HG	1:D:1756:MET:HE2	1.94	0.50
1:E:2019:VAL:HG21	1:E:2349:VAL:HG22	1.94	0.50
1:E:2073:LEU:O	1:E:2077:LEU:HB2	2.12	0.50
1:F:2844:ALA:O	1:F:2877:ARG:HD2	2.12	0.50
1:G:3067:PRO:HG3	1:G:3261:ARG:CZ	2.37	0.50
1:A:356:ALA:O	1:A:359:HIS:HB2	2.11	0.49
1:B:783:GLU:N	1:B:786:ARG:HD3	2.27	0.49
1:B:840:ARG:O	1:B:843:GLU:HB2	2.12	0.49
1:D:1536:LEU:HD12	1:D:1866:THR:CG2	2.40	0.49
1:D:1670:VAL:HG23	1:D:1681:TYR:CE1	2.45	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:B:627:SER:O	1:B:631:MET:HG2	2.12	0.49
1:B:747:CYS:HA	1:B:753:ILE:CD1	2.41	0.49
1:D:1524:LEU:C	1:D:1525:GLU:HG3	2.37	0.49
1:G:3252:VAL:CG2	1:G:3256:MET:HE3	2.42	0.49
1:H:3570:ILE:HG13	1:H:3573:LEU:HB2	1.94	0.49
1:H:3585:ASN:O	1:H:3720:ARG:NE	2.44	0.49
1:H:3707:GLU:HG3	1:H:3708:HIS:N	2.28	0.49
1:B:617:GLU:OE1	1:B:664:ARG:NH1	2.45	0.49
1:B:705:ILE:HG23	1:B:706:TYR:N	2.27	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:G:3372:ARG:O	1:G:3376:GLU:HG3	2.11	0.49
1:H:3598:VAL:HG23	1:H:3602:GLN:OE1	2.12	0.49
1:C:1122:SER:HA	1:C:1123:PRO:C	2.37	0.49
1:C:1204:GLU:O	1:C:1206:TYR:N	2.45	0.49
1:G:3082:ARG:HG2	1:G:3087:LEU:O	2.11	0.49
1:A:64:TYR:CD2	2:A:914:TRP:CZ3	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:HG3	1:A:216:PHE:CG	2.47	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:B:546:PRO:HG3	1:B:788:PHE:CD1	2.46	0.49
1:C:1301:ASP:O	1:C:1305:GLU:HG3	2.13	0.49
1:E:2312:LEU:HD22	1:E:2325:MET:SD	2.52	0.49
1:H:3536:LEU:HB3	1:H:3863:SER:H	1.76	0.49
1:D:1711:TYR:HB2	1:D:1712:GLU:OE2	2.12	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:F:2582:ARG:HH11	1:F:2583:ARG:N	2.09	0.49
1:H:3821:PHE:CG	1:H:3865:ALA:HB2	2.47	0.49
1:A:292:ALA:O	1:A:295:ALA:HB3	2.12	0.49
1:C:1227:LEU:HD22	1:C:1256:MET:HE1	1.95	0.49
1:D:1582:ARG:HB3	1:D:1582:ARG:NH1	2.27	0.49
1:D:1687:GLU:HG3	1:D:1691:ARG:HH21	1.77	0.49
1:E:2001:MET:O	1:F:2698:PHE:HA	2.13	0.49
1:B:569:GLY:HA3	1:B:596:VAL:HG13	1.95	0.49
1:B:880:ARG:HH22	1:D:1843:GLU:HG3	1.77	0.49
1:E:2070:ILE:HG13	1:E:2073:LEU:HB2	1.95	0.49
1:E:2150:PHE:HE1	1:E:2315:VAL:HG21	1.77	0.49
1:F:2608:PHE:CD2	1:F:2612:LEU:CD2	2.95	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:H:3555:ARG:O	1:H:3559:GLN:HG3	2.12	0.49
1:D:1831:ALA:HB1	1:D:1832:PRO:HD2	1.95	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: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:H:3687:GLU:O	1:H:3691:ARG:HG3	2.13	0.49
1:A:175:ASN:ND2	3:A:413:PLP:O3	2.46	0.48
1:C:1029:GLN:HG2	1:C:1029:GLN:O	2.13	0.48
1:E:2025:GLU:O	1:E:2026:LEU:HG	2.12	0.48
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:B:782:GLN:HB3	1:B:786:ARG:NH2	2.28	0.48
1:D:1792:ALA:O	1:D:1795:ALA:HB3	2.13	0.48
1:F:2590:THR:HB	1:F:2591:PRO:HD2	1.95	0.48
1:C:1008:VAL:O	1:C:1011:MET:HG2	2.14	0.48
1:C:1321:PHE:HA	1:C:1364:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1799:ARG:HB3	1:D:1871:LEU:CD1	2.41	0.48
1:E:2041:PRO:HB3	1:E:2296:TYR:OH	2.13	0.48
1:E:2190:ALA:HB2	1:E:2218:PRO:HB3	1.95	0.48
1:E:2224:GLU:O	1:E:2224:GLU:HG2	2.13	0.48
1:F:2690:ALA:HB2	1:F:2718:PRO:HB3	1.95	0.48
1:G:3190:ALA:HB2	1:G:3218:PRO:HB3	1.95	0.48
1:H:3839:GLU:O	1:H:3843:GLU:HG2	2.14	0.48
1:A:102:GLN:O	1:A:102:GLN:HG3	2.14	0.48
1:B:567:PRO:CG	1:B:761:ARG:HH21	2.17	0.48
1:B:598:VAL:HG23	1:B:602:GLN:OE1	2.12	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:1803:LEU:HD12	1:D:1864:TYR:HD2	1.78	0.48
1:F:2545:THR:HA	1:F:2737:ALA:HB3	1.95	0.48
1:G:3129:PRO:O	1:G:3132:VAL:HG12	2.13	0.48
1:D:1821:PHE:CG	1:D:1865:ALA:HB2	2.49	0.48
1:E:2072:GLU:HB3	1:E:2276:LEU:HD11	1.96	0.48
1:F:2769:THR:HA	1:F:2772:GLN:HG3	1.94	0.48
1:G:3045:THR:HA	1:G:3237:ALA:HB3	1.94	0.48
1:H:3524:LEU:HG	1:H:3524:LEU:O	2.12	0.48
1:H:3528:ARG:O	1:H:3529:GLN:HB2	2.12	0.48
1:A:82:ARG:HG2	1:A:87:LEU:O	2.13	0.48
1:A:345:GLY:HA3	1:A:377:ARG:NH1	2.28	0.48
1:B:531:VAL:HA	1:D:1840:ARG:HH22	1.78	0.48
1:B:540:GLU:HB3	1:B:739:THR:HG21	1.96	0.48
1:B:570:ILE:HG13	1:B:573:LEU:HB2	1.94	0.48
1:B:690:ALA:HB2	1:B:718:PRO:HB3	1.95	0.48
1:D:1628:TYR:N	1:D:1629:PRO:HD2	2.29	0.48
1:G:3070:ILE:HG13	1:G:3073:LEU:HB2	1.95	0.48
1:G:3102:GLN:O	1:G:3102:GLN:HG3	2.12	0.48
1:H:3799:ARG:HB3	1:H:3871:LEU:HD11	1.95	0.48
1:C:1098:VAL:HG22	1:C:1267:PRO:HG3	1.96	0.48
1:C:1175:ASN:ND2	3:C:1413:PLP:O3	2.47	0.48
1:E:2087:LEU:CD2	1:E:2247:CYS:SG	3.02	0.48
1:E:2321:PHE:HA	1:E:2364:TYR:CZ	2.48	0.48
1:F:2546:PRO:HG3	1:F:2788:PHE:CG	2.48	0.48
1:F:2598:VAL:HG12	1:F:2598:VAL:O	2.12	0.48
1:F:2810:LEU:HD21	1:F:2879:ALA:HA	1.95	0.48
1:G:3085:ASN:HB3	1:G:3087:LEU:HD13	1.94	0.48
1:G:3097:THR:HB	1:G:3102:GLN:HG2	1.96	0.48
1:A:184:GLU:HA	1:A:187:GLU:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:LEU:O	1:B:577:LEU:HB2	2.14	0.48
1:D:1598:VAL:HG23	1:D:1602:GLN:OE1	2.13	0.48
1:D:1704:GLU:HG2	1:D:1715:HIS:NE2	2.29	0.48
1:E:2016:VAL:C	1:E:2018:ALA:N	2.71	0.48
1:G:3026:LEU:O	1:G:3031:VAL:HB	2.13	0.48
1:G:3067:PRO:CD	1:G:3261:ARG:NH1	2.76	0.48
1:B:806:GLY:CA	1:B:875:LEU:HD11	2.44	0.48
1:C:1024:LEU:O	1:C:1024:LEU:CD1	2.62	0.48
1:C:1064:TYR:CE2	1:D:1742:ARG:NH1	2.82	0.48
1:C:1186:LEU:HD12	1:C:1218:PRO:HG3	1.96	0.48
1:C:1367:SER:O	1:C:1371:LEU:HD22	2.14	0.48
1:G:3345:GLY:HA3	1:G:3377:ARG:NH1	2.29	0.48
1:B:525:GLU:HG2	1:B:529:GLN:HE21	1.79	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:C:1005:SER:HG	1:C:1008:VAL:HB	1.78	0.48
1:C:1190:ALA:HB2	1:C:1218:PRO:HB3	1.96	0.48
1:E:2303:LEU:HD22	1:E:2307:LEU:HD12	1.96	0.48
1:E:2330:ILE:HG22	1:E:2337:ALA:HB1	1.96	0.48
1:H:3574:ARG:NH2	1:H:3592:GLU:HA	2.29	0.48
1:C:1212:GLU:CD	1:C:1316:ARG:HH12	2.21	0.47
1:D:1690:ALA:HB2	1:D:1718:PRO:HB3	1.96	0.47
1:E:2261:ARG:HG3	1:E:2262:GLN:HG2	1.96	0.47
1:F:2607:LEU:HG	1:F:2756:MET:CE	2.43	0.47
1:G:3283:GLU:CD	1:G:3283:GLU:H	2.22	0.47
1:G:3371:LEU:O	1:G:3375:LEU:HG	2.14	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: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:A:27:ARG:HG2	1:A:27:ARG:O	2.14	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:G:3014:ASP:CB	1:G:3017:VAL:HG22	2.41	0.47
1:G:3312:LEU:HD22	1:G:3325:MET:SD	2.54	0.47
1:H:3551:GLU:HA	1:H:3554:ARG:HD2	1.96	0.47
1:H:3597:THR:HG21	1:H:3603:ALA:HA	1.97	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:D:1797:ARG:O	1:D:1800:ARG:HB3	2.15	0.47
1:E:2077:LEU:HD21	1:E:2245:TYR:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3687:GLU:HG2	1:H:3691:ARG:NH2	2.29	0.47
1:A:248:GLY:CA	1:A:253:ILE:HD11	2.45	0.47
1:B:541:PRO:HB3	1:B:796:TYR:OH	2.15	0.47
1:B:796:TYR:O	1:B:800:ARG:HB2	2.15	0.47
1:B:804:LEU:O	1:B:808:THR:HB	2.14	0.47
1:E:2027:ARG:HA	1:E:2031:VAL:O	2.14	0.47
1:E:2292:ALA:O	1:E:2295:ALA:HB3	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:G:3132:VAL:HG11	1:G:3139:VAL:CG2	2.44	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:190:ALA:HB2	1:A:218:PRO:HB3	1.96	0.47
1:B:645:LEU:O	1:B:648:GLU:HG3	2.15	0.47
1:C:1070:ILE:HG13	1:C:1073:LEU:HB2	1.96	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:E:2265:THR:O	1:E:2266:SER:HB2	2.13	0.47
1:F:2608:PHE:HB3	1:F:2612:LEU:HD23	1.97	0.47
1:A:300:ARG:NH1	1:A:317:PRO:O	2.48	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:G:3017:VAL:HG21	1:H:3761:ARG:NH1	2.28	0.47
1:G:3067:PRO:CB	1:G:3261:ARG:HD2	2.45	0.47
1:G:3325:MET:O	1:G:3359:HIS:HA	2.15	0.47
1:H:3831:ALA:HB1	1:H:3832:PRO:HD2	1.97	0.47
1:A:46:PRO:HB2	1:A:49:VAL:HG23	1.96	0.47
1:A:64:TYR:CG	2:A:914:TRP:CZ3	3.03	0.47
1:B:683:LYS:HZ3	1:B:687:GLU:CD	2.23	0.47
1:E:2328:SER:HB3	1:E:2329:PRO:HD3	1.97	0.47
1:G:3027:ARG:NH1	1:G:3028:ARG:HH11	2.12	0.47
1:G:3205:ILE:CG2	1:G:3206:TYR:CD2	2.96	0.47
1:G:3242:ARG:HG2	1:H:3768:ASP:HA	1.95	0.47
1:H:3825:MET:O	1:H:3859:HIS:HA	2.15	0.47
1:A:126:VAL:HG23	1:A:354:PHE:CZ	2.49	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:G:3158:ARG:NH1	1:G:3196:HIS:HE1	2.12	0.47
1:B:621:LEU:CD2	1:B:652:PRO:HB3	2.45	0.47
1:C:1206:TYR:CE2	3:C:1413:PLP:H2A3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1306:GLY:C	1:C:1375:LEU:HD21	2.39	0.47
1:D:1581:PHE:O	1:D:1585:ASN:HB2	2.14	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:E:2153:ASP:O	1:E:2157:VAL:HG23	2.15	0.47
1:H:3617:GLU:CD	1:H:3664:ARG:HG3	2.40	0.47
1:D:1545:THR:HG21	1:D:1741:TRP:NE1	2.19	0.46
1:E:2026:LEU:C	1:E:2031:VAL:HG13	2.41	0.46
1:E:2107:LEU:HG	1:E:2256:MET:HE2	1.96	0.46
1:F:2691:ARG:O	1:F:2694:VAL:HG12	2.15	0.46
1:F:2876:GLU:O	1:F:2879:ALA:HB3	2.15	0.46
1:G:3045:THR:HG21	1:G:3241:TRP:NE1	2.28	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:B:525:GLU:CG	1:B:529:GLN:HE21	2.27	0.46
1:B:782:GLN:CB	1:B:786:ARG:HD2	2.45	0.46
1:E:2064:TYR:CZ	2:E:2914:TRP:HE3	2.33	0.46
1:A:25:GLU:O	1:A:25:GLU:CG	2.63	0.46
1:B:519:VAL:HG11	1:B:849:VAL:HG22	1.96	0.46
1:B:843:GLU:C	1:B:845:GLY:H	2.23	0.46
1:C:1108:PHE:CD2	1:C:1112:LEU:CD2	2.97	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:2527:ARG:HE	1:F:2533:LEU:HD21	1.80	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:H:3742:ARG:HH22	3:H:3913:PLP:P	2.38	0.46
1:A:307:LEU:HD22	1:A:312:LEU:HB2	1.97	0.46
1:C:1286:ARG:HG3	1:C:1286:ARG:NH1	2.27	0.46
1:D:1587:LEU:HD23	1:D:1747:CYS:SG	2.56	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:G:3132:VAL:CG1	1:G:3133:ARG:N	2.79	0.46
1:G:3184:GLU:CD	1:G:3184:GLU:H	2.23	0.46
1:D:1684:GLU:HA	1:D:1687:GLU:CB	2.46	0.46
1:F:2514:ASP:HB3	1:F:2517:VAL:CG1	2.46	0.46
1:G:3025:GLU:O	1:G:3028:ARG:C	2.59	0.46
1:B:717:SER:HB2	1:B:720:ARG:NH1	2.28	0.46
1:B:764:THR:O	1:B:765:THR:HB	2.14	0.46
1:C:1064:TYR:CD1	2:D:1914:TRP:CZ3	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2093:GLU:HB3	1:E:2248:GLY:O	2.16	0.46
1:E:2112:LEU:HD11	1:E:2118:VAL:CG2	2.45	0.46
1:E:2324:LEU:HD23	1:E:2324:LEU:HA	1.69	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:A:70:ILE:HG13	1:A:73:LEU:HB2	1.96	0.46
1:A:254:LYS:O	1:A:254:LYS:HG2	2.16	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:G:3020:ASN:O	1:G:3024:LEU:HG	2.15	0.46
1:G:3292:ALA:O	1:G:3295:ALA:HB3	2.16	0.46
1:H:3803:LEU:O	1:H:3807:LEU:HB2	2.16	0.46
1:C:1122:SER:HB3	1:C:1124:TYR:HD2	1.81	0.46
1:D:1622:SER:HB3	1:D:1624:TYR:HD2	1.81	0.46
1:F:2524:LEU:CD1	1:F:2527:ARG:HG2	2.46	0.46
1:F:2769:THR:O	1:F:2772:GLN:HB2	2.16	0.46
1:H:3533:LEU:HD22	1:H:3533:LEU:N	2.27	0.46
1:H:3612:LEU:HD11	1:H:3618:VAL:CG2	2.46	0.46
1:H:3655:GLU:O	1:H:3658:ARG:HB3	2.16	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:2528:ARG:O	1:F:2529:GLN:HG2	2.15	0.46
1:F:2533:LEU:C	1:F:2533:LEU:HD23	2.41	0.46
1:F:2845:GLY:HA3	1:F:2877:ARG:NH1	2.31	0.46
1:B:607:LEU:HG	1:B:756:MET:CE	2.45	0.45
1:B:625:TRP:HB2	1:B:675:ASN:CB	2.46	0.45
1:C:1040:GLU:HB3	1:C:1239:THR:HG21	1.98	0.45
1:F:2523:ALA:HB3	1:F:2524:LEU:HD22	1.97	0.45
1:F:2608:PHE:HD2	1:F:2612:LEU:CD2	2.29	0.45
1:G:3025:GLU:O	1:G:3026:LEU:C	2.59	0.45
1:H:3841:LEU:O	1:H:3846:VAL:HG12	2.16	0.45
1:B:800:ARG:HD2	1:B:800:ARG:O	2.15	0.45
1:C:1097:THR:HG21	1:C:1103:ALA:HA	1.97	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:B:882:LEU:HD23	1:B:882:LEU:HA	1.83	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:E:2248:GLY:C	1:E:2253:ILE:HD11	2.42	0.45
1:H:3602:GLN:O	1:H:3602:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1782:GLN:O	1:D:1783:GLU:HB2	2.17	0.45
1:E:2077:LEU:HD21	1:E:2245:TYR:CB	2.46	0.45
1:E:2205:ILE:HG23	1:E:2206:TYR:CD2	2.52	0.45
1:A:2:ARG:NH2	1:B:725:HIS:CE1	2.85	0.45
1:B:531:VAL:HG13	1:D:1840:ARG:HH12	1.82	0.45
1:C:1024:LEU:C	1:C:1028:ARG:HB2	2.42	0.45
1:D:1803:LEU:HD12	1:D:1864:TYR:CD2	2.52	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: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:H:3750:LYS:HE3	1:H:3750:LYS:HB2	1.80	0.45
1:B:758:SER:HA	1:B:761:ARG:HG2	1.98	0.45
1:B:832:PRO:CB	1:B:836:ARG:HH21	2.29	0.45
1:B:880:ARG:NH1	1:D:1843:GLU:OE1	2.50	0.45
1:C:1185:VAL:O	1:C:1189:LEU:HG	2.17	0.45
1:C:1205:ILE:HG23	1:C:1206:TYR:N	2.32	0.45
1:C:1341:LEU:O	1:C:1346:VAL:HG12	2.17	0.45
1:F:2502:ARG:NH1	1:G:3082:ARG:NH1	2.65	0.45
1:F:2545:THR:HG21	1:F:2741:TRP:NE1	2.28	0.45
1:F:2833:ASP:CB	1:F:2836:ARG:HH21	2.29	0.45
1:G:3077:LEU:HD21	1:G:3245:TYR:HB3	1.99	0.45
1:G:3132:VAL:HG22	1:G:3137:GLY:HA3	1.97	0.45
1:C:1112:LEU:HD21	1:C:1118:VAL:HG21	1.99	0.45
1:C:1327:THR:HB	1:C:1337:ALA:HB1	1.98	0.45
1:D:1612:LEU:HD11	1:D:1618:VAL:CG2	2.47	0.45
1:E:2252:VAL:HG22	1:E:2256:MET:HE3	1.98	0.45
1:F:2674:ASN:OD1	1:F:2677:THR:HG23	2.16	0.45
1:F:2881:VAL:HG12	1:F:2882:LEU:N	2.32	0.45
1:H:3792:ALA:O	1:H:3795:ALA:HB3	2.17	0.45
1:A:248:GLY:C	1:A:253:ILE:HD11	2.42	0.45
1:A:264:THR:O	1:A:265:THR:HB	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:F:2527:ARG:HG3	1:F:2527:ARG:O	2.16	0.45
1:G:3025:GLU:O	1:G:3028:ARG:N	2.50	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1748:GLY:CA	1:D:1753:ILE:HD11	2.45	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:D:1877:ARG:HG2	1:D:1880:ARG:NH2	2.32	0.44
1:F:2761:ARG:CD	1:F:2762:GLN:HG2	2.47	0.44
1:A:14:ASP:HB3	1:A:17:VAL:HG12	1.99	0.44
1:A:204:GLU:O	1:A:206:TYR:N	2.50	0.44
1:B:612:LEU:HD11	1:B:618:VAL:CG2	2.47	0.44
1:C:1107:LEU:HG	1:C:1256:MET:CE	2.44	0.44
2:C:1414:TRP:CE3	1:D:1564:TYR:CG	3.06	0.44
1:E:2107:LEU:HD21	1:E:2227:LEU:HD13	2.00	0.44
1:E:2108:PHE:CB	1:E:2112:LEU:HD23	2.42	0.44
1:G:3262:GLN:OE1	1:H:3630:GLU:HB3	2.17	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:H:3670:VAL:HG23	1:H:3681:TYR:CE1	2.47	0.44
1:A:143:GLU:HG3	1:A:144:THR:N	2.33	0.44
1:B:798:ARG:HG3	1:B:798:ARG:HH11	1.83	0.44
1:D:1585:ASN:CB	1:D:1587:LEU:HD13	2.48	0.44
1:G:3108:PHE:CD2	1:G:3112:LEU:CD2	2.99	0.44
2:G:3414:TRP:CZ3	1:H:3564:TYR:CB	2.98	0.44
1:A:12:LYS:HB2	1:A:12:LYS:HE3	1.72	0.44
1:B:851:GLY:HA3	1:B:856:ALA:O	2.16	0.44
1:C:1105:PHE:HA	1:C:1131:MET:HE2	2.00	0.44
1:C:1261:ARG:NH2	1:D:1517:VAL:HG11	2.33	0.44
1:A:340:ARG:NH2	1:A:381:VAL:O	2.50	0.44
1:C:1112:LEU:HD11	1:C:1118:VAL:CG2	2.47	0.44
1:C:1205:ILE:HG23	1:C:1206:TYR:HD2	1.80	0.44
1:D:1619:ILE:HA	1:D:1640:VAL:O	2.18	0.44
1:D:1684:GLU:HA	1:D:1687:GLU:HB2	1.99	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:G:3077:LEU:HD11	1:G:3245:TYR:CG	2.53	0.44
1:A:5:SER:OG	1:A:8:VAL:HB	2.18	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:1151:VAL:HG22	1:C:1181:TYR:CD2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3765:THR:O	1:H:3766:SER:HB2	2.17	0.44
1:A:321:PHE:CG	1:A:365:ALA:HB2	2.53	0.44
1:E:2097:THR:HB	1:E:2102:GLN:CG	2.36	0.44
1:E:2312:LEU:HD11	1:E:2382:LEU:HD11	2.00	0.44
1:F:2643:GLU:HG3	1:F:2644:THR:N	2.33	0.44
1:G:3170:VAL:HG23	1:G:3181:TYR:HE1	1.82	0.44
1:G:3300:ARG:NH1	1:G:3317:PRO:O	2.51	0.44
1:H:3508:VAL:O	1:H:3511:MET:HG2	2.18	0.44
1:H:3621:LEU:HD12	1:H:3621:LEU:N	2.33	0.44
1:H:3727:LEU:HD22	1:H:3756:MET:HE1	2.00	0.44
1:A:22:LYS:HE2	1:A:26:LEU:HD11	1.98	0.43
1:A:286:ARG:O	1:A:286:ARG:HG2	2.18	0.43
1:B:848:VAL:HG21	1:B:860:VAL:HG21	1.99	0.43
1:C:1216:PHE:HD1	1:C:1220:ARG:HH11	1.66	0.43
1:E:2029:GLN:CG	1:E:2029:GLN:O	2.66	0.43
1:F:2747:CYS:C	1:F:2753:ILE:HD11	2.42	0.43
1:F:2799:ARG:HB3	1:F:2871:LEU:CD1	2.48	0.43
1:A:112:LEU:HD11	1:A:118:VAL:CG2	2.49	0.43
1:D:1579:GLU:O	1:D:1583:ARG:HB2	2.18	0.43
1:E:2089:VAL:HA	1:E:2093:GLU:OE1	2.18	0.43
1:E:2364:TYR:C	1:E:2366:THR:H	2.26	0.43
1:G:3077:LEU:HD21	1:G:3245:TYR:CB	2.47	0.43
1:C:1024:LEU:O	1:C:1028:ARG:HB2	2.18	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:A:321:PHE:HA	1:A:364:TYR:OH	2.19	0.43
1:C:1028:ARG:O	1:C:1029:GLN:CB	2.66	0.43
1:C:1307:LEU:HD21	1:C:1325:MET:SD	2.58	0.43
1:E:2268:ASP:HA	1:F:2742:ARG:HG2	2.00	0.43
1:F:2804:LEU:O	1:F:2808:THR:HB	2.18	0.43
1:G:3027:ARG:HA	1:G:3031:VAL:O	2.18	0.43
1:G:3321:PHE:HA	1:G:3364:TYR:CZ	2.53	0.43
1:H:3674:ASN:OD1	1:H:3677:THR:HG23	2.19	0.43
1:A:233:ALA:HB1	1:A:239:THR:HG22	2.00	0.43
1:C:1034:VAL:O	1:C:1346:VAL:HA	2.19	0.43
1:D:1522:LYS:HA	1:D:1525:GLU:OE2	2.18	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:3204:GLU:HG2	1:G:3215:HIS:CE1	2.53	0.43
1:G:3310:LEU:HD11	1:G:3379:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:THR:HB	1:B:664:ARG:NH2	2.33	0.43
1:C:1007:ARG:HG3	1:C:1008:VAL:N	2.33	0.43
1:C:1176:PRO:HD3	1:C:1354:PHE:CD2	2.54	0.43
1:E:2051:GLU:O	1:E:2054:ARG:HB2	2.18	0.43
1:F:2546:PRO:HG3	1:F:2788:PHE:CD1	2.54	0.43
1:F:2612:LEU:HD11	1:F:2618:VAL:CG2	2.47	0.43
1:F:2705:ILE:HG23	1:F:2706:TYR:CD2	2.53	0.43
1:F:2748:GLY:N	1:F:2753:ILE:CD1	2.81	0.43
1:G:3112:LEU:HD11	1:G:3118:VAL:CG2	2.47	0.43
1:G:3324:LEU:HD23	1:G:3324:LEU:HA	1.83	0.43
1:B:825:MET:O	1:B:859:HIS:HA	2.19	0.43
1:C:1026:LEU:O	1:C:1031:VAL:HB	2.18	0.43
1:C:1211:TYR:C	1:C:1212:GLU:HG2	2.43	0.43
1:C:1372:ARG:HA	1:C:1372:ARG:HD3	1.84	0.43
1:E:2112:LEU:HD21	1:E:2118:VAL:HG21	2.01	0.43
1:E:2265:THR:O	1:E:2266:SER:CB	2.67	0.43
1:G:3014:ASP:HB3	1:G:3017:VAL:HG13	2.01	0.43
1:G:3126:VAL:HG23	1:G:3354:PHE:CZ	2.53	0.43
1:G:3205:ILE:HG22	1:G:3206:TYR:HD2	1.79	0.43
1:G:3312:LEU:HD21	1:G:3330:ILE:HD12	2.01	0.43
1:G:3341:LEU:O	1:G:3346:VAL:HG12	2.19	0.43
1:H:3514:ASP:O	1:H:3517:VAL:HG12	2.18	0.43
1:B:717:SER:N	1:B:720:ARG:NH1	2.66	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:A:28:ARG:HD2	1:A:28:ARG:HA	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:H:3585:ASN:CB	1:H:3587:LEU:HD13	2.49	0.43
1:A:12:LYS:HG3	1:A:13:PRO:CD	2.47	0.43
1:A:119:ILE:HA	1:A:140:VAL:O	2.19	0.43
1:A:248:GLY:H	1:A:253:ILE:HD11	1.79	0.43
1:C:1376:GLU:O	1:C:1379:ALA:HB3	2.19	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:F:2841:LEU:O	1:F:2846:VAL:HG12	2.19	0.43
1:G:3067:PRO:HB3	1:G:3261:ARG:CD	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HG11	1:A:374:ALA:HB2	2.00	0.42
1:A:184:GLU:HA	1:A:187:GLU:HB2	2.01	0.42
1:B:545:THR:HG22	1:B:737:ALA:O	2.19	0.42
1:B:758:SER:HA	1:B:761:ARG:NH1	2.24	0.42
1:B:848:VAL:CG2	1:B:860:VAL:HG21	2.49	0.42
1:C:1124:TYR:O	1:C:1354:PHE:CD2	2.72	0.42
1:E:2121:LEU:O	1:E:2124:TYR:HB3	2.19	0.42
1:E:2146:PRO:HB3	1:E:2150:PHE:CZ	2.54	0.42
1:E:2249:PRO:O	1:E:2250:LYS:C	2.62	0.42
1:E:2341:LEU:O	1:E:2346:VAL:HG12	2.19	0.42
1:H:3645:LEU:HB2	1:H:3648:GLU:HG2	2.00	0.42
1:B:619:ILE:HA	1:B:640:VAL:O	2.20	0.42
1:B:671:ASN:C	1:B:671:ASN:ND2	2.77	0.42
1:B:717:SER:OG	1:B:720:ARG:NH1	2.52	0.42
1:B:758:SER:CA	1:B:761:ARG:HD2	2.44	0.42
1:C:1226:THR:CG2	1:C:1227:LEU:N	2.81	0.42
1:C:1345:GLY:HA3	1:C:1377:ARG:NH1	2.34	0.42
1:D:1823:VAL:HG23	1:D:1864:TYR:CE2	2.53	0.42
1:F:2720:ARG:HH11	1:F:2720:ARG:CB	2.32	0.42
1:A:23:ALA:HB3	1:A:24:LEU:H	1.68	0.42
1:A:170:VAL:HG23	1:A:181:TYR:HE1	1.84	0.42
1:A:321:PHE:CD1	1:A:365:ALA:HB2	2.54	0.42
1:A:341:LEU:O	1:A:346:VAL:HG12	2.20	0.42
1:C:1015:ALA:HB2	1:C:1353:ASP:OD1	2.19	0.42
1:D:1727:LEU:HD22	1:D:1756:MET:HE1	2.02	0.42
1:B:534:VAL:CG1	1:B:874:ALA:HB2	2.46	0.42
1:C:1121:LEU:HD22	1:C:1152:PRO:HB3	2.01	0.42
1:D:1540:GLU:HB3	1:D:1739:THR:HG21	2.02	0.42
1:D:1683:LYS:HG3	1:D:1716:PHE:CG	2.54	0.42
1:E:2077:LEU:HD11	1:E:2245:TYR:CG	2.54	0.42
1:E:2085:ASN:HB2	1:E:2087:LEU:HD13	2.00	0.42
1:F:2627:SER:O	1:F:2628:TYR:C	2.63	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:A:2:ARG:HE	1:B:725:HIS:CD2	2.37	0.42
1:A:64:TYR:CE2	1:B:742:ARG:NH1	2.85	0.42
1:C:1024:LEU:C	1:C:1025:GLU:HG2	2.44	0.42
1:F:2670:VAL:HG23	1:F:2681:TYR:HE1	1.83	0.42
1:A:74:ARG:NH2	1:A:92:GLU:HA	2.35	0.42
1:A:112:LEU:HD21	1:A:118:VAL:HG21	2.01	0.42
1:A:187:GLU:HG3	1:A:191:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:LEU:HD11	1:B:816:ARG:HA	2.01	0.42
1:B:841:LEU:O	1:B:846:VAL:HG12	2.19	0.42
1:C:1119:ILE:HA	1:C:1140:VAL:O	2.20	0.42
1:C:1286:ARG:O	1:C:1290:GLU:HG2	2.20	0.42
1:F:2656:ARG:HA	1:F:2659:ARG:HG2	2.02	0.42
1:G:3112:LEU:HD21	1:G:3118:VAL:HG21	2.02	0.42
1:G:3122:SER:HA	1:G:3123:PRO:C	2.44	0.42
1:G:3212:GLU:OE2	1:G:3316:ARG:NH2	2.51	0.42
1:G:3227:LEU:HD11	1:G:3252:VAL:HG21	2.02	0.42
1:H:3534:VAL:CG2	1:H:3873:LYS:HD2	2.48	0.42
1:H:3827:THR:CG2	1:H:3860:VAL:HB	2.50	0.42
1:A:249:PRO:O	1:A:253:ILE:HG13	2.20	0.42
1:B:792:ALA:HB1	1:B:796:TYR:CE1	2.55	0.42
1:D:1521:ALA:C	1:D:1523:ALA:H	2.28	0.42
1:D:1826:ASP:C	1:D:1828:SER:H	2.28	0.42
1:E:2252:VAL:CG2	1:E:2256:MET:HE3	2.50	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:H:3612:LEU:HD21	1:H:3618:VAL:HG21	2.02	0.42
1:H:3776:LEU:HD23	1:H:3776:LEU:O	2.19	0.42
1:A:45:THR:HA	1:A:46:PRO:HD3	1.88	0.42
1:A:330:ILE:HD11	1:A:341:LEU:HD21	2.02	0.42
1:B:611:ILE:CG1	1:B:612:LEU:H	2.20	0.42
1:D:1841:LEU:O	1:D:1846:VAL:HG12	2.20	0.42
1:E:2323:VAL:HG23	1:E:2364:TYR:CE2	2.54	0.42
1:E:2345:GLY:HA3	1:E:2377:ARG:NH1	2.35	0.42
1:F:2587:LEU:HD12	1:F:2587:LEU:HA	1.89	0.42
1:A:45:THR:HG22	1:A:237:ALA:O	2.19	0.42
1:A:111:ILE:CG1	1:A:112:LEU:H	2.19	0.42
1:A:255:ALA:HB1	1:B:508:VAL:HG11	2.02	0.42
1:B:612:LEU:HD21	1:B:618:VAL:HG21	2.02	0.42
1:B:717:SER:H	1:B:720:ARG:HH11	1.65	0.42
1:C:1102:GLN:O	1:C:1102:GLN:HG3	2.20	0.42
1:C:1111:ILE:CG1	1:C:1112:LEU:H	2.21	0.42
1:D:1748:GLY:N	1:D:1753:ILE:CD1	2.73	0.42
1:E:2186:LEU:HB3	1:E:2218:PRO:HG3	2.02	0.42
1:E:2224:GLU:O	1:E:2224:GLU:CG	2.68	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:E:2325:MET:O	1:E:2359:HIS:HA	2.20	0.42
1:E:2362:LEU:HD11	1:E:2378:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2662:THR:HB	1:F:2664:ARG:NH2	2.35	0.42
1:G:3118:VAL:HB	1:G:3132:VAL:HG21	2.02	0.42
1:H:3619:ILE:HA	1:H:3640:VAL:O	2.19	0.42
1:A:20:ASN:O	1:A:24:LEU:HG	2.20	0.42
1:B:675:ASN:HD22	3:B:913:PLP:H2A1	1.85	0.42
1:D:1825:MET:O	1:D:1859:HIS:HA	2.20	0.42
1:G:3005:SER:HG	1:G:3008:VAL:HB	1.85	0.42
1:A:64:TYR:CE2	2:A:914:TRP:CZ3	3.08	0.41
1:A:265:THR:O	1:A:266:SER:CB	2.68	0.41
1:B:533:LEU:H	1:B:533:LEU:CD2	2.33	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:F:2619:ILE:HA	1:F:2640:VAL:O	2.20	0.41
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:G:3174:ASN:ND2	1:G:3174:ASN:C	2.78	0.41
1:A:227:LEU:CD2	1:A:256:MET:HE1	2.50	0.41
1:B:690:ALA:O	1:B:694:VAL:HG23	2.19	0.41
1:B:782:GLN:HG2	1:B:786:ARG:NH2	2.17	0.41
1:D:1573:LEU:O	1:D:1577:LEU:HB2	2.20	0.41
1:D:1621:LEU:O	1:D:1624:TYR:HB3	2.20	0.41
1:D:1840:ARG:NH2	1:D:1881:VAL:O	2.49	0.41
1:B:717:SER:HA	1:B:718:PRO:HD3	1.92	0.41
1:B:749:PRO:HB2	1:B:752:VAL:HG12	2.01	0.41
1:B:821:PHE:CG	1:B:865:ALA:HB2	2.54	0.41
1:C:1227:LEU:CD2	1:C:1256:MET:HE1	2.49	0.41
1:D:1844:ALA:O	1:D:1877:ARG:HD3	2.21	0.41
1:E:2346:VAL:O	1:E:2346:VAL:HG13	2.20	0.41
1:G:3023:ALA:O	1:G:3025:GLU:N	2.46	0.41
1:H:3840:ARG:NH2	1:H:3881:VAL:O	2.52	0.41
1:C:1085:ASN:CB	1:C:1087:LEU:HD13	2.48	0.41
1:C:1242:ARG:HG2	1:D:1768:ASP:HA	2.02	0.41
1:C:1297:ARG:O	1:C:1300:ARG:HB3	2.20	0.41
1:D:1525:GLU:CA	1:D:1528:ARG:HB3	2.51	0.41
1:E:2153:ASP:OD2	1:E:2156:ARG:HD3	2.20	0.41
1:F:2830:ILE:HD13	1:F:2830:ILE:O	2.20	0.41
1:B:626:VAL:HG23	1:B:854:PHE:CE2	2.55	0.41
1:B:694:VAL:HA	1:B:725:HIS:NE2	2.36	0.41
1:E:2112:LEU:HD11	1:E:2118:VAL:HG23	2.03	0.41
1:E:2174:ASN:OD1	1:E:2175:ASN:N	2.53	0.41
1:F:2802:LEU:HD23	1:F:2868:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2824:LEU:HD23	1:F:2824:LEU:HA	1.80	0.41
1:G:3071:PRO:O	1:G:3075:GLU:HG3	2.20	0.41
1:H:3842:LEU:HD23	1:H:3842:LEU:HA	1.73	0.41
1:A:342:LEU:HA	1:A:342:LEU:HD23	1.84	0.41
1:C:1324:LEU:HD23	1:C:1324:LEU:HA	1.77	0.41
1:D:1562:THR:O	1:D:1562:THR:OG1	2.36	0.41
1:H:3562:THR:O	1:H:3562:THR:OG1	2.37	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:C:1046:PRO:HB2	1:C:1049:VAL:CG2	2.45	0.41
1:C:1234:LYS:HZ2	3:C:1413:PLP:C4A	2.34	0.41
1:D:1506:ARG:HH11	1:D:1506:ARG:CG	2.33	0.41
1:D:1621:LEU:CD2	1:D:1652:PRO:HB3	2.51	0.41
1:D:1803:LEU:HD22	1:D:1807:LEU:CD1	2.51	0.41
1:F:2514:ASP:HB3	1:F:2517:VAL:HB	2.02	0.41
1:F:2753:ILE:O	1:F:2753:ILE:CG2	2.63	0.41
1:F:2761:ARG:O	1:F:2761:ARG:HG2	2.17	0.41
1:G:3158:ARG:NH1	1:G:3196:HIS:CE1	2.89	0.41
1:G:3303:LEU:HD23	1:G:3375:LEU:HD21	2.02	0.41
1:H:3622:SER:C	1:H:3624:TYR:N	2.77	0.41
1:B:554:ARG:HA	1:B:557:LEU:HD12	2.01	0.41
1:C:1147:GLU:C	1:C:1149:GLY:H	2.29	0.41
1:D:1782:GLN:O	1:D:1783:GLU:CB	2.68	0.41
1:F:2831:ALA:HB1	1:F:2832:PRO:CD	2.50	0.41
1:A:57:LEU:HD21	1:B:741:TRP:CH2	2.56	0.41
1:B:581:PHE:O	1:B:585:ASN:HB2	2.21	0.41
1:B:804:LEU:CD1	1:B:816:ARG:HG3	2.51	0.41
1:B:816:ARG:HA	1:B:817:PRO:HD2	1.98	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:C:1253:ILE:O	1:C:1253:ILE:CG2	2.67	0.41
1:C:1381:VAL:HG12	1:C:1382:LEU:N	2.35	0.41
1:D:1575:GLU:O	1:D:1579:GLU:HG3	2.21	0.41
1:D:1819:GLY:O	1:D:1820:ALA:HB3	2.21	0.41
1:E:2045:THR:HA	1:E:2046:PRO:HD3	1.91	0.41
1:E:2184:GLU:HA	1:E:2187:GLU:HB3	2.03	0.41
1:E:2296:TYR:O	1:E:2300:ARG:HB2	2.20	0.41
1:F:2526:LEU:C	1:F:2528:ARG:N	2.78	0.41
1:F:2529:GLN:HG3	1:F:2529:GLN:O	2.20	0.41
1:F:2681:TYR:HA	1:F:2682:PRO:HD3	1.80	0.41
1:G:3330:ILE:O	1:G:3331:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3622:SER:CB	1:H:3643:GLU:HA	2.51	0.41
1:H:3683:LYS:HG3	1:H:3716:PHE:CG	2.56	0.41
1:H:3800:ARG:O	1:H:3804:LEU:HD23	2.20	0.41
1:H:3876:GLU:O	1:H:3879:ALA:HB3	2.21	0.41
1:B:574:ARG:NH2	1:B:592:GLU:HA	2.36	0.41
1:B:625:TRP:HB2	1:B:675:ASN:HB3	2.03	0.41
1:B:864:TYR:HA	1:B:871:LEU:HD21	2.02	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:D:1741:TRP:O	1:D:1742:ARG:HB2	2.21	0.41
1:F:2621:LEU:HD22	1:F:2652:PRO:HB3	2.03	0.41
1:G:3205:ILE:CG2	1:G:3206:TYR:N	2.84	0.41
1:H:3693:ALA:HA	1:H:3698:PHE:CZ	2.56	0.41
1:A:45:THR:CG2	1:B:562:THR:OG1	2.69	0.40
1:A:108:PHE:HB3	1:A:112:LEU:HD23	2.03	0.40
1:C:1017:VAL:CG1	1:D:1761:ARG:HH21	2.31	0.40
1:C:1033:LEU:N	1:C:1033:LEU:HD22	2.35	0.40
1:D:1550:LYS:O	1:D:1554:ARG:HG3	2.22	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:B:572:GLU:HB3	1:B:776:LEU:HD11	2.03	0.40
1:B:646:PRO:HB3	1:B:650:PHE:CZ	2.57	0.40
1:B:656:ARG:HA	1:B:659:ARG:HG2	2.02	0.40
1:B:672:SER:HA	1:B:674:ASN:N	2.37	0.40
1:B:680:VAL:O	1:B:680:VAL:HG13	2.21	0.40
1:B:686:LEU:HB2	1:B:716:PHE:CD2	2.56	0.40
1:E:2373:LYS:O	1:E:2376:GLU:HB3	2.21	0.40
1:F:2683:LYS:HG3	1:F:2716:PHE:CG	2.56	0.40
1:F:2831:ALA:HB3	1:F:2837:ALA:CB	2.42	0.40
1:F:2869:GLU:O	1:F:2873:LYS:HG3	2.21	0.40
1:G:3127:SER:HB3	1:H:3762:GLN:OE1	2.21	0.40
1:G:3156:ARG:HA	1:G:3159:ARG:HG2	2.04	0.40
1:H:3612:LEU:HD11	1:H:3618:VAL:HG23	2.04	0.40
1:A:47:GLU:O	1:A:51:GLU:HB2	2.21	0.40
1:A:122:SER:HB3	1:A:124:TYR:CD2	2.57	0.40
1:A:184:GLU:CD	1:A:184:GLU:H	2.28	0.40
1:B:842:LEU:HD23	1:B:842:LEU:HA	1.81	0.40
1:C:1005:SER:HB3	1:D:1611:ILE:O	2.21	0.40
1:C:1298:ARG:HD3	1:C:1368:GLU:OE2	2.21	0.40
1:C:1342:LEU:HA	1:C:1342:LEU:HD23	1.84	0.40
1:D:1536:LEU:HB3	1:D:1863:SER:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1705:ILE:HG23	1:D:1706:TYR:N	2.36	0.40
1:D:1810:LEU:HD23	1:D:1810:LEU:HA	1.95	0.40
1:F:2612:LEU:HD21	1:F:2618:VAL:HG21	2.04	0.40
1:G:3077:LEU:C	1:G:3079:GLU:N	2.75	0.40
1:H:3539:GLY:O	1:H:3821:PHE:HZ	2.04	0.40
1:H:3845:GLY:HA3	1:H:3877:ARG:HH11	1.87	0.40
1:A:90:THR:HB	1:A:91:PRO:HD2	2.02	0.40
1:A:193:ALA:HA	1:A:198:PHE:CZ	2.56	0.40
1:A:268:ASP:HA	1:B:742:ARG:HG2	2.04	0.40
1:A:323:VAL:HG23	1:A:364:TYR:CE2	2.55	0.40
1:B:823:VAL:HG23	1:B:864:TYR:CE2	2.55	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:D:1716:PHE:CE1	1:D:1720:ARG:HD3	2.56	0.40
1:D:1742:ARG:NH2	3:D:1913:PLP:O3P	2.51	0.40
1:E:2193:ALA:HA	1:E:2198:PHE:CZ	2.56	0.40
1:E:2312:LEU:HD21	1:E:2330:ILE:HD12	2.04	0.40
1:H:3828:SER:HB3	1:H:3829:PRO:HD3	2.04	0.40
1:A:40:GLU:H	1:A:40:GLU:HG2	1.73	0.40
1:A:184:GLU:HA	1:A:187:GLU:HB3	2.03	0.40
1:C:1180:VAL:O	1:C:1180:VAL:HG13	2.22	0.40
1:D:1526:LEU:HD23	1:D:1526:LEU:HA	1.89	0.40
1:D:1612:LEU:HD21	1:D:1618:VAL:HG21	2.02	0.40
1:F:2526:LEU:C	1:F:2528:ARG:H	2.28	0.40
1:F:2700:LEU:HD23	1:F:2700:LEU:HA	1.94	0.40
1:H:3520:ASN:O	1:H:3523:ALA:HB3	2.21	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%)	3	19
1	B	380/385 (99%)	322 (85%)	42 (11%)	16 (4%)	2	14
1	C	380/385 (99%)	321 (84%)	41 (11%)	18 (5%)	2	12
1	D	380/385 (99%)	322 (85%)	41 (11%)	17 (4%)	2	13
1	E	380/385 (99%)	323 (85%)	42 (11%)	15 (4%)	2	16
1	F	380/385 (99%)	321 (84%)	45 (12%)	14 (4%)	2	17
1	G	380/385 (99%)	325 (86%)	41 (11%)	14 (4%)	2	17
1	H	380/385 (99%)	323 (85%)	43 (11%)	14 (4%)	2	17
All	All	3040/3080 (99%)	2589 (85%)	331 (11%)	120 (4%)	2	16

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	255 (84%)	50 (16%)	2	11
1	B	305/306 (100%)	256 (84%)	49 (16%)	2	12
1	C	305/306 (100%)	254 (83%)	51 (17%)	2	11
1	D	305/306 (100%)	260 (85%)	45 (15%)	3	13
1	E	305/306 (100%)	245 (80%)	60 (20%)	1	6
1	F	305/306 (100%)	246 (81%)	59 (19%)	1	6
1	G	305/306 (100%)	257 (84%)	48 (16%)	2	12
1	H	305/306 (100%)	262 (86%)	43 (14%)	3	14
All	All	2440/2448 (100%)	2035 (83%)	405 (17%)	2	11

All (405) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	VAL
1	A	16	VAL
1	A	19	VAL
1	A	24	LEU
1	A	25	GLU

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Mol	Chain	Res	Type
1	A	28	ARG
1	A	32	ASP
1	A	33	LEU
1	A	45	THR
1	A	55	ARG
1	A	62	THR
1	A	73	LEU
1	A	77	LEU
1	A	80	LYS
1	A	94	THR
1	A	96	VAL
1	A	102	GLN
1	A	107	LEU
1	A	112	LEU
1	A	156	ARG
1	A	175	ASN
1	A	177	THR
1	A	184	GLU
1	A	192	LEU
1	A	200	LEU
1	A	205	ILE
1	A	212	GLU
1	A	214	GLU
1	A	226	THR
1	A	227	LEU
1	A	228	THR
1	A	243	ILE
1	A	251	GLU
1	A	265	THR
1	A	268	ASP
1	A	276	LEU
1	A	282	GLN
1	A	286	ARG
1	A	298	ARG
1	A	302	LEU
1	A	303	LEU
1	A	315	VAL
1	A	342	LEU
1	A	360	VAL
1	A	367	SER
1	A	368	GLU
1	A	372	ARG

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Mol	Chain	Res	Type
1	A	375	LEU
1	A	381	VAL
1	B	505	SER
1	B	508	VAL
1	B	512	LYS
1	B	516	VAL
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	573	LEU
1	B	577	LEU
1	B	583	ARG
1	B	594	THR
1	B	596	VAL
1	B	602	GLN
1	B	612	LEU
1	B	651	VAL
1	B	656	ARG
1	B	669	VAL
1	B	670	VAL
1	B	671	ASN
1	B	676	PRO
1	B	677	THR
1	B	684	GLU
1	B	692	LEU
1	B	700	LEU
1	B	712	GLU
1	B	726	THR
1	B	727	LEU
1	B	728	THR
1	B	743	ILE
1	B	752	VAL
1	B	754	LYS
1	B	765	THR
1	B	776	LEU
1	B	782	GLN
1	B	786	ARG
1	B	802	LEU
1	B	803	LEU

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Mol	Chain	Res	Type
1	B	808	THR
1	B	815	VAL
1	B	821	PHE
1	B	828	SER
1	B	840	ARG
1	B	842	LEU
1	B	869	GLU
1	B	875	LEU
1	B	881	VAL
1	C	1008	VAL
1	C	1012	LYS
1	C	1014	ASP
1	C	1032	ASP
1	C	1033	LEU
1	C	1045	THR
1	C	1059	GLN
1	C	1062	THR
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	1192	LEU
1	C	1200	LEU
1	C	1212	GLU
1	C	1214	GLU
1	C	1226	THR
1	C	1227	LEU
1	C	1228	THR
1	C	1234	LYS
1	C	1243	ILE
1	C	1254	LYS
1	C	1261	ARG
1	C	1265	THR

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Mol	Chain	Res	Type
1	C	1268	ASP
1	C	1276	LEU
1	C	1282	GLN
1	C	1298	ARG
1	C	1302	LEU
1	C	1303	LEU
1	C	1315	VAL
1	C	1316	ARG
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	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	1525	GLU
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	1573	LEU
1	D	1577	LEU
1	D	1594	THR
1	D	1596	VAL
1	D	1602	GLN
1	D	1607	LEU
1	D	1612	LEU
1	D	1645	LEU
1	D	1647	GLU
1	D	1656	ARG
1	D	1677	THR
1	D	1684	GLU

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Mol	Chain	Res	Type
1	D	1686	LEU
1	D	1694	VAL
1	D	1700	LEU
1	D	1712	GLU
1	D	1727	LEU
1	D	1728	THR
1	D	1751	GLU
1	D	1765	THR
1	D	1776	LEU
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	2080	LYS
1	E	2082	ARG

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Mol	Chain	Res	Type
1	E	2094	THR
1	E	2102	GLN
1	E	2107	LEU
1	E	2112	LEU
1	E	2113	ASP
1	E	2127	SER
1	E	2145	LEU
1	E	2147	GLU
1	E	2164	ARG
1	E	2172	SER
1	E	2177	THR
1	E	2184	GLU
1	E	2192	LEU
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	2252	VAL
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	2362	LEU
1	E	2367	SER
1	E	2375	LEU
1	E	2381	VAL
1	F	2506	ARG
1	F	2508	VAL
1	F	2512	LYS

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Mol	Chain	Res	Type
1	F	2516	VAL
1	F	2517	VAL
1	F	2519	VAL
1	F	2522	LYS
1	F	2524	LEU
1	F	2526	LEU
1	F	2531	VAL
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	2602	GLN
1	F	2612	LEU
1	F	2613	ASP
1	F	2614	PRO
1	F	2645	LEU
1	F	2647	GLU
1	F	2651	VAL
1	F	2675	ASN
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	2751	GLU
1	F	2752	VAL
1	F	2761	ARG

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Mol	Chain	Res	Type
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	2815	VAL
1	F	2830	ILE
1	F	2842	LEU
1	F	2860	VAL
1	F	2867	SER
1	F	2868	GLU
1	F	2872	ARG
1	F	2881	VAL
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	3032	ASP
1	G	3033	LEU
1	G	3045	THR
1	G	3055	ARG
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	3131	MET
1	G	3156	ARG
1	G	3174	ASN
1	G	3176	PRO
1	G	3184	GLU
1	G	3186	LEU
1	G	3200	LEU
1	G	3205	ILE

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Mol	Chain	Res	Type
1	G	3214	GLU
1	G	3226	THR
1	G	3227	LEU
1	G	3228	THR
1	G	3243	ILE
1	G	3252	VAL
1	G	3265	THR
1	G	3266	SER
1	G	3276	LEU
1	G	3277	GLU
1	G	3283	GLU
1	G	3286	ARG
1	G	3298	ARG
1	G	3302	LEU
1	G	3303	LEU
1	G	3310	LEU
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	3531	VAL
1	H	3532	ASP
1	H	3533	LEU
1	H	3545	THR
1	H	3562	THR
1	H	3573	LEU
1	H	3577	LEU
1	H	3594	THR
1	H	3596	VAL
1	H	3602	GLN
1	H	3612	LEU
1	H	3613	ASP
1	H	3623	PRO
1	H	3655	GLU
1	H	3656	ARG
1	H	3659	ARG
1	H	3664	ARG
1	H	3675	ASN
1	H	3676	PRO

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Mol	Chain	Res	Type
1	H	3677	THR
1	H	3684	GLU
1	H	3700	LEU
1	H	3714	GLU
1	H	3726	THR
1	H	3727	LEU
1	H	3728	THR
1	H	3743	ILE
1	H	3752	VAL
1	H	3761	ARG
1	H	3765	THR
1	H	3776	LEU
1	H	3800	ARG
1	H	3802	LEU
1	H	3805	GLU
1	H	3815	VAL
1	H	3830	ILE
1	H	3842	LEU
1	H	3860	VAL
1	H	3875	LEU
1	H	3881	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	102	GLN
1	A	171	ASN
1	A	359	HIS
1	A	370	ASN
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	C	1215	HIS
1	C	1359	HIS
1	D	1509	GLN
1	D	1671	ASN
1	D	1859	HIS
1	E	2009	GLN

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Mol	Chain	Res	Type
1	E	2048	HIS
1	E	2059	GLN
1	E	2106	ASN
1	E	2171	ASN
1	E	2175	ASN
1	E	2282	GLN
1	F	2671	ASN
1	F	2715	HIS
1	F	2772	GLN
1	F	2859	HIS
1	F	2870	ASN
1	G	3009	GLN
1	G	3171	ASN
1	G	3174	ASN
1	G	3196	HIS
1	G	3215	HIS
1	G	3262	GLN
1	G	3359	HIS
1	H	3674	ASN
1	H	3782	GLN
1	H	3870	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	TRP	A	414	3	15,16,16	1.12	1 (6%)	18,22,22	0.62	0
2	TRP	A	914	3	15,16,16	1.85	4 (26%)	18,22,22	1.81	3 (16%)
2	TRP	C	1414	3	15,16,16	1.67	3 (20%)	18,22,22	2.42	4 (22%)
2	TRP	E	2914	3	15,16,16	3.58	5 (33%)	18,22,22	1.68	5 (27%)
2	TRP	G	3414	3	15,16,16	1.48	2 (13%)	18,22,22	2.01	3 (16%)
3	PLP	A	413	2	15,15,16	2.41	5 (33%)	21,22,23	2.26	7 (33%)
2	TRP	D	1914	3	15,16,16	2.13	4 (26%)	18,22,22	1.07	1 (5%)
2	TRP	E	2414	3	15,16,16	1.51	3 (20%)	18,22,22	2.31	4 (22%)
3	PLP	B	913	2	15,15,16	4.47	7 (46%)	21,22,23	2.34	8 (38%)
3	PLP	E	2413	2	15,15,16	1.87	5 (33%)	21,22,23	5.54	9 (42%)
3	PLP	G	3413	2	15,15,16	3.64	6 (40%)	21,22,23	3.17	11 (52%)
3	PLP	F	2913	2	15,15,16	3.48	5 (33%)	21,22,23	1.60	5 (23%)
3	PLP	H	3913	2	15,15,16	4.30	8 (53%)	21,22,23	1.53	4 (19%)
2	TRP	H	3914	3	15,16,16	2.14	1 (6%)	18,22,22	0.83	1 (5%)
3	PLP	C	1413	2	15,15,16	2.12	8 (53%)	21,22,23	5.81	11 (52%)
3	PLP	D	1913	2	15,15,16	3.52	7 (46%)	21,22,23	3.43	6 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	A	414	3	-	7/8/8/8	0/2/2/2
2	TRP	A	914	3	-	3/8/8/8	0/2/2/2
2	TRP	C	1414	3	-	7/8/8/8	0/2/2/2
2	TRP	E	2914	3	-	0/8/8/8	0/2/2/2
2	TRP	G	3414	3	-	4/8/8/8	0/2/2/2
3	PLP	A	413	2	-	0/6/6/8	0/1/1/1
2	TRP	D	1914	3	-	4/8/8/8	0/2/2/2
2	TRP	E	2414	3	-	2/8/8/8	0/2/2/2
3	PLP	B	913	2	-	1/6/6/8	0/1/1/1
3	PLP	E	2413	2	-	2/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	G	3413	2	-	1/6/6/8	0/1/1/1
3	PLP	F	2913	2	-	3/6/6/8	0/1/1/1
3	PLP	H	3913	2	-	0/6/6/8	0/1/1/1
2	TRP	H	3914	3	-	6/8/8/8	0/2/2/2
3	PLP	C	1413	2	-	1/6/6/8	0/1/1/1
3	PLP	D	1913	2	-	0/6/6/8	0/1/1/1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	913	PLP	C5-C4	14.06	1.56	1.40
3	H	3913	PLP	C4A-C4	10.82	1.73	1.51
3	D	1913	PLP	C5-C4	10.34	1.52	1.40
3	H	3913	PLP	C5-C4	10.24	1.52	1.40
3	G	3413	PLP	C5-C4	9.83	1.51	1.40
3	F	2913	PLP	C5-C4	8.67	1.50	1.40
2	H	3914	TRP	CB-CG	7.70	1.64	1.50
3	B	913	PLP	C4A-C4	7.66	1.66	1.51
3	G	3413	PLP	C4A-C4	7.51	1.66	1.51
2	E	2914	TRP	CD1-CG	-7.24	1.26	1.36
2	E	2914	TRP	CZ2-CE2	7.08	1.51	1.39
3	F	2913	PLP	C3-C4	-6.81	1.27	1.40
3	A	413	PLP	C4A-C4	6.71	1.65	1.51
2	D	1914	TRP	CB-CG	6.22	1.62	1.50
2	E	2914	TRP	CB-CG	-6.06	1.38	1.50
2	E	2914	TRP	CH2-CZ2	5.46	1.48	1.38
3	F	2913	PLP	C3-C2	-5.21	1.35	1.41
3	D	1913	PLP	C4A-C4	4.96	1.61	1.51
2	A	914	TRP	O-C	4.46	1.35	1.22
3	D	1913	PLP	C3-C2	4.07	1.45	1.41
2	C	1414	TRP	O-C	4.01	1.34	1.22
3	C	1413	PLP	C3-C2	3.77	1.44	1.41
3	A	413	PLP	C3-C2	3.76	1.44	1.41
2	A	914	TRP	CD1-CG	3.66	1.42	1.36
2	E	2414	TRP	CB-CG	-3.61	1.43	1.50
3	E	2413	PLP	C4A-C4	-3.56	1.44	1.51
3	C	1413	PLP	C5A-C5	3.53	1.60	1.50
2	G	3414	TRP	CB-CG	3.51	1.56	1.50
3	B	913	PLP	C2A-C2	3.39	1.55	1.50
3	D	1913	PLP	C6-C5	3.35	1.44	1.37
3	C	1413	PLP	C4A-C4	3.33	1.58	1.51
3	H	3913	PLP	C3-C2	3.28	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	413	PLP	C5-C4	3.05	1.44	1.40
2	E	2914	TRP	CD1-NE1	3.04	1.42	1.37
3	F	2913	PLP	C4A-C4	3.04	1.57	1.51
2	A	414	TRP	CB-CG	2.99	1.55	1.50
3	H	3913	PLP	C3-C4	-2.94	1.34	1.40
3	G	3413	PLP	C5A-C5	2.91	1.58	1.50
3	E	2413	PLP	P-O2P	2.90	1.65	1.54
3	D	1913	PLP	C2A-C2	2.90	1.55	1.50
3	F	2913	PLP	C5A-C5	-2.89	1.43	1.50
3	G	3413	PLP	O3-C3	-2.87	1.30	1.36
3	H	3913	PLP	C2A-C2	2.79	1.54	1.50
2	C	1414	TRP	CB-CA	2.77	1.65	1.53
3	H	3913	PLP	C2-N1	2.72	1.38	1.33
3	B	913	PLP	C6-C5	2.69	1.43	1.37
3	H	3913	PLP	C6-C5	2.69	1.43	1.37
3	C	1413	PLP	C3-C4	2.68	1.45	1.40
2	D	1914	TRP	CD1-CG	2.65	1.40	1.36
2	E	2414	TRP	OXT-C	-2.65	1.22	1.30
3	E	2413	PLP	O3-C3	2.63	1.42	1.36
3	C	1413	PLP	C2-N1	2.60	1.38	1.33
2	D	1914	TRP	O-C	2.57	1.29	1.22
3	E	2413	PLP	C6-C5	-2.55	1.32	1.37
3	G	3413	PLP	C6-C5	2.51	1.42	1.37
3	G	3413	PLP	C3-C4	-2.49	1.35	1.40
2	A	914	TRP	CH2-CZ2	-2.43	1.34	1.38
3	B	913	PLP	P-O3P	-2.43	1.45	1.54
3	H	3913	PLP	P-O3P	-2.41	1.45	1.54
3	B	913	PLP	C3-C4	-2.39	1.35	1.40
3	A	413	PLP	P-O3P	-2.37	1.46	1.54
3	C	1413	PLP	O3-C3	-2.33	1.31	1.36
3	B	913	PLP	O3-C3	2.31	1.42	1.36
2	A	914	TRP	CD2-CE2	2.27	1.44	1.41
3	D	1913	PLP	P-O2P	2.21	1.63	1.54
2	G	3414	TRP	CZ3-CE3	2.19	1.42	1.38
3	E	2413	PLP	C2A-C2	2.18	1.53	1.50
3	D	1913	PLP	P-O3P	-2.14	1.46	1.54
2	C	1414	TRP	CH2-CZ3	2.14	1.43	1.38
3	C	1413	PLP	C2A-C2	2.09	1.53	1.50
3	C	1413	PLP	P-O3P	-2.09	1.47	1.54
2	D	1914	TRP	CB-CA	2.02	1.62	1.53
2	E	2414	TRP	CD2-CG	-2.02	1.40	1.44
3	A	413	PLP	C2A-C2	2.00	1.53	1.50

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2413	PLP	C4A-C4-C5	-23.79	96.42	120.94
3	C	1413	PLP	C6-C5-C4	15.63	130.91	118.10
3	C	1413	PLP	C4A-C4-C5	-14.79	105.69	120.94
3	C	1413	PLP	C4A-C4-C3	10.51	138.06	120.52
3	D	1913	PLP	C3-C4-C5	-8.98	107.81	118.59
2	C	1414	TRP	CA-CB-CG	8.74	130.09	113.49
2	E	2414	TRP	CA-CB-CG	8.12	128.89	113.49
3	D	1913	PLP	C6-C5-C4	7.63	124.35	118.10
3	D	1913	PLP	C4A-C4-C5	7.32	128.49	120.94
2	G	3414	TRP	CA-CB-CG	6.75	126.29	113.49
3	G	3413	PLP	C6-C5-C4	6.65	123.55	118.10
3	B	913	PLP	C3-C4-C5	-6.44	110.86	118.59
3	G	3413	PLP	C4A-C4-C5	-6.27	114.47	120.94
3	C	1413	PLP	C5A-C5-C6	-6.13	109.37	119.36
3	A	413	PLP	C6-C5-C4	5.88	122.92	118.10
2	A	914	TRP	CA-CB-CG	-5.52	103.02	113.49
3	G	3413	PLP	C4A-C4-C3	5.50	129.70	120.52
3	C	1413	PLP	C3-C4-C5	-5.47	112.02	118.59
3	G	3413	PLP	C3-C4-C5	-4.98	112.62	118.59
3	D	1913	PLP	C4-C3-C2	4.50	126.61	119.89
3	C	1413	PLP	C5-C6-N1	-4.43	116.62	123.83
3	A	413	PLP	C4A-C4-C3	4.14	127.42	120.52
2	G	3414	TRP	CB-CA-N	-4.10	94.46	112.42
3	G	3413	PLP	C5A-C5-C6	-3.99	112.85	119.36
3	B	913	PLP	C4-C3-C2	3.86	125.66	119.89
3	A	413	PLP	C4A-C4-C5	-3.82	117.00	120.94
3	E	2413	PLP	C6-C5-C4	3.64	121.08	118.10
2	A	914	TRP	OXT-C-O	-3.61	115.90	124.08
3	G	3413	PLP	O2P-P-O4P	-3.54	97.45	106.67
3	F	2913	PLP	C4-C3-C2	3.43	125.01	119.89
3	C	1413	PLP	C3-C2-N1	3.33	125.17	120.96
3	E	2413	PLP	C2A-C2-C3	3.33	124.69	120.80
2	E	2414	TRP	CB-CA-N	-3.33	97.86	112.42
3	G	3413	PLP	C5-C6-N1	-3.31	118.44	123.83
3	B	913	PLP	C5A-C5-C6	-3.26	114.04	119.36
3	H	3913	PLP	C3-C4-C5	-3.22	114.72	118.59
2	E	2914	TRP	CD2-CE2-NE1	-3.01	105.02	107.52
3	B	913	PLP	O4P-C5A-C5	3.00	114.99	109.36
2	E	2914	TRP	CZ2-CE2-NE1	2.99	135.53	130.74
3	F	2913	PLP	O3P-P-O1P	2.99	122.48	110.83
3	E	2413	PLP	O3-C3-C2	2.91	123.61	117.58
3	C	1413	PLP	O3-C3-C2	2.87	123.52	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2914	TRP	CZ2-CE2-CD2	-2.83	119.45	122.19
2	E	2414	TRP	CB-CG-CD2	-2.74	121.43	126.70
2	E	2914	TRP	OXT-C-O	-2.72	117.90	124.08
3	B	913	PLP	C4A-C4-C3	-2.72	115.99	120.52
3	C	1413	PLP	C4-C3-C2	-2.72	115.82	119.89
3	A	413	PLP	C3-C4-C5	-2.70	115.35	118.59
3	D	1913	PLP	O3-C3-C4	-2.66	111.16	118.10
3	E	2413	PLP	C4A-C4-C3	-2.65	116.11	120.52
3	A	413	PLP	C2A-C2-C3	2.62	123.86	120.80
3	H	3913	PLP	C6-C5-C4	2.59	120.22	118.10
3	G	3413	PLP	O3P-P-O1P	2.59	120.92	110.83
2	C	1414	TRP	OXT-C-O	-2.58	118.23	124.08
2	H	3914	TRP	CA-CB-CG	2.56	118.36	113.49
3	D	1913	PLP	C5A-C5-C6	-2.56	115.19	119.36
3	F	2913	PLP	C4A-C4-C3	-2.55	116.27	120.52
3	G	3413	PLP	O3-C3-C2	2.50	122.76	117.58
3	H	3913	PLP	C4-C3-C2	2.48	123.60	119.89
3	E	2413	PLP	O4P-C5A-C5	-2.45	104.76	109.36
2	C	1414	TRP	CB-CA-N	-2.43	101.80	112.42
3	C	1413	PLP	O3P-P-O1P	2.43	120.28	110.83
2	E	2914	TRP	CD2-CG-CD1	2.42	108.63	106.16
3	E	2413	PLP	C5-C6-N1	-2.41	119.91	123.83
3	B	913	PLP	C6-C5-C4	2.40	120.06	118.10
2	D	1914	TRP	OXT-C-O	-2.38	118.68	124.08
3	E	2413	PLP	O3P-P-O1P	2.37	120.08	110.83
2	E	2414	TRP	CB-CG-CD1	2.37	131.59	126.97
3	B	913	PLP	O3-C3-C4	-2.35	111.97	118.10
2	G	3414	TRP	OXT-C-O	-2.34	118.77	124.08
3	H	3913	PLP	O3P-P-O1P	2.34	119.95	110.83
3	B	913	PLP	O3P-P-O1P	2.33	119.91	110.83
3	F	2913	PLP	C5-C6-N1	-2.26	120.15	123.83
3	E	2413	PLP	C4-C3-C2	-2.25	116.53	119.89
3	G	3413	PLP	O4P-C5A-C5	-2.20	105.22	109.36
2	A	914	TRP	CZ3-CH2-CZ2	2.15	122.89	120.24
3	F	2913	PLP	O3-C3-C4	-2.13	112.53	118.10
2	C	1414	TRP	CB-CG-CD2	-2.12	122.62	126.70
3	G	3413	PLP	C3-C2-N1	2.12	123.63	120.96
3	A	413	PLP	O2P-P-O4P	2.04	111.98	106.67
3	C	1413	PLP	C2A-C2-C3	-2.03	118.42	120.80
3	A	413	PLP	C5-C6-N1	-2.01	120.56	123.83

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	414	TRP	N-CA-CB-CG
2	C	1414	TRP	N-CA-CB-CG
2	D	1914	TRP	N-CA-CB-CG
2	D	1914	TRP	C-CA-CB-CG
2	G	3414	TRP	N-CA-CB-CG
3	C	1413	PLP	C5A-O4P-P-O3P
3	F	2913	PLP	C5A-O4P-P-O1P
3	F	2913	PLP	C5A-O4P-P-O2P
3	F	2913	PLP	C5A-O4P-P-O3P
2	A	414	TRP	OXT-C-CA-CB
2	E	2414	TRP	OXT-C-CA-N
2	H	3914	TRP	O-C-CA-CB
2	A	414	TRP	O-C-CA-CB
2	H	3914	TRP	OXT-C-CA-CB
2	C	1414	TRP	OXT-C-CA-N
2	G	3414	TRP	CA-CB-CG-CD2
2	A	914	TRP	CA-CB-CG-CD2
2	C	1414	TRP	O-C-CA-N
2	E	2414	TRP	O-C-CA-N
2	C	1414	TRP	O-C-CA-CB
2	H	3914	TRP	CA-CB-CG-CD2
2	C	1414	TRP	CA-CB-CG-CD1
2	C	1414	TRP	OXT-C-CA-CB
3	B	913	PLP	C5A-O4P-P-O3P
3	G	3413	PLP	C5A-O4P-P-O3P
2	A	414	TRP	CA-CB-CG-CD2
2	C	1414	TRP	CA-CB-CG-CD2
2	D	1914	TRP	CA-CB-CG-CD2
2	A	414	TRP	CA-CB-CG-CD1
2	A	914	TRP	N-CA-CB-CG
2	H	3914	TRP	N-CA-CB-CG
2	H	3914	TRP	CA-CB-CG-CD1
2	D	1914	TRP	CA-CB-CG-CD1
2	G	3414	TRP	OXT-C-CA-CB
2	A	914	TRP	C-CA-CB-CG
2	H	3914	TRP	C-CA-CB-CG
2	A	414	TRP	OXT-C-CA-N
2	A	414	TRP	O-C-CA-N
3	E	2413	PLP	C5A-O4P-P-O3P
3	E	2413	PLP	C4-C5-C5A-O4P
2	G	3414	TRP	CA-CB-CG-CD1

There are no ring outliers.

15 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	414	TRP	2	0
2	A	914	TRP	8	0
2	C	1414	TRP	8	0
2	E	2914	TRP	11	0
2	G	3414	TRP	6	0
3	A	413	PLP	1	0
2	D	1914	TRP	11	0
2	E	2414	TRP	3	0
3	B	913	PLP	3	0
3	E	2413	PLP	1	0
3	G	3413	PLP	1	0
3	H	3913	PLP	1	0
2	H	3914	TRP	1	0
3	C	1413	PLP	5	0
3	D	1913	PLP	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	382/385 (99%)	-0.55	0 100 100	3, 17, 38, 57	0
1	B	382/385 (99%)	-0.58	1 (0%) 90 82	3, 18, 40, 66	0
1	C	382/385 (99%)	-0.58	0 100 100	2, 17, 38, 50	0
1	D	382/385 (99%)	-0.59	0 100 100	2, 16, 33, 50	0
1	E	382/385 (99%)	-0.62	1 (0%) 90 82	2, 16, 37, 53	0
1	F	382/385 (99%)	-0.61	0 100 100	2, 15, 33, 56	0
1	G	382/385 (99%)	-0.60	0 100 100	3, 15, 34, 54	0
1	H	382/385 (99%)	-0.60	0 100 100	3, 17, 37, 60	0
All	All	3056/3080 (99%)	-0.59	2 (0%) 92 90	2, 16, 37, 66	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	675	ASN	2.6
1	E	2032	ASP	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRP	G	3414	15/15	0.39	0.27	32,53,59,59	0
2	TRP	E	2914	15/15	0.59	0.27	29,61,76,77	0
2	TRP	D	1914	15/15	0.66	0.20	32,43,59,61	0
2	TRP	C	1414	15/15	0.67	0.23	41,64,68,70	0
2	TRP	E	2414	15/15	0.75	0.18	21,50,56,57	0
2	TRP	A	914	15/15	0.77	0.26	26,59,74,75	0
2	TRP	A	414	15/15	0.77	0.16	35,41,47,49	0
2	TRP	H	3914	15/15	0.80	0.14	23,43,48,49	0
3	PLP	C	1413	15/16	0.92	0.09	8,18,24,34	0
3	PLP	E	2413	15/16	0.93	0.10	2,7,23,33	0
3	PLP	D	1913	15/16	0.94	0.08	2,14,19,26	0
3	PLP	A	413	15/16	0.94	0.09	8,24,34,40	0
3	PLP	H	3913	15/16	0.95	0.07	7,17,27,30	0
3	PLP	F	2913	15/16	0.96	0.07	2,5,16,21	0
3	PLP	G	3413	15/16	0.97	0.06	2,5,17,27	0
3	PLP	B	913	15/16	0.98	0.04	2,7,13,20	0

6.5 Other polymers

There are no such residues in this entry.