



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:35 AM UTC

PDB ID : 7GPB / pdb_00007gpb
Title : STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE
CONTROL BY PHOSPHORYLATION AND AMP
Authors : Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on : 1990-11-13
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

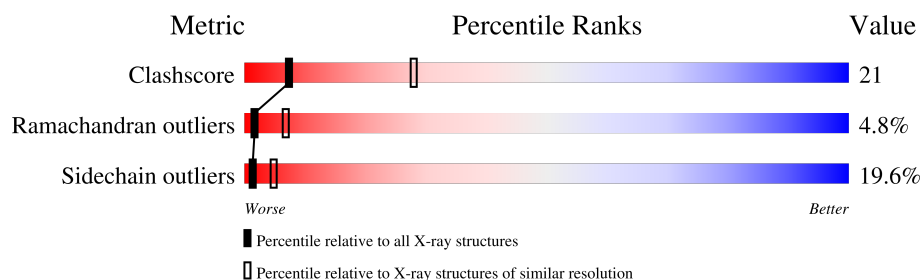
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	
1	B	842	
1	C	842	
1	D	842	

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	SO4	A	901	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26955 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.

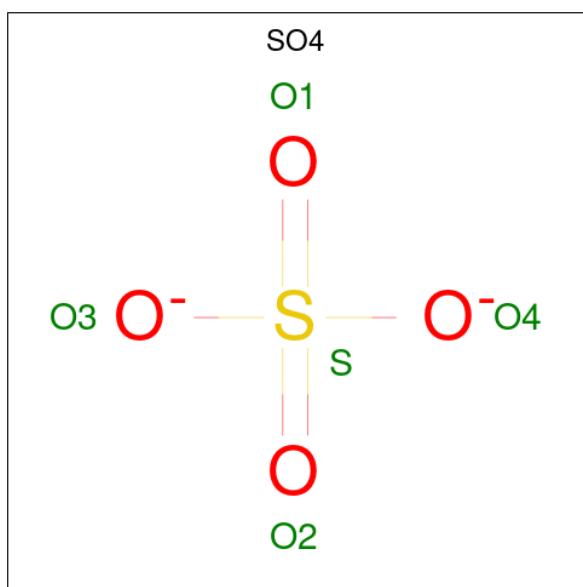
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	B	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	C	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	D	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			

There are 4 discrepancies between the modelled and reference sequences:

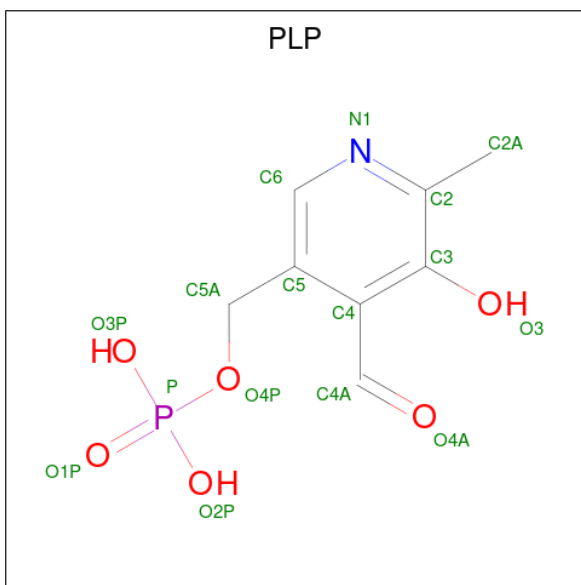
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



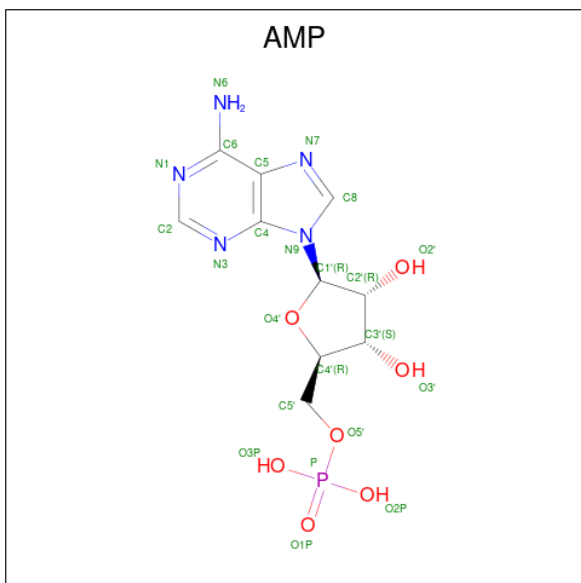
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- 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		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



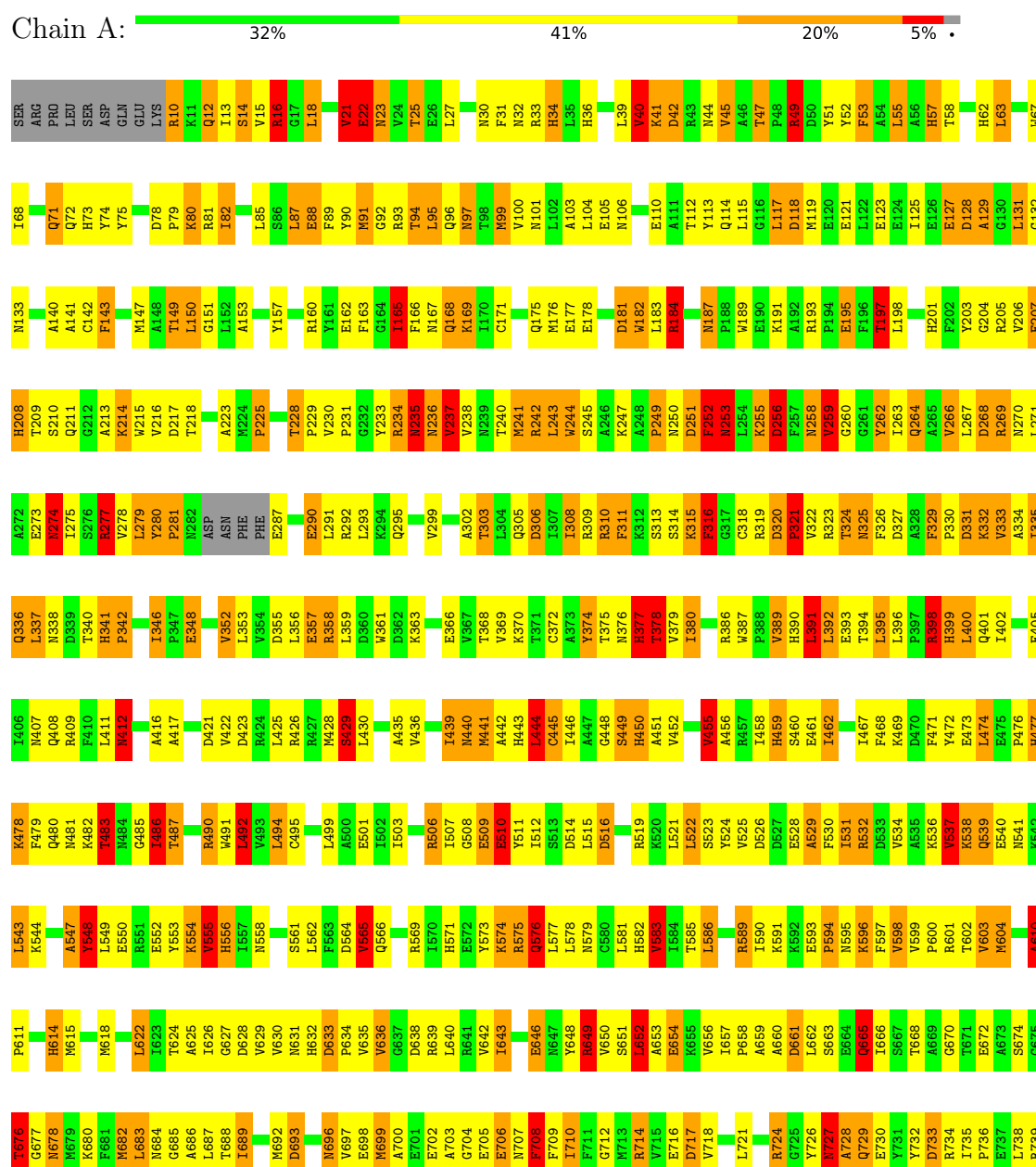
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	D	1	Total 23	C 10	N 5	O 7	P 1	0	0

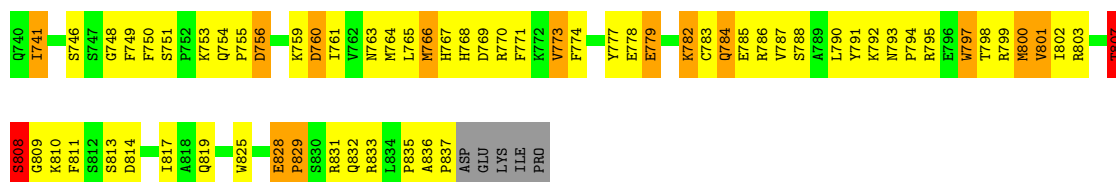
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

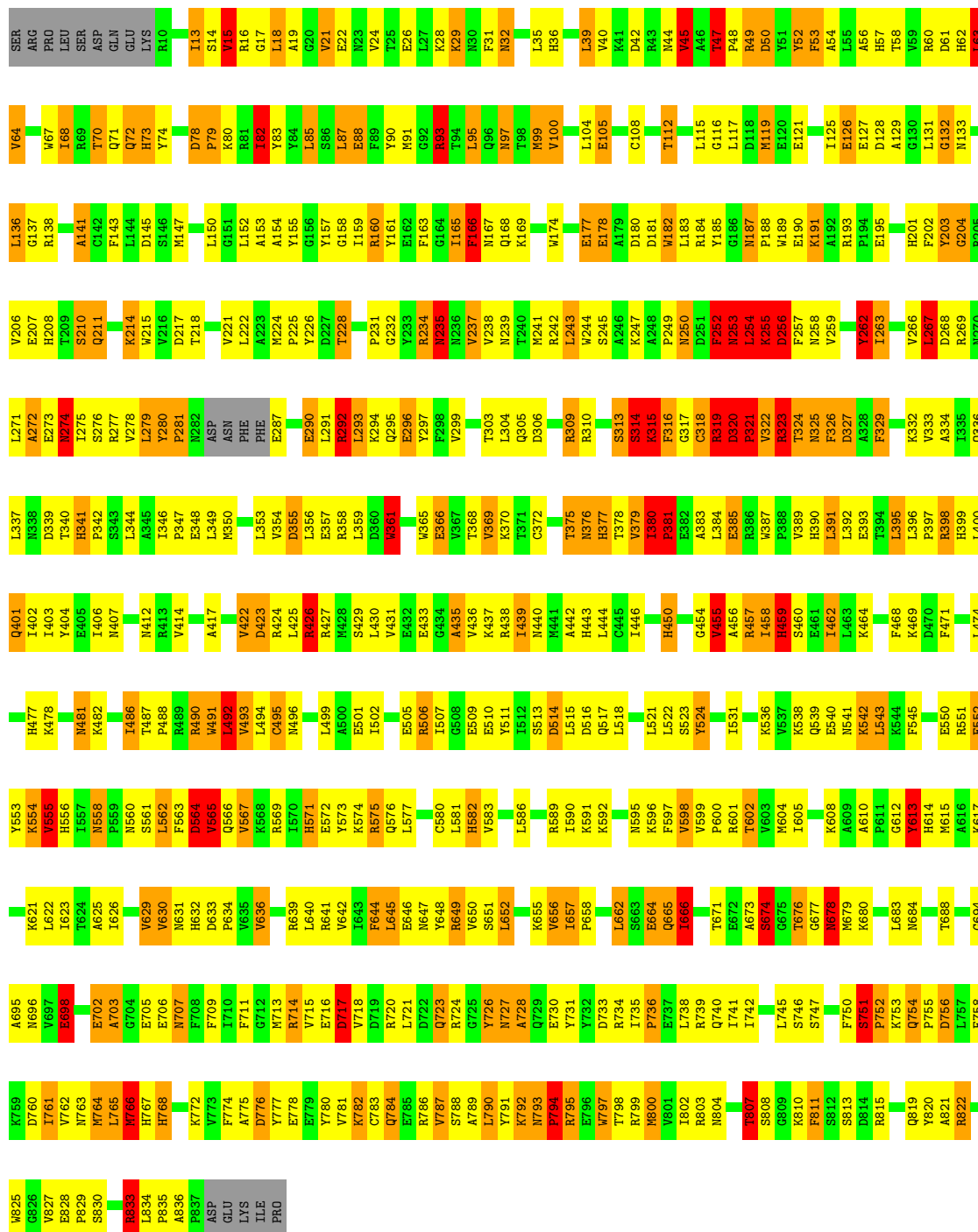
• Molecule 1: GLYCOGEN PHOSPHORYLASE B



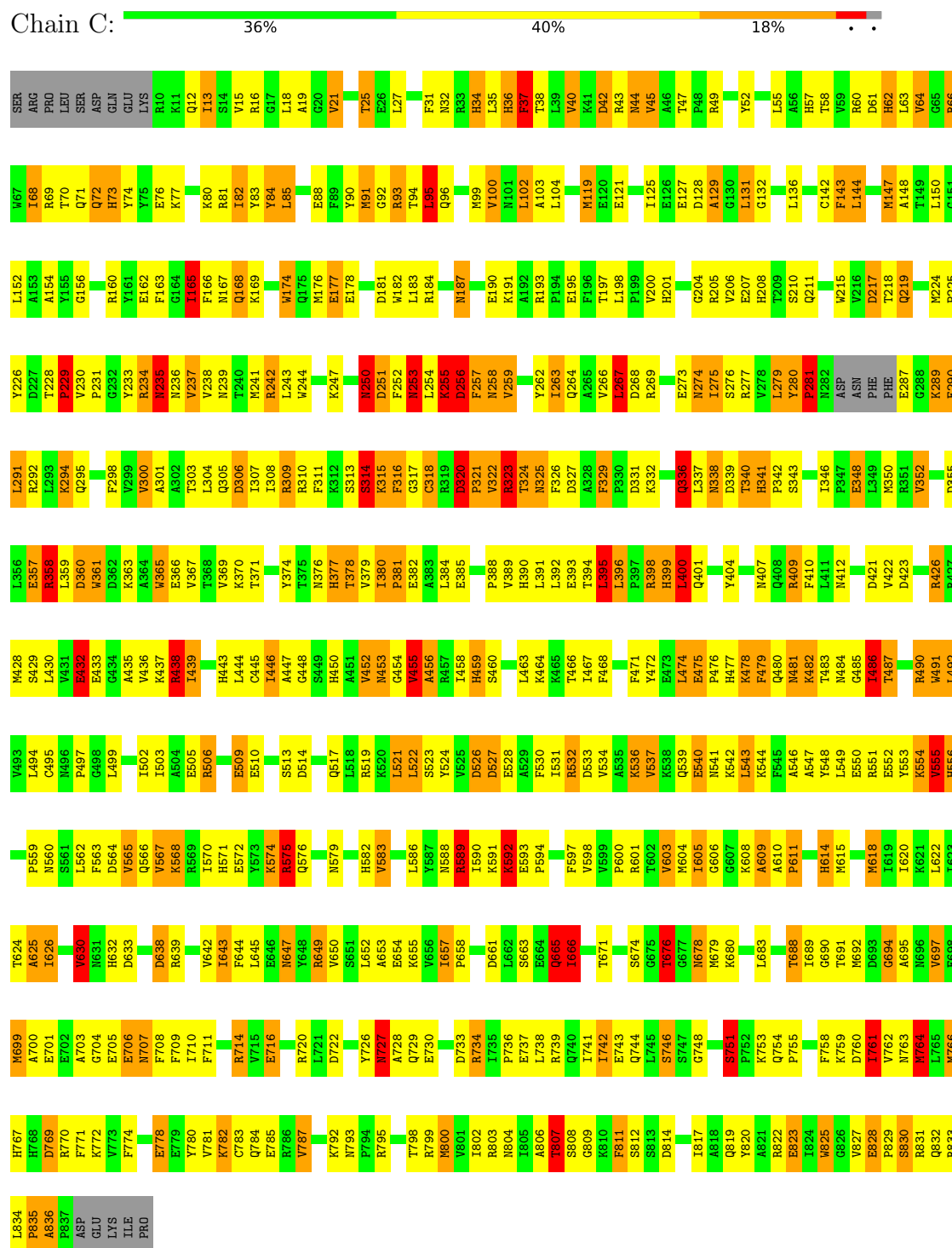


• Molecule 1: GLYCOGEN PHOSPHORYLASE B

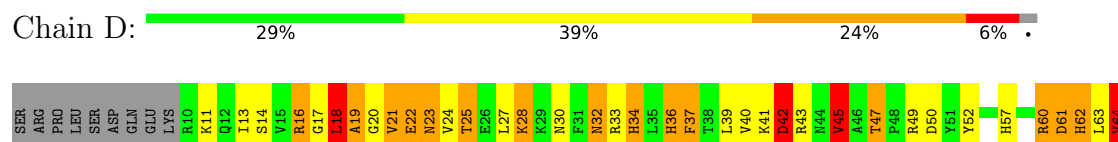
Chain B: 34% 41% 18% 5%



● Molecule 1: GLYCOGEN PHOSPHORYLASE B



● Molecule 1: GLYCOGEN PHOSPHORYLASE B



N793	R724	R658	A529	L463	E393	P330	L267	H201	L131	G65
F794	G725	A659	F530	A464	T394	D331	D268	R205	G132	R66
E796	Y726	A660	I531	K465	L395	K332	R269	R206	N133	W67
W797	N727	D661	R532	T466	L396	V333	N270	V206	G136	I68
T798	A728	L662	D533	F467	P397	A334	E273	E207	G137	R69
W799	Y732	S663	N595	F468	R398	I335	N274	H208	R138	T70
R800	D733	E664	K596	K469	H399	O386	I275	T209	G171	Q71
W801	R734	Q665	F597	D470	L400	L337	N276	S210	F143	Q72
R802	I735	I666	V537	L474	Q401	N338	S276	Q211	L144	H73
R803	Y735	A669	K538	L475	I402	D339	R277	Q211	Y74	Y75
N804	L738	A673	E540	F476	N407	H341	V278	K214	D145	E76
T805	R739	S674	R541	H477	Q408	P342	L279	V215	S146	E77
A806	Q740	G675	K542	K478	R409	S343	P281	V216	M147	K77
S807	I741	G676	L543	F479	F410	L344	T282	D217	A148	D78
S808	Q744	T676	K544	Q480	N412	A345	ASP	T218	L149	P79
G809	Q744	G677	F545	Q481	N413	I346	ASN	Q219	L150	K80
K810	Q744	G678	A546	K482	R413	P347	PHE	G151	G151	R81
F811	G748	N679	A547	T483	V414	E348	PHE	L152	L152	I82
S812	F749	K680	Y548	N484	A415	L349	E287	A153	A153	Y83
L813	F750	F681	L549	G485	A416	K350	E287	A154	A154	Y84
D814	S751	H614	E550	T486	N481	R351	K289	Y155	Y155	L85
R815	P752	L683	R551	T487	N412	V352	E290	G156	G156	
K816	K753	N684	A616	P488	D421	L291	K291	R160	R160	F89
T817	Q754	G684	Y552	R489	V422	R292	L291	Y161	Y161	F90
A818	P755	L687	K554	R490	D423	L356	L293	E162	E162	R81
Q819	D756	T688	Y555	W491	R424	E357	L293	F163	F163	G92
Y820	L757	R689	R556	L492	L425	R388	K294	G164	G164	R93
A821	F758	G690	R557	L492	R426	L359	Q295	R234	R234	T94
R822	K759	N691	N558	V493	R427	D360	E296	F165	F165	L95
E823	D760	N692	N559	L494	M428	V361	Y297	F166	F166	Q96
T824	Q761	G693	P559	C495	S429	K362	Y298	N236	N236	N97
N825	I762	G694	N560	N496	L430	K363	V299	V237	V237	T98
G826	Y763	G694	S561	P497	V431	A364	V300	K169	K169	M99
W827	N763	A695	L562	G498	A435	W365	A301	I170	I170	V100
L765	N764	N696	F563	L499	A500	E366	A302	C171	C171	
N766	L765	V697	D564	L500	V436	V367	T303	G172	G172	N101
H767	N766	E698	Y565	E501	R437	T368	L304	L102	L102	L102
H768	H767	N699	Q566	I502	R438	V369	Q305	W174	W174	A103
D769	H768	E701	Y567	I503	I439	K370	D306	Q175	Q175	E105
Y773	D769	E702	R569	R506	N440	T371	I307	M176	M176	L104
F774	Y773	A703	I570	I507	H443	C372	I308	E177	E177	N106
A775	F774	G704	H571	I507	L444	A373	R309	E178	E178	A107
E776	A775	E705	E572	Y511	C445	Y374	K312	A248	A248	E110
Y777	D776	E706	Y573	D514	L446	N376	S313	P249	P249	E110
E778	Y777	N707	K574	D514	L446	N376	S313	D251	D251	Y113
E779	E778	F708	R575	L515	S449	T378	K315	F252	F252	Y113
W782	E779	F709	Q576	D516	H450	V379	F316	L183	L183	Q114
C783	Q782	I710	L577	E646	A451	I380	G317	R184	R184	L115
Q784	C783	F711	L578	L518	V452	P381	C318	M187	M187	M119
E785	Q784	G712	N579	R519	M453	E382	R319	P188	P188	
R786	E785	M713	C580	K520	G454	A383	D320	W189	W189	L122
W787	R786	V715	L581	L521	V455	P321	N258	E190	E190	E123
S788	W787	L652	H582	L522	A456	V322	F257	E124	E124	E124
A789	S788	Y583	S523	S523	R457	R323	V259	R193	R193	I125
L790	A789	I584	Y524	Y524	I458	W387	Y262	T197	T197	E127
Y791	L790	Y587	V525	D526	R459	V389	I263	L198	L198	E127
K792	K792	N588	D527	E461	S460	H390	Q264	P199	P199	A129
		R589	E528	E528	I462	L392	V266	V200	V200	G130

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26955	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, PLP, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.29	43/6842 (0.6%)	2.34	408/9258 (4.4%)
1	B	1.28	44/6842 (0.6%)	2.25	324/9258 (3.5%)
1	C	1.28	45/6842 (0.7%)	2.27	349/9258 (3.8%)
1	D	1.26	38/6842 (0.6%)	2.31	360/9258 (3.9%)
All	All	1.28	170/27368 (0.6%)	2.29	1441/37032 (3.9%)

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	6
1	B	0	6
1	C	0	5
1	D	0	8
All	All	0	25

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	VAL	CA-CB	11.80	1.70	1.54
1	C	657	ILE	CA-CB	9.83	1.59	1.54
1	A	829	PRO	CA-CB	-8.38	1.41	1.53
1	D	626	ILE	CA-CB	8.34	1.64	1.54
1	C	630	VAL	CA-CB	8.31	1.64	1.54
1	B	323	ARG	CZ-NH1	8.18	1.44	1.32
1	B	318	CYS	C-N	7.95	1.44	1.33
1	B	165	ILE	CA-CB	7.71	1.63	1.54
1	B	567	VAL	CA-CB	7.71	1.65	1.54
1	A	225	PRO	CA-CB	-7.52	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	388	PRO	CA-CB	-7.48	1.43	1.53
1	B	459	HIS	CD2-NE2	-7.47	1.29	1.37
1	A	323	ARG	NE-CZ	7.40	1.41	1.33
1	C	237	VAL	CA-CB	7.38	1.63	1.54
1	C	256	ASP	C-N	7.34	1.44	1.33
1	B	322	VAL	CA-CB	7.31	1.63	1.54
1	B	278	VAL	CA-CB	7.16	1.63	1.54
1	B	582	HIS	CD2-NE2	-7.14	1.30	1.37
1	C	571	HIS	CD2-NE2	-7.09	1.30	1.37
1	C	582	HIS	CD2-NE2	-7.06	1.30	1.37
1	C	62	HIS	CD2-NE2	-7.03	1.30	1.37
1	D	459	HIS	CD2-NE2	-7.03	1.30	1.37
1	C	68	ILE	CA-CB	7.01	1.62	1.54
1	C	341	HIS	CD2-NE2	-6.94	1.30	1.37
1	B	40	VAL	CA-CB	6.92	1.63	1.54
1	C	200	VAL	CA-CB	-6.91	1.46	1.54
1	A	201	HIS	CD2-NE2	-6.88	1.30	1.37
1	A	666	ILE	CA-CB	6.88	1.63	1.54
1	B	341	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	57	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	36	HIS	CD2-NE2	-6.77	1.30	1.37
1	B	319	ARG	CZ-NH1	6.76	1.42	1.32
1	A	632	HIS	CD2-NE2	-6.75	1.30	1.37
1	B	767	HIS	CD2-NE2	-6.75	1.30	1.37
1	D	281	PRO	C-N	-6.73	1.24	1.33
1	C	399	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	341	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	459	HIS	CD2-NE2	-6.59	1.30	1.37
1	B	556	HIS	CD2-NE2	-6.59	1.30	1.37
1	D	450	HIS	CD2-NE2	-6.56	1.30	1.37
1	C	73	HIS	CD2-NE2	-6.55	1.30	1.37
1	C	281	PRO	C-N	-6.52	1.24	1.33
1	C	556	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	377	HIS	CG-ND1	-6.49	1.31	1.38
1	D	571	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	201	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	443	HIS	CG-ND1	-6.38	1.31	1.38
1	D	443	HIS	CD2-NE2	-6.37	1.30	1.37
1	D	57	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.34	1.30	1.37
1	D	34	HIS	CG-ND1	-6.34	1.31	1.38
1	B	57	HIS	CD2-NE2	-6.33	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	HIS	CD2-NE2	-6.33	1.30	1.37
1	C	459	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	34	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	443	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	377	HIS	CD2-NE2	-6.28	1.30	1.37
1	D	819	GLN	CA-CB	-6.26	1.43	1.53
1	D	767	HIS	CD2-NE2	-6.23	1.31	1.37
1	C	614	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	767	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	323	ARG	CZ-NH2	6.16	1.41	1.33
1	A	57	HIS	CG-ND1	-6.15	1.31	1.38
1	C	352	VAL	CA-CB	-6.15	1.47	1.54
1	D	632	HIS	CD2-NE2	-6.15	1.31	1.37
1	B	632	HIS	CD2-NE2	-6.14	1.31	1.37
1	B	281	PRO	C-N	-6.13	1.24	1.33
1	B	73	HIS	CD2-NE2	-6.12	1.31	1.37
1	D	201	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	208	HIS	CD2-NE2	-6.11	1.31	1.37
1	D	377	HIS	CD2-NE2	-6.11	1.31	1.37
1	D	36	HIS	CG-ND1	-6.10	1.31	1.38
1	C	82	ILE	CA-CB	6.06	1.61	1.54
1	A	614	HIS	CD2-NE2	-6.05	1.31	1.37
1	C	201	HIS	CD2-NE2	-6.04	1.31	1.37
1	D	34	HIS	CD2-NE2	-6.04	1.31	1.37
1	D	36	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	281	PRO	C-N	-6.01	1.25	1.33
1	D	200	VAL	CA-CB	-6.00	1.47	1.54
1	B	443	HIS	CD2-NE2	-6.00	1.31	1.37
1	D	556	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	571	HIS	CD2-NE2	-5.99	1.31	1.37
1	D	208	HIS	CD2-NE2	-5.99	1.31	1.37
1	C	477	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	36	HIS	CG-ND1	-5.98	1.31	1.38
1	A	477	HIS	CD2-NE2	-5.97	1.31	1.37
1	D	399	HIS	CD2-NE2	-5.94	1.31	1.37
1	C	34	HIS	CG-ND1	-5.93	1.31	1.38
1	B	390	HIS	CD2-NE2	-5.92	1.31	1.37
1	D	614	HIS	CD2-NE2	-5.91	1.31	1.37
1	D	82	ILE	CA-CB	5.88	1.60	1.53
1	A	443	HIS	CD2-NE2	-5.88	1.31	1.37
1	B	15	VAL	CA-CB	5.87	1.60	1.54
1	B	450	HIS	CD2-NE2	-5.87	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	450	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	21	VAL	CA-CB	5.84	1.62	1.54
1	B	136	LEU	CA-C	-5.84	1.47	1.52
1	C	767	HIS	CD2-NE2	-5.84	1.31	1.37
1	C	399	HIS	CG-ND1	-5.83	1.31	1.38
1	D	73	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	73	HIS	CG-ND1	-5.79	1.31	1.38
1	C	377	HIS	CD2-NE2	-5.78	1.31	1.37
1	D	62	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	377	HIS	CD2-NE2	-5.76	1.31	1.37
1	C	83	TYR	CA-C	-5.75	1.45	1.52
1	A	768	HIS	CD2-NE2	-5.74	1.31	1.37
1	D	582	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	62	HIS	CD2-NE2	-5.72	1.31	1.37
1	C	632	HIS	CD2-NE2	-5.70	1.31	1.37
1	D	64	VAL	CA-CB	5.70	1.61	1.54
1	C	208	HIS	CD2-NE2	-5.70	1.31	1.37
1	C	57	HIS	CD2-NE2	-5.67	1.31	1.37
1	B	614	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	556	HIS	CD2-NE2	-5.66	1.31	1.37
1	C	390	HIS	CD2-NE2	-5.65	1.31	1.37
1	C	83	TYR	CA-CB	-5.63	1.45	1.53
1	B	318	CYS	C-O	5.62	1.31	1.24
1	C	40	VAL	CA-CB	5.62	1.62	1.54
1	B	82	ILE	CA-CB	5.61	1.61	1.54
1	D	253	ASN	C-N	5.60	1.41	1.33
1	D	388	PRO	CA-CB	-5.58	1.46	1.53
1	D	379	VAL	CA-CB	5.58	1.61	1.54
1	D	318	CYS	C-O	5.56	1.30	1.24
1	B	208	HIS	CD2-NE2	-5.56	1.31	1.37
1	A	656	VAL	CA-CB	5.56	1.60	1.54
1	D	361	TRP	CG-CD2	-5.56	1.33	1.43
1	B	556	HIS	CB-CG	5.55	1.57	1.50
1	D	188	PRO	CA-CB	-5.54	1.45	1.53
1	B	477	HIS	CD2-NE2	-5.53	1.31	1.37
1	D	820	TYR	CA-CB	5.52	1.62	1.53
1	A	450	HIS	CG-ND1	-5.51	1.32	1.38
1	A	399	HIS	CD2-NE2	-5.51	1.31	1.37
1	B	450	HIS	CG-ND1	-5.51	1.32	1.38
1	A	450	HIS	CD2-NE2	-5.49	1.31	1.37
1	C	466	THR	CA-CB	5.49	1.60	1.53
1	C	325	ASN	CA-C	-5.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ASN	C-N	5.44	1.41	1.33
1	B	582	HIS	CG-ND1	-5.42	1.32	1.38
1	A	571	HIS	CD2-NE2	-5.41	1.31	1.37
1	D	399	HIS	CG-ND1	-5.38	1.32	1.38
1	B	404	TYR	CA-CB	-5.35	1.44	1.53
1	A	399	HIS	CG-ND1	-5.33	1.32	1.38
1	A	323	ARG	CZ-NH1	5.33	1.40	1.32
1	B	657	ILE	CA-CB	5.32	1.61	1.54
1	A	259	VAL	CA-CB	5.31	1.61	1.54
1	C	827	VAL	CA-CB	5.31	1.62	1.54
1	D	768	HIS	CD2-NE2	-5.29	1.32	1.37
1	A	201	HIS	CG-ND1	-5.28	1.32	1.38
1	B	399	HIS	CD2-NE2	-5.27	1.32	1.37
1	C	643	ILE	CA-CB	5.27	1.61	1.54
1	D	390	HIS	CD2-NE2	-5.27	1.32	1.37
1	B	768	HIS	CD2-NE2	-5.27	1.32	1.37
1	A	582	HIS	CD2-NE2	-5.26	1.32	1.37
1	C	34	HIS	CD2-NE2	-5.22	1.32	1.37
1	C	263	ILE	CA-CB	5.17	1.61	1.54
1	B	319	ARG	NE-CZ	5.15	1.38	1.33
1	A	223	ALA	CA-CB	-5.14	1.45	1.53
1	A	626	ILE	CA-CB	-5.13	1.48	1.54
1	B	787	VAL	CA-CB	5.12	1.60	1.54
1	C	242	ARG	CA-CB	-5.09	1.45	1.53
1	A	565	VAL	CA-CB	5.08	1.62	1.55
1	C	201	HIS	CG-ND1	-5.07	1.32	1.38
1	C	396	LEU	N-CA	-5.07	1.41	1.46
1	A	165	ILE	CA-CB	5.06	1.61	1.54
1	D	477	HIS	CD2-NE2	-5.05	1.32	1.37
1	C	331	ASP	CA-C	-5.05	1.46	1.52
1	C	438	ARG	CA-C	-5.03	1.46	1.52
1	A	311	PHE	CA-CB	-5.02	1.45	1.53
1	D	244	TRP	CG-CD2	-5.01	1.34	1.43
1	A	335	ILE	CA-CB	5.01	1.63	1.55

All (1441) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	TRP	CG-CD2-CE3	-36.55	97.35	133.90
1	D	67	TRP	NE1-CE2-CZ2	-24.67	93.09	130.10
1	B	477	HIS	CA-CB-CG	13.92	127.72	113.80
1	A	181	ASP	CA-CB-CG	13.84	126.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	575	ARG	N-CA-C	13.75	130.00	113.23
1	A	509	GLU	N-CA-C	13.67	129.25	111.75
1	D	61	ASP	CA-CB-CG	12.73	125.33	112.60
1	C	45	VAL	N-CA-CB	-12.48	96.13	112.36
1	B	320	ASP	CA-CB-CG	12.25	124.85	112.60
1	A	332	LYS	N-CA-C	12.11	127.55	113.02
1	B	455	VAL	N-CA-CB	-12.11	94.15	112.67
1	B	324	THR	N-CA-C	-12.05	95.01	111.28
1	C	807	THR	N-CA-CB	-12.01	92.90	110.80
1	C	324	THR	N-CA-C	-11.97	94.86	111.39
1	A	575	ARG	N-CA-C	11.90	127.72	111.54
1	C	252	PHE	CA-CB-CG	11.86	125.66	113.80
1	B	180	ASP	CA-CB-CG	11.70	124.30	112.60
1	B	250	ASN	N-CA-C	11.64	127.94	111.30
1	C	306	ASP	CA-CB-CG	11.58	124.18	112.60
1	A	320	ASP	CA-CB-CG	11.45	124.05	112.60
1	D	575	ARG	N-CA-C	11.41	126.50	112.58
1	D	533	ASP	CA-CB-CG	11.38	123.98	112.60
1	A	515	LEU	N-CA-C	11.17	124.78	111.82
1	B	18	LEU	N-CA-C	11.10	129.83	107.41
1	B	575	ARG	N-CA-C	11.06	126.34	111.30
1	B	163	PHE	N-CA-C	11.02	127.10	112.88
1	A	654	GLU	CA-CB-CG	11.02	136.15	114.10
1	B	235	ASN	CA-CB-CG	10.92	123.52	112.60
1	A	727	ASN	CA-CB-CG	10.87	123.47	112.60
1	C	552	GLU	N-CA-C	-10.81	88.85	107.99
1	D	582	HIS	CA-CB-CG	10.79	124.59	113.80
1	A	336	GLN	OE1-CD-NE2	-10.75	111.85	122.60
1	A	455	VAL	N-CA-CB	-10.72	98.00	111.94
1	D	278	VAL	N-CA-C	10.69	122.91	108.27
1	C	338	ASN	OD1-CG-ND2	-10.65	111.95	122.60
1	A	578	LEU	N-CA-C	-10.54	99.48	110.97
1	D	631	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	A	716	GLU	CB-CG-CD	10.49	130.44	112.60
1	C	626	ILE	N-CA-C	-10.49	100.35	110.42
1	D	564	ASP	CA-CB-CG	10.45	123.05	112.60
1	A	175	GLN	OE1-CD-NE2	-10.42	112.18	122.60
1	B	602	THR	N-CA-C	-10.34	91.39	108.34
1	A	277	ARG	NH1-CZ-NH2	-10.23	106.00	119.30
1	B	552	GLU	N-CA-C	-10.19	92.00	108.41
1	A	262	TYR	N-CA-C	9.97	123.88	107.23
1	B	507	ILE	N-CA-C	9.97	123.54	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ASP	CA-CB-CG	9.94	122.54	112.60
1	C	571	HIS	CB-CG-CD2	-9.92	118.31	131.20
1	A	49	ARG	NE-CZ-NH2	-9.80	110.38	119.20
1	B	455	VAL	CB-CA-C	9.77	120.37	110.70
1	A	727	ASN	OD1-CG-ND2	-9.71	112.89	122.60
1	A	274	ASN	CB-CG-ND2	9.70	130.94	116.40
1	D	326	PHE	N-CA-C	-9.69	101.25	112.87
1	B	133	ASN	CA-CB-CG	9.64	122.24	112.60
1	C	423	ASP	CA-CB-CG	-9.62	102.98	112.60
1	D	148	ALA	CA-C-O	-9.60	111.01	120.90
1	B	126	GLU	CA-CB-CG	-9.60	94.89	114.10
1	A	631	ASN	CA-CB-CG	9.60	122.20	112.60
1	A	217	ASP	CA-CB-CG	9.56	122.16	112.60
1	A	16	ARG	NE-CZ-NH2	9.54	127.79	119.20
1	A	16	ARG	N-CA-C	9.53	122.65	111.02
1	D	148	ALA	N-CA-C	-9.53	100.45	111.03
1	C	19	ALA	N-CA-C	9.53	121.97	108.54
1	A	331	ASP	N-CA-C	-9.51	100.48	111.03
1	D	18	LEU	N-CA-C	9.45	123.25	112.57
1	C	274	ASN	CA-CB-CG	9.45	122.05	112.60
1	A	97	ASN	OD1-CG-ND2	-9.42	113.18	122.60
1	D	313	SER	CA-C-O	-9.37	108.59	120.31
1	A	727	ASN	CB-CG-ND2	9.31	130.36	116.40
1	A	440	ASN	CA-CB-CG	-9.29	103.31	112.60
1	D	230	VAL	N-CA-C	9.29	117.54	107.60
1	D	676	THR	CA-CB-OG1	-9.25	95.72	109.60
1	C	45	VAL	CB-CA-C	9.24	121.10	110.93
1	D	325	ASN	CA-C-O	9.23	132.18	121.28
1	C	380	ILE	N-CA-CB	-9.21	98.31	111.21
1	D	267	LEU	CA-C-O	-9.19	110.68	120.42
1	A	57	HIS	CA-C-O	-9.19	111.23	120.70
1	B	626	ILE	N-CA-C	-9.19	100.71	110.36
1	A	277	ARG	N-CA-C	9.18	122.27	111.71
1	A	389	VAL	CA-C-O	-9.16	111.14	120.85
1	D	324	THR	N-CA-C	-9.16	99.57	111.02
1	A	313	SER	N-CA-C	9.15	123.46	111.75
1	B	513	SER	CA-CB-OG	9.12	129.34	111.10
1	D	760	ASP	CA-CB-CG	9.12	121.72	112.60
1	C	706	GLU	CA-CB-CG	9.11	132.31	114.10
1	C	428	MET	CA-CB-CG	-9.09	95.92	114.10
1	C	255	LYS	O-C-N	9.09	134.05	122.87
1	B	136	LEU	N-CA-C	-9.04	99.75	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	VAL	CA-C-O	-9.02	109.51	120.78
1	C	31	PHE	CA-CB-CG	9.01	122.81	113.80
1	A	96	GLN	CA-C-O	-9.01	111.42	120.70
1	C	647	ASN	CA-CB-CG	8.96	121.56	112.60
1	D	477	HIS	CA-CB-CG	8.96	122.76	113.80
1	C	455	VAL	N-CA-CB	-8.94	96.48	111.23
1	A	366	GLU	N-CA-C	-8.93	101.23	110.97
1	B	571	HIS	CB-CG-CD2	-8.92	119.60	131.20
1	C	325	ASN	OD1-CG-ND2	-8.89	113.71	122.60
1	D	571	HIS	CB-CG-CD2	-8.89	119.65	131.20
1	A	412	ASN	CA-CB-CG	-8.88	103.72	112.60
1	A	582	HIS	CA-CB-CG	8.88	122.68	113.80
1	B	267	LEU	CA-C-O	-8.85	111.59	120.70
1	A	575	ARG	CB-CG-CD	-8.84	90.97	111.30
1	A	325	ASN	N-CA-C	8.84	123.27	110.10
1	A	305	GLN	N-CA-C	-8.84	99.32	112.04
1	C	205	ARG	CA-CB-CG	8.82	131.75	114.10
1	A	324	THR	N-CA-C	-8.81	99.23	111.39
1	D	435	ALA	N-CA-C	-8.78	94.58	108.63
1	A	274	ASN	OD1-CG-ND2	-8.77	113.83	122.60
1	C	42	ASP	CA-CB-CG	8.74	121.34	112.60
1	A	555	VAL	N-CA-C	8.74	127.51	109.34
1	B	647	ASN	CA-CB-CG	8.69	121.29	112.60
1	C	61	ASP	CA-CB-CG	8.68	121.28	112.60
1	D	496	ASN	CA-CB-CG	-8.63	103.97	112.60
1	D	789	ALA	N-CA-C	-8.63	99.61	112.04
1	B	678	ASN	CA-CB-CG	8.63	121.23	112.60
1	C	699	MET	N-CA-C	-8.63	100.87	111.40
1	D	253	ASN	CA-CB-CG	8.59	121.19	112.60
1	A	275	ILE	N-CA-C	-8.56	102.50	111.58
1	C	331	ASP	N-CA-C	-8.53	101.20	111.69
1	D	175	GLN	OE1-CD-NE2	-8.53	114.08	122.60
1	B	717	ASP	CA-CB-CG	8.52	121.12	112.60
1	B	555	VAL	N-CA-C	8.52	127.05	109.34
1	D	23	ASN	CA-CB-CG	-8.51	104.09	112.60
1	C	678	ASN	CA-CB-CG	8.47	121.07	112.60
1	A	548	TYR	N-CA-C	-8.45	102.15	111.36
1	A	649	ARG	CG-CD-NE	-8.45	93.42	112.00
1	C	537	VAL	CB-CA-C	-8.44	101.17	111.97
1	B	250	ASN	OD1-CG-ND2	-8.42	114.18	122.60
1	A	391	LEU	N-CA-C	-8.41	102.19	111.36
1	B	252	PHE	CA-CB-CG	8.41	122.21	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASN	OD1-CG-ND2	-8.40	114.20	122.60
1	D	450	HIS	CB-CG-CD2	-8.36	120.33	131.20
1	A	306	ASP	CA-CB-CG	8.33	120.93	112.60
1	A	449	SER	N-CA-C	8.29	122.60	109.50
1	A	676	THR	CA-CB-OG1	-8.26	97.21	109.60
1	A	583	VAL	CB-CA-C	-8.23	101.03	112.14
1	A	509	GLU	CB-CG-CD	8.22	126.57	112.60
1	C	676	THR	N-CA-CB	-8.20	97.98	110.20
1	B	281	PRO	N-CA-C	8.19	132.58	112.10
1	D	332	LYS	CA-CB-CG	-8.18	97.75	114.10
1	A	18	LEU	N-CA-C	8.15	123.81	112.72
1	B	767	HIS	CA-CB-CG	-8.15	105.65	113.80
1	A	555	VAL	CB-CA-C	-8.14	97.93	111.29
1	A	128	ASP	CA-CB-CG	8.13	120.73	112.60
1	B	274	ASN	CA-CB-CG	8.10	120.70	112.60
1	D	613	TYR	N-CA-C	-8.08	95.24	108.41
1	B	459	HIS	CB-CG-CD2	-8.07	120.70	131.20
1	A	422	VAL	N-CA-C	-8.06	104.88	111.81
1	A	25	THR	CA-CB-OG1	-8.04	97.54	109.60
1	A	149	THR	N-CA-CB	-8.03	98.31	110.12
1	D	325	ASN	O-C-N	8.03	132.34	123.10
1	A	395	LEU	CA-C-N	-8.02	113.45	123.15
1	A	395	LEU	C-N-CA	-8.02	113.45	123.15
1	C	274	ASN	N-CA-C	8.00	121.45	112.97
1	B	357	GLU	N-CA-C	-8.00	99.31	110.35
1	C	459	HIS	CB-CG-CD2	-8.00	120.81	131.20
1	B	325	ASN	CA-C-O	7.99	130.16	121.05
1	C	316	PHE	CA-CB-CG	-7.98	105.82	113.80
1	A	268	ASP	CA-CB-CG	7.98	120.58	112.60
1	C	785	GLU	N-CA-C	-7.97	102.53	111.14
1	D	727	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	B	62	HIS	CA-C-O	7.96	129.10	120.10
1	A	547	ALA	N-CA-C	7.96	120.03	111.36
1	C	638	ASP	CA-CB-CG	7.95	120.55	112.60
1	D	455	VAL	N-CA-CB	-7.94	98.12	111.23
1	B	154	ALA	N-CA-C	7.93	122.16	108.76
1	A	665	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	D	809	GLY	N-CA-C	7.90	122.47	112.83
1	D	652	LEU	N-CA-C	-7.89	103.80	113.50
1	A	564	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	408	GLN	OE1-CD-NE2	-7.87	114.73	122.60
1	A	101	ASN	CA-CB-CG	-7.86	104.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	769	ASP	CA-CB-CG	7.84	120.44	112.60
1	D	97	ASN	CB-CG-ND2	7.84	128.16	116.40
1	A	638	ASP	CA-CB-CG	7.84	120.44	112.60
1	A	469	LYS	N-CA-C	7.83	119.44	111.07
1	C	211	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	C	650	VAL	CA-C-O	-7.80	112.95	121.29
1	B	341	HIS	CB-CG-CD2	-7.79	121.07	131.20
1	C	807	THR	CB-CA-C	7.79	123.54	109.99
1	B	684	ASN	CA-CB-CG	-7.77	104.83	112.60
1	D	676	THR	N-CA-CB	-7.77	99.12	110.47
1	A	676	THR	CA-CB-CG2	7.74	123.66	110.50
1	D	644	PHE	CA-CB-CG	-7.73	106.07	113.80
1	C	486	ILE	N-CA-CB	-7.71	98.51	111.23
1	C	16	ARG	N-CA-C	7.71	124.09	111.37
1	A	305	GLN	CA-C-O	-7.71	110.68	120.31
1	B	766	MET	N-CA-C	7.70	119.75	111.36
1	B	422	VAL	N-CA-CB	-7.69	99.84	110.68
1	C	785	GLU	CB-CG-CD	7.68	125.66	112.60
1	D	325	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	A	12	GLN	CA-CB-CG	7.66	129.42	114.10
1	A	811	PHE	CA-CB-CG	-7.65	106.15	113.80
1	B	542	LYS	N-CA-C	-7.65	103.02	111.36
1	D	588	ASN	CA-CB-CG	7.64	120.24	112.60
1	D	338	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	B	820	TYR	N-CA-C	-7.61	102.93	111.07
1	B	313	SER	N-CA-C	7.60	120.30	111.02
1	D	768	HIS	N-CA-C	7.60	119.95	109.54
1	B	257	PHE	CA-CB-CG	7.60	121.40	113.80
1	A	341	HIS	CB-CG-CD2	-7.59	121.34	131.20
1	D	323	ARG	CA-CB-CG	7.58	129.26	114.10
1	A	461	GLU	CA-C-O	-7.56	112.91	120.70
1	A	646	GLU	CA-C-O	7.56	128.62	120.38
1	D	49	ARG	CA-CB-CG	7.56	129.21	114.10
1	D	793	ASN	N-CA-C	-7.56	98.04	109.30
1	B	15	VAL	N-CA-C	-7.56	102.97	110.30
1	B	696	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	D	361	TRP	CE2-CD2-CE3	7.54	126.34	118.80
1	C	72	GLN	N-CA-C	-7.54	103.00	111.14
1	D	270	ASN	CA-CB-CG	-7.52	105.08	112.60
1	D	258	ASN	N-CA-C	-7.51	102.69	112.68
1	D	431	VAL	N-CA-CB	-7.51	102.43	111.00
1	D	816	THR	CA-CB-CG2	-7.51	97.74	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	808	SER	CB-CA-C	-7.50	97.92	110.68
1	B	165	ILE	N-CA-C	-7.50	96.92	107.80
1	D	571	HIS	CB-CG-ND1	7.48	133.91	122.70
1	B	380	ILE	N-CA-CB	-7.46	101.26	111.86
1	A	72	GLN	N-CA-C	-7.46	103.09	111.07
1	A	807	THR	N-CA-CB	-7.46	97.88	110.41
1	D	650	VAL	CA-C-O	-7.45	113.66	121.41
1	C	268	ASP	CA-CB-CG	7.44	120.04	112.60
1	B	116	GLY	O-C-N	7.43	132.36	122.70
1	D	459	HIS	CB-CG-CD2	-7.43	121.54	131.20
1	C	487	THR	CA-CB-OG1	-7.42	98.47	109.60
1	B	187	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	B	97	ASN	CB-CG-ND2	7.41	127.52	116.40
1	A	803	ARG	CA-CB-CG	-7.41	99.28	114.10
1	D	127	GLU	CA-CB-CG	7.41	128.92	114.10
1	D	114	GLN	CA-CB-CG	-7.41	99.29	114.10
1	B	249	PRO	O-C-N	-7.40	114.07	123.03
1	D	485	GLY	CA-C-N	7.40	132.04	120.34
1	D	485	GLY	C-N-CA	7.40	132.04	120.34
1	C	94	THR	N-CA-C	7.39	122.59	113.50
1	A	554	LYS	CA-C-O	-7.37	111.75	120.60
1	C	792	LYS	N-CA-CB	-7.36	98.05	110.49
1	D	643	ILE	O-C-N	-7.36	116.35	122.97
1	D	534	VAL	N-CA-C	-7.35	103.36	110.42
1	A	258	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	D	568	LYS	CA-CB-CG	7.35	128.79	114.10
1	D	808	SER	N-CA-C	7.35	121.15	111.75
1	A	329	PHE	O-C-N	-7.32	115.22	120.27
1	A	714	ARG	N-CA-C	-7.32	99.62	110.46
1	A	582	HIS	CA-C-O	-7.32	113.14	120.82
1	A	80	LYS	CA-C-O	-7.31	113.15	121.19
1	C	564	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	571	HIS	CB-CG-CD2	-7.30	121.70	131.20
1	A	67	TRP	NE1-CE2-CZ2	-7.30	119.15	130.10
1	D	688	THR	CB-CA-C	-7.30	98.21	109.89
1	B	372	CYS	N-CA-C	7.29	122.21	109.96
1	A	14	SER	N-CA-C	7.28	121.34	109.85
1	B	634	PRO	N-CA-C	7.26	123.45	113.65
1	A	16	ARG	O-C-N	-7.25	114.32	122.08
1	B	412	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	C	348	GLU	CA-C-O	-7.23	113.25	120.70
1	D	727	ASN	CB-CG-ND2	7.23	127.24	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	776	ASP	CA-CB-CG	7.23	119.83	112.60
1	D	372	CYS	N-CA-C	7.23	120.77	110.14
1	B	401	GLN	N-CA-C	-7.23	103.01	111.03
1	C	571	HIS	CB-CG-ND1	7.22	133.53	122.70
1	D	16	ARG	N-CA-C	7.22	126.18	110.80
1	A	332	LYS	CA-CB-CG	-7.22	99.66	114.10
1	B	380	ILE	N-CA-C	7.22	119.11	107.71
1	A	435	ALA	N-CA-C	-7.21	96.79	108.41
1	D	394	THR	CA-CB-OG1	-7.21	98.78	109.60
1	C	395	LEU	CA-C-N	-7.21	114.82	122.89
1	C	395	LEU	C-N-CA	-7.21	114.82	122.89
1	D	561	SER	N-CA-C	7.20	126.13	110.80
1	D	551	ARG	N-CA-C	-7.19	95.48	110.80
1	B	613	TYR	N-CA-C	-7.18	98.80	109.15
1	C	727	ASN	CA-CB-CG	7.18	119.78	112.60
1	D	579	ASN	CA-CB-CG	7.18	119.78	112.60
1	B	608	LYS	N-CA-C	-7.17	98.04	109.59
1	C	217	ASP	N-CA-C	7.17	121.05	111.30
1	C	338	ASN	CB-CG-ND2	7.17	127.15	116.40
1	D	493	VAL	N-CA-C	7.17	117.27	110.53
1	D	749	PHE	N-CA-C	-7.17	103.16	110.97
1	C	676	THR	CA-CB-OG1	-7.16	98.86	109.60
1	C	707	ASN	CB-CG-ND2	7.16	127.14	116.40
1	B	340	THR	N-CA-C	7.15	121.45	112.87
1	B	13	ILE	N-CA-C	-7.15	94.47	109.34
1	B	383	ALA	N-CA-C	7.15	121.10	112.38
1	B	664	GLU	N-CA-C	7.14	120.74	109.39
1	A	201	HIS	CA-C-O	-7.13	112.86	121.28
1	A	82	ILE	CB-CA-C	7.13	121.25	110.62
1	D	643	ILE	N-CA-C	7.13	119.52	107.18
1	D	545	PHE	CA-CB-CG	-7.13	106.67	113.80
1	C	95	LEU	CB-CA-C	-7.11	100.01	110.96
1	C	563	PHE	CA-CB-CG	7.09	120.89	113.80
1	B	455	VAL	CA-C-O	7.09	124.99	119.46
1	D	97	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	C	541	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	D	697	VAL	O-C-N	-7.07	113.73	122.57
1	A	401	GLN	CB-CG-CD	-7.06	100.60	112.60
1	B	551	ARG	N-CA-C	-7.05	102.67	112.12
1	A	332	LYS	CB-CG-CD	7.05	127.52	111.30
1	A	733	ASP	CA-CB-CG	-7.05	105.55	112.60
1	A	253	ASN	CA-CB-CG	7.05	119.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	571	HIS	CB-CG-ND1	7.05	133.27	122.70
1	B	716	GLU	CB-CG-CD	7.04	124.56	112.60
1	D	106	ASN	N-CA-C	7.04	118.60	111.07
1	B	740	GLN	CB-CG-CD	-7.04	100.64	112.60
1	A	23	ASN	CA-C-O	7.03	128.20	119.98
1	A	241	MET	N-CA-C	-7.03	97.44	108.90
1	A	509	GLU	CB-CA-C	-7.02	96.83	110.46
1	C	74	TYR	N-CA-C	-7.02	103.62	111.28
1	D	501	GLU	CA-CB-CG	7.02	128.14	114.10
1	B	575	ARG	CB-CG-CD	-7.02	95.16	111.30
1	C	321	PRO	CA-N-CD	-7.02	102.18	112.00
1	A	564	ASP	CA-C-O	-7.01	113.62	120.92
1	B	72	GLN	N-CA-C	-7.01	103.33	110.97
1	B	417	ALA	N-CA-C	7.00	118.70	111.14
1	D	684	ASN	CA-CB-CG	-7.00	105.60	112.60
1	B	780	TYR	CA-C-O	-7.00	113.65	121.00
1	B	825	TRP	CG-CD2-CE3	7.00	140.90	133.90
1	B	464	LYS	CB-CG-CD	-7.00	95.21	111.30
1	C	575	ARG	CB-CG-CD	-6.99	95.22	111.30
1	B	558	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	C	466	THR	CA-C-O	-6.98	115.29	119.55
1	C	275	ILE	N-CA-C	-6.98	102.09	111.44
1	B	459	HIS	CB-CG-ND1	6.97	133.16	122.70
1	A	106	ASN	CA-CB-CG	6.97	119.57	112.60
1	A	807	THR	N-CA-C	6.97	121.61	113.18
1	C	746	SER	N-CA-C	6.97	118.53	111.07
1	C	763	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	D	314	SER	CA-CB-OG	6.96	125.02	111.10
1	D	440	ASN	CA-CB-CG	-6.95	105.65	112.60
1	C	44	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	B	565	VAL	CB-CA-C	-6.95	99.80	110.50
1	A	831	ARG	N-CA-C	-6.94	105.61	112.97
1	D	412	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	D	792	LYS	CA-CB-CG	6.94	127.98	114.10
1	B	62	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	C	52	TYR	N-CA-C	-6.93	103.65	111.07
1	B	238	VAL	N-CA-C	-6.93	98.15	108.12
1	A	310	ARG	CG-CD-NE	-6.92	96.77	112.00
1	C	215	TRP	N-CA-C	-6.92	97.24	108.52
1	A	380	ILE	N-CA-CB	-6.91	103.65	110.08
1	C	393	GLU	CA-CB-CG	6.91	127.91	114.10
1	D	666	ILE	N-CA-C	6.91	123.70	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	597	PHE	CA-CB-CG	-6.90	106.90	113.80
1	B	486	ILE	N-CA-CB	-6.90	100.88	112.47
1	C	565	VAL	N-CA-C	6.89	120.10	108.86
1	B	166	PHE	CA-CB-CG	6.88	120.68	113.80
1	C	435	ALA	N-CA-C	-6.88	98.00	108.67
1	A	663	SER	CA-CB-OG	6.88	124.87	111.10
1	A	749	PHE	N-CA-C	-6.88	103.70	111.07
1	D	253	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	D	801	VAL	O-C-N	-6.88	115.19	121.87
1	A	784	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	A	236	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	D	547	ALA	N-CA-C	6.87	118.85	111.36
1	D	713	MET	N-CA-C	6.87	119.92	110.24
1	C	84	TYR	O-C-N	-6.86	115.37	122.64
1	C	452	VAL	N-CA-C	-6.86	98.24	108.12
1	B	295	GLN	OE1-CD-NE2	-6.86	115.74	122.60
1	C	825	TRP	CG-CD2-CE3	6.85	140.75	133.90
1	D	224	MET	CA-C-N	6.82	126.99	120.31
1	D	224	MET	C-N-CA	6.82	126.99	120.31
1	B	325	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	A	778	GLU	CB-CG-CD	6.80	124.16	112.60
1	D	98	THR	CA-CB-OG1	-6.79	99.41	109.60
1	A	228	THR	CA-C-N	6.79	126.83	119.90
1	A	228	THR	C-N-CA	6.79	126.83	119.90
1	C	242	ARG	CB-CG-CD	-6.78	95.70	111.30
1	C	564	ASP	CA-C-O	-6.78	112.88	120.54
1	D	511	TYR	N-CA-C	6.78	119.53	111.33
1	A	274	ASN	CA-CB-CG	6.78	119.38	112.60
1	C	197	THR	N-CA-C	6.77	120.05	109.96
1	B	784	GLN	CG-CD-NE2	6.77	126.55	116.40
1	C	560	ASN	CA-CB-CG	6.77	119.37	112.60
1	A	643	ILE	N-CA-C	6.76	117.58	108.11
1	D	490	ARG	NE-CZ-NH2	-6.76	113.11	119.20
1	C	407	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	C	40	VAL	CG1-CB-CG2	-6.76	95.93	110.80
1	D	351	ARG	CA-CB-CG	6.76	127.61	114.10
1	D	614	HIS	CB-CG-CD2	-6.74	122.43	131.20
1	C	438	ARG	O-C-N	6.74	131.79	123.10
1	D	68	ILE	N-CA-C	-6.73	104.20	110.53
1	C	352	VAL	N-CA-CB	-6.72	103.05	110.51
1	C	707	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	B	398	ARG	NE-CZ-NH2	-6.71	113.16	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	568	LYS	CA-C-O	-6.71	113.58	121.44
1	B	39	LEU	N-CA-C	6.70	119.59	111.82
1	A	710	ILE	O-C-N	-6.70	115.84	122.67
1	A	273	GLU	O-C-N	-6.69	115.03	122.12
1	A	386	ARG	N-CA-C	6.69	118.39	107.23
1	C	341	HIS	CB-CG-CD2	-6.68	122.51	131.20
1	D	19	ALA	O-C-N	-6.68	115.53	123.28
1	A	274	ASN	N-CA-C	6.68	122.29	113.20
1	B	797	TRP	N-CA-C	-6.68	103.69	110.97
1	A	236	ASN	CA-CB-CG	-6.67	105.92	112.60
1	B	78	ASP	N-CA-C	6.67	124.56	109.81
1	B	745	LEU	O-C-N	6.67	128.94	122.07
1	B	811	PHE	CA-CB-CG	-6.67	107.12	113.80
1	D	391	LEU	N-CA-C	-6.67	102.64	111.24
1	D	569	ARG	CA-CB-CG	6.67	127.43	114.10
1	C	459	HIS	CB-CG-ND1	6.66	132.70	122.70
1	A	277	ARG	CG-CD-NE	6.66	126.65	112.00
1	D	73	HIS	CB-CG-CD2	-6.66	122.55	131.20
1	C	830	SER	CA-CB-OG	-6.66	97.79	111.10
1	C	807	THR	CA-C-N	6.65	129.52	120.54
1	C	807	THR	C-N-CA	6.65	129.52	120.54
1	A	63	LEU	CA-C-O	-6.65	113.50	120.55
1	B	703	ALA	N-CA-C	6.65	120.61	112.23
1	C	257	PHE	CA-C-N	6.65	129.49	120.44
1	C	257	PHE	C-N-CA	6.65	129.49	120.44
1	C	566	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	D	558	ASN	O-C-N	-6.65	113.67	121.32
1	B	217	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	574	LYS	CA-C-N	6.64	131.56	122.07
1	A	574	LYS	C-N-CA	6.64	131.56	122.07
1	C	187	ASN	O-C-N	-6.64	115.93	121.44
1	B	563	PHE	CA-CB-CG	6.63	120.43	113.80
1	D	555	VAL	N-CA-C	6.62	123.12	109.34
1	C	323	ARG	N-CA-C	6.62	124.90	110.80
1	C	475	GLU	CA-C-N	6.62	126.20	119.19
1	C	475	GLU	C-N-CA	6.62	126.20	119.19
1	A	52	TYR	O-C-N	-6.61	113.34	122.46
1	D	631	ASN	CB-CG-ND2	6.61	126.31	116.40
1	C	783	CYS	CA-CB-SG	-6.60	99.23	114.40
1	C	258	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	79	PRO	CA-C-O	-6.59	113.95	122.12
1	A	33	ARG	CA-CB-CG	6.58	127.26	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	HIS	CA-C-O	6.58	127.33	118.38
1	A	25	THR	N-CA-CB	-6.58	100.45	110.12
1	C	325	ASN	CB-CG-ND2	6.57	126.26	116.40
1	B	341	HIS	O-C-N	-6.57	114.31	120.55
1	C	421	ASP	N-CA-CB	6.57	120.45	109.94
1	A	142	CYS	N-CA-C	-6.56	103.75	111.03
1	C	491	TRP	N-CA-C	6.56	121.14	113.20
1	D	163	PHE	CA-CB-CG	-6.56	107.24	113.80
1	D	380	ILE	N-CA-CB	-6.56	103.16	111.23
1	C	36	HIS	CB-CG-CD2	-6.56	122.68	131.20
1	C	793	ASN	CA-CB-CG	6.55	119.15	112.60
1	C	537	VAL	N-CA-CB	6.55	118.22	110.55
1	D	816	THR	CA-CB-OG1	6.55	119.42	109.60
1	A	321	PRO	CA-N-CD	-6.55	102.83	112.00
1	C	13	ILE	N-CA-C	-6.55	97.13	107.15
1	A	417	ALA	N-CA-C	6.54	119.39	111.40
1	D	423	ASP	CA-CB-CG	6.54	119.14	112.60
1	C	665	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	D	593	GLU	CA-CB-CG	-6.54	101.02	114.10
1	C	143	PHE	N-CA-C	-6.54	104.15	111.28
1	A	264	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	A	405	GLU	N-CA-C	-6.53	103.78	111.03
1	D	341	HIS	O-C-N	-6.53	114.57	120.71
1	D	527	ASP	O-C-N	6.53	131.19	122.96
1	B	514	ASP	O-C-N	-6.53	115.70	123.28
1	C	148	ALA	CA-C-O	-6.53	113.94	120.80
1	D	558	ASN	N-CA-C	-6.51	95.42	109.81
1	D	714	ARG	N-CA-C	-6.51	99.72	109.94
1	A	666	ILE	N-CA-C	6.50	122.87	109.34
1	B	513	SER	N-CA-C	-6.50	105.26	113.72
1	A	387	TRP	N-CA-C	6.50	117.99	109.93
1	B	820	TYR	CA-C-O	-6.50	113.99	120.82
1	D	325	ASN	CA-CB-CG	6.50	119.10	112.60
1	C	807	THR	OG1-CB-CG2	6.50	122.30	109.30
1	D	161	TYR	N-CA-C	-6.50	98.31	108.90
1	A	561	SER	N-CA-C	6.50	120.49	110.42
1	B	168	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	A	593	GLU	O-C-N	-6.50	115.13	121.17
1	D	821	ALA	O-C-N	6.50	128.78	122.03
1	D	47	THR	CA-CB-OG1	-6.49	99.86	109.60
1	B	131	LEU	N-CA-C	-6.49	103.79	112.94
1	A	552	GLU	CA-C-N	6.49	133.93	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	GLU	C-N-CA	6.49	133.93	121.54
1	C	514	ASP	CA-CB-CG	6.49	119.09	112.60
1	C	479	PHE	CA-CB-CG	-6.49	107.31	113.80
1	C	31	PHE	N-CA-C	-6.49	104.13	111.07
1	B	666	ILE	N-CA-C	6.48	122.83	109.34
1	B	426	ARG	CA-CB-CG	6.48	127.06	114.10
1	A	541	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	B	389	VAL	CA-C-O	-6.46	114.23	120.95
1	B	126	GLU	CB-CG-CD	6.46	123.58	112.60
1	B	268	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	342	PRO	CA-N-CD	-6.46	102.96	112.00
1	B	727	ASN	CA-CB-CG	-6.46	106.14	112.60
1	B	54	ALA	CA-C-O	-6.45	114.00	120.90
1	C	716	GLU	O-C-N	6.45	129.52	122.11
1	D	96	GLN	CA-CB-CG	-6.45	101.21	114.10
1	D	301	ALA	CA-C-O	6.44	127.33	120.70
1	D	233	TYR	O-C-N	6.43	131.14	122.59
1	A	249	PRO	O-C-N	-6.43	115.04	123.01
1	A	341	HIS	CB-CG-ND1	6.43	132.34	122.70
1	A	509	GLU	O-C-N	-6.43	114.87	122.20
1	D	338	ASN	CB-CG-ND2	6.42	126.03	116.40
1	B	486	ILE	O-C-N	-6.42	116.10	122.97
1	B	435	ALA	N-CA-C	-6.42	99.91	109.15
1	A	412	ASN	OD1-CG-ND2	-6.42	116.19	122.60
1	A	574	LYS	CB-CG-CD	6.41	126.05	111.30
1	C	325	ASN	O-C-N	6.41	131.54	123.01
1	A	244	TRP	CA-C-N	6.41	131.17	122.84
1	A	244	TRP	C-N-CA	6.41	131.17	122.84
1	C	391	LEU	N-CA-C	-6.41	102.81	112.04
1	B	565	VAL	N-CA-C	6.41	118.01	108.46
1	C	73	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	B	329	PHE	N-CA-C	-6.40	103.78	112.35
1	D	28	LYS	CA-CB-CG	-6.39	101.31	114.10
1	B	309	ARG	CA-C-O	-6.39	114.05	121.07
1	C	407	ASN	CB-CG-ND2	6.39	125.98	116.40
1	A	252	PHE	CA-CB-CG	6.38	120.19	113.80
1	B	290	GLU	CB-CG-CD	6.38	123.45	112.60
1	B	319	ARG	CA-CB-CG	6.38	126.87	114.10
1	B	385	GLU	N-CA-C	6.38	120.29	110.20
1	D	822	ARG	NE-CZ-NH2	6.38	124.95	119.20
1	C	439	ILE	N-CA-C	-6.38	99.24	108.36
1	C	486	ILE	CA-CB-CG1	-6.38	99.55	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	PHE	N-CA-CB	-6.38	99.71	110.49
1	A	329	PHE	CA-C-O	-6.38	113.26	119.13
1	C	566	GLN	CG-CD-NE2	6.37	125.96	116.40
1	A	258	ASN	N-CA-C	-6.37	105.16	113.12
1	A	595	ASN	N-CA-C	-6.37	102.89	111.87
1	B	262	TYR	CA-CB-CG	-6.37	102.44	113.90
1	C	187	ASN	CA-C-O	-6.37	113.08	120.34
1	A	184	ARG	N-CA-C	6.36	118.75	111.11
1	A	510	GLU	CB-CG-CD	6.36	123.41	112.60
1	D	264	GLN	N-CA-C	-6.36	105.51	113.20
1	A	656	VAL	CA-C-O	-6.36	114.66	121.27
1	D	484	ASN	N-CA-C	6.35	119.56	110.10
1	B	422	VAL	CB-CA-C	6.35	119.29	111.80
1	D	421	ASP	CA-CB-CG	6.35	118.95	112.60
1	C	307	ILE	O-C-N	-6.34	115.72	121.87
1	C	236	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	C	300	VAL	CA-CB-CG2	-6.32	99.65	110.40
1	C	688	THR	CA-C-O	-6.32	113.35	120.43
1	B	597	PHE	CA-C-O	6.32	127.82	120.49
1	D	314	SER	CB-CA-C	-6.32	97.85	110.42
1	A	801	VAL	N-CA-CB	-6.31	103.17	110.55
1	D	314	SER	N-CA-CB	6.31	121.15	110.49
1	B	714	ARG	N-CA-C	-6.30	102.41	110.53
1	D	677	GLY	CA-C-N	6.30	128.63	120.44
1	D	677	GLY	C-N-CA	6.30	128.63	120.44
1	D	696	ASN	CA-CB-CG	6.29	118.89	112.60
1	B	464	LYS	CA-CB-CG	6.29	126.68	114.10
1	C	215	TRP	CG-CD1-NE1	-6.29	102.02	110.20
1	C	447	ALA	O-C-N	-6.29	115.45	122.12
1	D	407	ASN	CA-CB-CG	6.29	118.89	112.60
1	B	369	VAL	N-CA-CB	-6.28	103.77	110.62
1	C	200	VAL	O-C-N	-6.28	116.58	123.18
1	D	99	MET	CA-C-O	-6.28	114.23	120.70
1	D	700	ALA	CA-C-O	-6.28	114.23	120.70
1	A	379	VAL	N-CA-C	-6.27	106.66	111.62
1	A	782	LYS	O-C-N	-6.27	115.47	122.12
1	B	355	ASP	CA-CB-CG	6.27	118.87	112.60
1	B	401	GLN	CG-CD-NE2	-6.27	106.99	116.40
1	A	633	ASP	CA-CB-CG	-6.27	106.33	112.60
1	C	176	MET	N-CA-C	-6.27	99.48	109.76
1	D	377	HIS	ND1-CG-CD2	6.26	112.36	106.10
1	A	12	GLN	OE1-CD-NE2	-6.25	116.35	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	LYS	O-C-N	6.25	131.33	123.01
1	D	454	GLY	N-CA-C	-6.25	102.70	112.58
1	B	310	ARG	CG-CD-NE	-6.25	98.25	112.00
1	D	483	THR	N-CA-C	6.25	119.43	110.24
1	D	689	ILE	O-C-N	-6.25	114.76	122.57
1	B	178	GLU	O-C-N	-6.24	113.77	122.76
1	B	481	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	C	376	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	C	513	SER	N-CA-CB	-6.24	101.19	110.61
1	A	716	GLU	CA-CB-CG	6.24	126.58	114.10
1	C	95	LEU	N-CA-C	6.23	117.76	110.97
1	D	522	LEU	O-C-N	6.23	128.57	122.09
1	B	174	TRP	CG-CD2-CE3	6.23	140.13	133.90
1	A	571	HIS	CB-CG-ND1	6.22	132.04	122.70
1	D	450	HIS	CB-CG-ND1	6.22	132.03	122.70
1	B	253	ASN	CA-CB-CG	6.22	118.82	112.60
1	C	409	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	A	534	VAL	N-CA-C	-6.21	104.27	110.30
1	B	376	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	D	57	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	610	ALA	N-CA-CB	6.20	121.41	110.37
1	A	595	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	B	754	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	C	743	GLU	CB-CG-CD	6.19	123.13	112.60
1	A	491	TRP	N-CA-C	6.19	119.53	112.97
1	B	804	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	C	57	HIS	CB-CG-CD2	-6.19	123.16	131.20
1	C	267	LEU	CA-C-O	-6.18	113.38	120.24
1	B	372	CYS	CA-C-O	-6.18	113.81	120.92
1	A	763	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	D	374	TYR	N-CA-CB	-6.18	101.26	110.90
1	A	537	VAL	CA-CB-CG2	-6.18	99.90	110.40
1	C	233	TYR	N-CA-C	6.17	119.56	110.30
1	A	558	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	D	380	ILE	CB-CA-C	6.17	117.87	110.78
1	D	88	GLU	N-CA-C	-6.15	99.04	108.76
1	A	555	VAL	O-C-N	-6.15	114.88	122.57
1	B	160	ARG	N-CA-C	-6.15	98.71	108.73
1	D	165	ILE	N-CA-C	-6.14	99.36	108.45
1	B	393	GLU	CA-CB-CG	6.14	126.39	114.10
1	C	527	ASP	N-CA-C	-6.14	99.15	108.67
1	A	380	ILE	CB-CA-C	6.13	117.52	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	717	ASP	CB-CA-C	-6.13	100.61	110.79
1	C	446	ILE	CA-C-O	-6.13	114.67	121.17
1	C	61	ASP	N-CA-C	-6.12	104.52	111.07
1	C	771	PHE	CA-CB-CG	-6.12	107.68	113.80
1	D	193	ARG	O-C-N	-6.12	116.28	121.23
1	A	308	ILE	N-CA-CB	-6.11	102.23	110.54
1	B	339	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	260	GLY	CA-C-N	6.11	126.72	120.00
1	A	260	GLY	C-N-CA	6.11	126.72	120.00
1	A	682	MET	CG-SD-CE	-6.11	87.47	100.90
1	A	240	THR	O-C-N	6.10	130.71	123.33
1	A	760	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	258	ASN	N-CA-C	-6.10	105.13	113.30
1	A	175	GLN	O-C-N	6.10	130.17	123.22
1	C	486	ILE	CB-CA-C	6.10	121.29	111.29
1	D	79	PRO	N-CA-C	6.09	120.05	111.33
1	A	168	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	C	614	HIS	N-CA-C	6.09	117.92	111.28
1	B	274	ASN	N-CA-C	6.09	120.71	113.16
1	D	76	GLU	CB-CG-CD	6.09	122.95	112.60
1	D	560	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	C	455	VAL	CB-CA-C	6.09	121.27	111.29
1	C	526	ASP	N-CA-C	6.08	121.45	113.30
1	A	97	ASN	CB-CG-ND2	6.08	125.52	116.40
1	B	707	ASN	CA-CB-CG	-6.08	106.52	112.60
1	D	184	ARG	CA-CB-CG	6.08	126.26	114.10
1	C	119	MET	CA-C-O	-6.07	114.11	120.55
1	B	365	TRP	CB-CG-CD1	-6.07	117.79	126.90
1	B	45	VAL	N-CA-CB	-6.07	101.21	111.23
1	D	459	HIS	CB-CG-ND1	6.07	131.80	122.70
1	C	678	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	B	36	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	A	631	ASN	CB-CG-ND2	-6.06	107.31	116.40
1	C	536	LYS	N-CA-C	-6.06	104.58	111.07
1	C	219	GLN	N-CA-C	-6.05	99.79	109.96
1	A	514	ASP	CA-CB-CG	6.05	118.65	112.60
1	D	669	ALA	O-C-N	6.05	130.12	123.04
1	D	708	PHE	O-C-N	-6.05	116.00	123.44
1	C	611	PRO	O-C-N	6.05	129.44	123.03
1	A	650	VAL	CG1-CB-CG2	-6.05	97.50	110.80
1	D	507	ILE	N-CA-C	6.04	121.91	109.34
1	A	71	GLN	OE1-CD-NE2	-6.04	116.56	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	660	ALA	CA-C-O	-6.04	114.40	121.16
1	D	317	GLY	N-CA-C	-6.04	106.85	114.16
1	A	94	THR	CA-C-O	-6.04	112.73	119.67
1	B	431	VAL	N-CA-C	6.04	116.39	107.15
1	C	688	THR	CA-CB-OG1	-6.04	100.55	109.60
1	A	769	ASP	CA-C-O	6.03	127.03	120.58
1	D	177	GLU	CA-CB-CG	6.03	126.17	114.10
1	A	507	ILE	CB-CA-C	-6.03	101.40	111.29
1	C	350	MET	CG-SD-CE	-6.03	87.63	100.90
1	C	95	LEU	CA-C-O	-6.03	114.67	121.00
1	C	262	TYR	N-CA-C	6.02	118.49	108.13
1	B	438	ARG	N-CA-C	6.02	119.02	109.81
1	D	676	THR	CA-CB-CG2	6.02	120.73	110.50
1	B	62	HIS	O-C-N	6.02	129.26	122.22
1	C	290	GLU	N-CA-C	-6.02	104.84	111.82
1	B	777	TYR	CA-C-O	-6.02	114.17	120.55
1	D	615	MET	CA-C-O	-6.01	114.51	120.70
1	A	686	ALA	N-CA-C	-6.01	98.81	108.55
1	B	656	VAL	N-CA-C	6.01	116.79	110.72
1	B	339	ASP	O-C-N	-6.01	114.60	122.59
1	A	209	THR	N-CA-C	6.01	118.53	108.02
1	C	429	SER	CA-CB-OG	6.01	123.11	111.10
1	D	273	GLU	CA-CB-CG	6.00	126.11	114.10
1	D	22	GLU	CA-C-N	-6.00	112.60	121.24
1	D	22	GLU	C-N-CA	-6.00	112.60	121.24
1	C	404	TYR	O-C-N	-6.00	115.55	122.03
1	C	25	THR	CA-CB-OG1	-6.00	100.60	109.60
1	D	754	GLN	N-CA-C	-6.00	97.81	108.55
1	A	785	GLU	N-CA-C	-6.00	104.65	111.07
1	B	375	THR	CA-CB-OG1	-6.00	100.61	109.60
1	A	55	LEU	CA-C-O	-5.99	114.48	121.07
1	B	808	SER	N-CA-C	5.99	123.55	110.80
1	C	836	ALA	N-CA-C	5.99	123.04	109.81
1	C	66	ARG	CA-CB-CG	-5.99	102.13	114.10
1	C	605	ILE	O-C-N	-5.99	117.03	123.14
1	A	717	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	586	LEU	CA-C-O	-5.98	114.08	120.42
1	C	68	ILE	N-CA-C	-5.98	104.50	110.30
1	C	317	GLY	N-CA-C	-5.98	105.26	112.49
1	C	320	ASP	N-CA-C	-5.97	104.05	112.17
1	D	716	GLU	CB-CG-CD	5.97	122.75	112.60
1	D	380	ILE	CA-C-N	5.97	125.65	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	380	ILE	C-N-CA	5.97	125.65	119.56
1	D	477	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	A	693	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	277	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	C	592	LYS	N-CA-C	-5.96	104.42	111.03
1	D	602	THR	N-CA-C	-5.95	97.52	107.99
1	D	678	ASN	N-CA-C	5.95	117.44	111.07
1	B	652	LEU	CA-C-O	-5.95	114.11	120.42
1	C	661	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	315	LYS	CA-C-O	-5.94	112.01	120.51
1	C	195	GLU	CB-CA-C	-5.94	98.93	110.46
1	C	483	THR	CA-CB-OG1	-5.94	100.69	109.60
1	A	278	VAL	CA-C-O	-5.94	115.51	121.45
1	B	556	HIS	N-CA-CB	5.94	120.53	110.49
1	B	752	PRO	N-CA-C	5.94	124.71	112.47
1	C	400	LEU	CB-CA-C	-5.94	100.75	110.85
1	A	117	LEU	N-CA-C	-5.94	100.31	109.52
1	D	266	VAL	CB-CA-C	-5.93	104.27	112.04
1	B	310	ARG	N-CA-CB	5.93	120.23	110.39
1	C	264	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	D	33	ARG	CA-CB-CG	5.92	125.94	114.10
1	A	529	ALA	N-CA-C	-5.92	104.75	111.14
1	D	255	LYS	CA-C-N	5.92	132.84	121.54
1	D	255	LYS	C-N-CA	5.92	132.84	121.54
1	A	251	ASP	CA-C-O	5.92	126.66	119.38
1	D	455	VAL	CB-CA-C	5.91	120.98	111.29
1	A	92	GLY	O-C-N	-5.91	115.02	122.70
1	A	828	GLU	CA-C-N	5.91	127.22	119.84
1	A	828	GLU	C-N-CA	5.91	127.22	119.84
1	B	17	GLY	CA-C-O	-5.91	114.02	120.40
1	D	85	LEU	O-C-N	-5.91	116.13	123.04
1	C	831	ARG	N-CA-C	-5.90	105.39	112.59
1	D	275	ILE	N-CA-C	-5.90	103.71	111.09
1	B	349	LEU	N-CA-C	-5.90	104.21	111.40
1	C	281	PRO	N-CA-C	5.90	126.84	112.10
1	A	603	VAL	N-CA-C	-5.90	99.91	108.87
1	C	505	GLU	CB-CA-C	-5.90	101.88	110.96
1	D	145	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	380	ILE	CA-C-O	5.89	123.50	119.20
1	C	129	ALA	N-CA-C	-5.89	99.55	108.67
1	A	661	ASP	N-CA-C	-5.88	106.64	113.88
1	A	398	ARG	N-CA-C	-5.88	104.79	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	36	HIS	CB-CG-ND1	5.88	131.52	122.70
1	D	199	PRO	N-CA-C	5.88	120.31	111.14
1	D	678	ASN	CA-CB-CG	5.88	118.48	112.60
1	B	387	TRP	CB-CA-C	5.88	117.16	108.87
1	A	277	ARG	CA-C-O	-5.87	113.46	120.10
1	B	807	THR	N-CA-CB	-5.87	100.83	110.40
1	A	399	HIS	CA-CB-CG	-5.87	107.93	113.80
1	B	225	PRO	O-C-N	5.87	130.53	123.13
1	B	256	ASP	CA-C-N	5.87	131.79	122.93
1	B	256	ASP	C-N-CA	5.87	131.79	122.93
1	B	325	ASN	O-C-N	5.87	129.94	123.01
1	D	412	ASN	N-CA-C	-5.87	104.80	111.14
1	C	565	VAL	CB-CA-C	-5.86	101.31	110.69
1	A	598	VAL	N-CA-C	-5.86	99.91	108.11
1	D	250	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	B	78	ASP	CA-CB-CG	-5.86	106.75	112.60
1	C	487	THR	CA-CB-CG2	5.86	120.45	110.50
1	D	506	ARG	CB-CG-CD	5.86	124.77	111.30
1	B	491	TRP	N-CA-C	5.85	119.18	112.57
1	C	589	ARG	CA-C-O	-5.85	114.86	121.00
1	C	527	ASP	CA-CB-CG	5.85	118.45	112.60
1	D	348	GLU	CB-CG-CD	5.85	122.54	112.60
1	B	63	LEU	CA-C-O	-5.83	114.67	120.80
1	B	336	GLN	N-CA-C	5.83	117.71	108.67
1	C	491	TRP	CG-CD2-CE3	5.83	139.73	133.90
1	B	471	PHE	CA-C-O	5.83	126.67	119.79
1	A	25	THR	CA-CB-CG2	5.83	120.40	110.50
1	B	429	SER	CB-CA-C	-5.83	101.10	109.84
1	C	400	LEU	N-CA-CB	5.83	118.78	110.16
1	B	424	ARG	CB-CA-C	-5.82	101.74	110.88
1	B	723	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	C	37	PHE	CA-CB-CG	5.82	119.62	113.80
1	D	187	ASN	O-C-N	-5.82	116.61	121.44
1	B	203	TYR	CA-CB-CG	-5.82	103.43	113.90
1	B	280	TYR	N-CA-C	5.82	121.50	109.11
1	C	237	VAL	N-CA-CB	5.81	119.16	111.25
1	C	432	GLU	CA-CB-CG	5.81	125.72	114.10
1	A	160	ARG	CB-CG-CD	-5.81	97.94	111.30
1	D	387	TRP	CA-C-N	5.81	125.74	119.76
1	D	387	TRP	C-N-CA	5.81	125.74	119.76
1	D	552	GLU	N-CA-C	-5.81	99.06	108.41
1	A	773	VAL	CA-C-O	-5.81	113.52	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	334	ALA	N-CA-CB	-5.81	101.40	110.87
1	D	581	LEU	N-CA-C	-5.81	104.86	111.07
1	B	132	GLY	O-C-N	5.80	129.60	123.45
1	D	322	VAL	CA-C-O	-5.80	114.25	121.04
1	D	200	VAL	O-C-N	-5.80	116.99	123.26
1	A	665	GLN	N-CA-CB	-5.80	103.85	110.35
1	B	365	TRP	CG-CD2-CE3	5.80	139.70	133.90
1	D	791	TYR	O-C-N	5.80	128.26	122.12
1	C	568	LYS	CA-CB-CG	5.79	125.69	114.10
1	A	243	LEU	CA-CB-CG	5.79	136.58	116.30
1	A	756	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	357	GLU	O-C-N	-5.79	114.52	122.23
1	D	817	ILE	O-C-N	5.79	127.80	121.83
1	D	69	ARG	CA-CB-CG	5.79	125.69	114.10
1	A	229	PRO	CA-C-O	-5.79	114.82	121.36
1	A	578	LEU	O-C-N	-5.79	116.01	122.03
1	C	195	GLU	N-CA-CB	5.78	119.28	110.14
1	C	281	PRO	N-CA-CB	-5.78	96.64	103.00
1	C	555	VAL	N-CA-C	5.78	121.36	109.34
1	D	421	ASP	N-CA-C	-5.77	97.49	108.17
1	A	837	PRO	N-CA-C	5.77	126.53	112.10
1	C	390	HIS	CA-CB-CG	5.77	119.57	113.80
1	A	331	ASP	CA-C-O	-5.77	114.96	120.90
1	A	653	ALA	N-CA-C	-5.77	104.99	111.28
1	B	201	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	C	191	LYS	N-CA-C	-5.77	99.78	109.07
1	D	574	LYS	CB-CG-CD	5.77	124.57	111.30
1	B	314	SER	CA-CB-OG	5.77	122.64	111.10
1	D	490	ARG	N-CA-C	5.77	118.31	111.33
1	D	786	ARG	CB-CG-CD	5.77	124.56	111.30
1	A	798	THR	O-C-N	-5.76	116.01	122.12
1	C	165	ILE	N-CA-C	-5.76	100.00	108.99
1	D	452	VAL	N-CA-C	-5.76	99.20	107.78
1	C	793	ASN	CA-C-N	5.75	125.61	119.28
1	C	793	ASN	C-N-CA	5.75	125.61	119.28
1	D	589	ARG	CB-CG-CD	5.75	124.53	111.30
1	C	688	THR	OG1-CB-CG2	5.75	120.80	109.30
1	C	771	PHE	N-CA-C	5.75	120.30	112.88
1	A	538	LYS	CA-CB-CG	-5.75	102.61	114.10
1	A	325	ASN	O-C-N	5.75	130.07	122.95
1	B	159	ILE	O-C-N	-5.74	116.79	122.76
1	C	229	PRO	CB-CA-C	5.74	118.84	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	541	ASN	CB-CG-ND2	5.74	125.01	116.40
1	A	459	HIS	CA-C-O	-5.73	114.80	120.82
1	A	235	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	341	HIS	O-C-N	-5.73	114.73	121.32
1	A	652	LEU	N-CA-C	-5.73	104.48	112.45
1	B	327	ASP	N-CA-C	-5.72	105.12	111.36
1	C	365	TRP	CG-CD2-CE3	5.72	139.62	133.90
1	C	421	ASP	CA-C-O	5.72	127.06	120.60
1	A	163	PHE	CA-CB-CG	-5.72	108.08	113.80
1	A	684	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	296	GLU	CB-CG-CD	5.71	122.31	112.60
1	B	143	PHE	N-CA-C	-5.71	105.06	111.28
1	B	496	ASN	CA-C-N	5.71	125.08	118.85
1	B	496	ASN	C-N-CA	5.71	125.08	118.85
1	C	614	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	D	67	TRP	CG-CD1-NE1	-5.71	102.78	110.20
1	C	649	ARG	CG-CD-NE	-5.71	99.44	112.00
1	C	184	ARG	CA-CB-CG	5.71	125.51	114.10
1	D	323	ARG	N-CA-C	5.71	122.95	110.80
1	B	348	GLU	CB-CG-CD	5.70	122.30	112.60
1	D	335	ILE	CA-C-O	-5.70	114.12	120.74
1	C	263	ILE	CA-CB-CG1	5.70	120.09	110.40
1	C	800	MET	N-CA-C	-5.70	105.05	112.23
1	B	310	ARG	CB-CA-C	-5.70	98.41	110.31
1	B	495	CYS	N-CA-C	5.70	118.26	111.71
1	D	178	GLU	O-C-N	-5.70	116.52	122.96
1	A	305	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	B	249	PRO	CA-C-N	-5.69	113.63	123.25
1	B	249	PRO	C-N-CA	-5.69	113.63	123.25
1	D	402	ILE	N-CA-CB	-5.69	102.80	110.54
1	C	526	ASP	CA-CB-CG	-5.69	106.91	112.60
1	A	554	LYS	N-CA-C	5.69	118.73	109.06
1	B	88	GLU	CB-CG-CD	5.69	122.27	112.60
1	B	166	PHE	N-CA-C	5.68	122.91	110.80
1	D	653	ALA	N-CA-C	-5.68	104.72	111.03
1	A	583	VAL	N-CA-C	5.68	116.41	110.62
1	B	277	ARG	CA-CB-CG	-5.68	102.74	114.10
1	A	62	HIS	CB-CG-CD2	-5.67	123.82	131.20
1	A	211	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	B	407	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	C	490	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	C	589	ARG	CB-CG-CD	5.67	124.34	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	B	93	ARG	N-CA-C	5.66	122.86	110.80
1	D	278	VAL	N-CA-CB	-5.66	101.66	111.63
1	A	175	GLN	CG-CD-NE2	5.66	124.89	116.40
1	C	329	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	145	ASP	N-CA-C	-5.66	105.02	111.07
1	B	341	HIS	CB-CG-ND1	5.66	131.19	122.70
1	B	62	HIS	N-CA-C	5.66	118.22	111.71
1	A	68	ILE	N-CA-C	-5.65	104.82	110.30
1	C	450	HIS	N-CA-C	-5.65	104.97	112.94
1	C	792	LYS	CA-CB-CG	5.65	125.40	114.10
1	A	41	LYS	N-CA-C	-5.65	100.94	108.34
1	D	793	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	595	ASN	CA-CB-CG	5.65	118.25	112.60
1	D	45	VAL	N-CA-CB	-5.64	101.92	111.23
1	D	322	VAL	N-CA-CB	-5.64	105.23	111.66
1	D	160	ARG	N-CA-C	-5.64	100.51	109.76
1	A	238	VAL	N-CA-C	-5.63	97.62	109.34
1	A	33	ARG	CB-CA-C	-5.63	102.22	110.95
1	C	764	MET	CA-CB-CG	5.63	125.36	114.10
1	D	578	LEU	N-CA-C	-5.63	105.06	111.14
1	A	610	ALA	CB-CA-C	-5.63	99.08	110.17
1	C	165	ILE	O-C-N	-5.63	116.95	122.97
1	B	800	MET	CA-C-N	5.63	128.14	120.77
1	B	800	MET	C-N-CA	5.63	128.14	120.77
1	B	177	GLU	CB-CG-CD	5.63	122.17	112.60
1	B	555	VAL	CA-C-N	5.63	132.28	121.54
1	B	555	VAL	C-N-CA	5.63	132.28	121.54
1	A	323	ARG	CA-CB-CG	5.62	125.35	114.10
1	C	310	ARG	CB-CG-CD	-5.62	98.37	111.30
1	C	804	ASN	CA-C-O	-5.62	114.99	120.89
1	C	541	ASN	CB-CG-ND2	5.62	124.83	116.40
1	C	160	ARG	CB-CG-CD	-5.62	98.38	111.30
1	A	96	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	A	391	LEU	CA-C-O	-5.62	114.47	120.42
1	D	306	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	477	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	D	626	ILE	N-CA-C	-5.61	105.03	110.42
1	C	555	VAL	CA-C-N	5.61	132.25	121.54
1	C	555	VAL	C-N-CA	5.61	132.25	121.54
1	B	646	GLU	CA-C-O	5.60	127.25	120.81
1	A	49	ARG	NE-CZ-NH1	5.60	127.10	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	728	ALA	N-CA-C	5.60	122.73	110.80
1	D	458	ILE	N-CA-CB	-5.60	104.29	110.51
1	B	754	GLN	N-CA-C	-5.60	97.43	109.81
1	D	210	SER	N-CA-C	5.60	122.72	110.80
1	D	555	VAL	CA-C-N	5.60	132.23	121.54
1	D	555	VAL	C-N-CA	5.60	132.23	121.54
1	B	614	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	D	525	VAL	N-CA-C	5.59	120.98	109.34
1	D	676	THR	CB-CA-C	5.59	119.03	109.24
1	B	99	MET	CA-C-O	-5.59	112.51	120.51
1	B	158	GLY	O-C-N	-5.59	117.26	123.58
1	C	80	LYS	N-CA-C	-5.59	101.58	109.96
1	B	63	LEU	N-CA-C	-5.59	104.03	111.24
1	B	761	ILE	N-CA-C	-5.59	105.66	111.58
1	C	552	GLU	N-CA-CB	5.59	119.74	110.47
1	A	250	ASN	CB-CG-ND2	5.58	124.78	116.40
1	A	336	GLN	CG-CD-NE2	5.58	124.78	116.40
1	A	444	LEU	CD1-CG-CD2	-5.58	98.52	110.80
1	A	777	TYR	CA-C-O	-5.58	114.95	120.70
1	B	439	ILE	CA-CB-CG1	-5.58	100.92	110.40
1	D	249	PRO	O-C-N	-5.58	116.05	122.85
1	D	47	THR	CA-CB-CG2	5.57	119.97	110.50
1	D	332	LYS	N-CA-C	5.57	119.25	112.23
1	D	565	VAL	CB-CA-C	-5.57	102.32	110.62
1	A	659	ALA	N-CA-C	5.57	119.92	113.18
1	C	649	ARG	CA-C-O	-5.57	115.32	121.28
1	C	727	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	D	208	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	D	569	ARG	CD-NE-CZ	-5.57	116.60	124.40
1	D	645	LEU	CA-C-O	5.57	126.71	120.92
1	D	20	GLY	CA-C-N	5.57	131.99	121.97
1	D	20	GLY	C-N-CA	5.57	131.99	121.97
1	D	60	ARG	N-CA-C	5.56	117.42	111.36
1	D	33	ARG	CB-CA-C	-5.56	102.15	110.88
1	A	579	ASN	CB-CG-ND2	5.56	124.74	116.40
1	B	57	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	B	649	ARG	CA-C-O	-5.55	115.19	121.25
1	C	258	ASN	CB-CG-ND2	5.55	124.73	116.40
1	A	321	PRO	N-CA-C	5.55	123.91	112.47
1	B	750	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	532	ARG	CA-CB-CG	5.55	125.20	114.10
1	A	708	PHE	CA-CB-CG	-5.55	108.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	VAL	N-CA-C	-5.55	100.07	108.17
1	D	73	HIS	CB-CG-ND1	5.55	131.02	122.70
1	D	572	GLU	N-CA-C	5.55	117.77	111.11
1	C	332	LYS	CA-CB-CG	-5.55	103.00	114.10
1	D	383	ALA	N-CA-C	5.55	119.89	113.18
1	B	747	SER	O-C-N	5.55	128.71	122.22
1	B	210	SER	CA-CB-OG	5.54	122.19	111.10
1	B	174	TRP	CB-CG-CD1	-5.54	118.59	126.90
1	A	807	THR	CA-C-N	5.53	127.96	120.38
1	A	807	THR	C-N-CA	5.53	127.96	120.38
1	A	245	SER	O-C-N	-5.53	116.47	123.05
1	C	722	ASP	CA-CB-CG	-5.53	107.07	112.60
1	B	723	GLN	CA-CB-CG	5.53	125.16	114.10
1	C	228	THR	CA-CB-OG1	-5.53	101.30	109.60
1	B	88	GLU	CA-CB-CG	5.53	125.16	114.10
1	B	517	GLN	OE1-CD-NE2	5.53	128.13	122.60
1	C	235	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	C	253	ASN	CA-CB-CG	5.53	118.12	112.60
1	A	508	GLY	O-C-N	-5.52	115.52	122.70
1	D	78	ASP	O-C-N	-5.52	114.97	121.32
1	B	361	TRP	N-CA-C	5.52	117.75	111.02
1	B	679	MET	CG-SD-CE	-5.52	88.76	100.90
1	A	187	ASN	CA-C-O	-5.51	114.69	120.09
1	C	239	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	45	VAL	CA-C-N	-5.51	113.93	122.09
1	A	45	VAL	C-N-CA	-5.51	113.93	122.09
1	C	127	GLU	N-CA-C	-5.51	101.56	110.32
1	A	143	PHE	CA-C-O	-5.51	114.68	120.63
1	A	729	GLN	O-C-N	-5.51	116.28	122.12
1	C	412	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	B	244	TRP	N-CA-C	5.50	117.87	108.90
1	B	703	ALA	CA-C-O	5.50	126.28	119.79
1	A	393	GLU	CA-CB-CG	5.50	125.10	114.10
1	A	684	ASN	CB-CG-ND2	5.50	124.65	116.40
1	C	360	ASP	CA-CB-CG	-5.50	107.10	112.60
1	A	205	ARG	CA-CB-CG	5.50	125.10	114.10
1	C	546	ALA	N-CA-C	-5.50	105.29	111.28
1	A	668	THR	CA-CB-OG1	-5.50	101.36	109.60
1	A	769	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	643	ILE	N-CA-CB	-5.50	105.20	112.34
1	C	666	ILE	N-CA-C	5.49	120.77	109.34
1	B	541	ASN	OD1-CG-ND2	-5.49	117.11	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	764	MET	O-C-N	5.49	127.72	122.07
1	A	558	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	254	LEU	CB-CA-C	-5.48	99.51	110.42
1	D	205	ARG	N-CA-CB	-5.48	101.21	111.13
1	A	118	ASP	CA-CB-CG	5.48	118.08	112.60
1	D	37	PHE	N-CA-C	5.48	119.14	112.23
1	C	478	LYS	CB-CG-CD	-5.48	98.70	111.30
1	D	767	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	A	486	ILE	CA-C-O	-5.47	115.92	121.67
1	A	657	ILE	CA-C-O	-5.47	112.62	119.95
1	B	833	ARG	CB-CA-C	-5.47	102.28	110.16
1	C	35	LEU	O-C-N	-5.47	116.43	122.07
1	C	93	ARG	NE-CZ-NH2	-5.47	114.27	119.20
1	A	539	GLN	N-CA-C	-5.47	105.32	111.28
1	A	696	ASN	CA-CB-CG	-5.47	107.13	112.60
1	B	380	ILE	CB-CA-C	5.47	116.59	110.52
1	D	341	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	C	772	LYS	CG-CD-CE	-5.46	98.73	111.30
1	A	310	ARG	CB-CA-C	-5.46	100.53	110.63
1	A	586	LEU	N-CA-CB	5.46	118.24	110.16
1	D	496	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	236	ASN	N-CA-C	5.45	122.42	110.80
1	C	168	GLN	O-C-N	-5.45	116.86	123.13
1	D	453	ASN	N-CA-C	-5.45	100.78	109.23
1	B	633	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	181	ASP	N-CA-CB	5.45	116.45	110.35
1	B	523	SER	N-CA-C	-5.44	106.14	112.89
1	B	407	ASN	CA-C-N	5.43	127.50	120.44
1	B	407	ASN	C-N-CA	5.43	127.50	120.44
1	C	273	GLU	CB-CA-C	-5.43	101.44	110.68
1	C	371	THR	CA-C-O	-5.43	113.37	120.00
1	D	409	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	A	117	LEU	CA-C-N	-5.43	114.80	122.94
1	A	117	LEU	C-N-CA	-5.43	114.80	122.94
1	D	89	PHE	O-C-N	-5.43	118.50	123.50
1	D	487	THR	N-CA-C	-5.43	102.82	110.31
1	B	598	VAL	N-CA-CB	-5.43	104.58	111.64
1	A	491	TRP	CE2-CD2-CG	-5.43	100.69	107.20
1	B	257	PHE	CA-C-O	5.43	129.60	122.44
1	B	387	TRP	CA-C-O	-5.43	115.63	120.19
1	D	104	LEU	N-CA-C	5.43	122.36	110.80
1	B	490	ARG	N-CA-C	5.42	117.62	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	TRP	CB-CG-CD1	-5.42	118.77	126.90
1	C	295	GLN	CB-CA-C	-5.42	102.37	110.88
1	A	632	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	B	765	LEU	O-C-N	5.42	127.67	122.03
1	C	226	TYR	CA-C-O	-5.42	114.85	120.70
1	D	295	GLN	OE1-CD-NE2	-5.42	117.19	122.60
1	B	337	LEU	O-C-N	-5.41	114.94	122.41
1	C	156	GLY	CA-C-O	-5.41	115.66	120.75
1	C	244	TRP	CB-CG-CD1	-5.41	118.78	126.90
1	D	739	ARG	O-C-N	5.41	127.72	122.09
1	A	494	LEU	N-CA-CB	-5.41	102.16	110.01
1	D	329	PHE	CA-CB-CG	5.41	119.21	113.80
1	D	183	LEU	N-CA-C	5.41	122.32	110.80
1	B	645	LEU	N-CA-C	5.41	117.05	108.67
1	D	678	ASN	CA-C-O	5.41	126.50	120.82
1	A	356	LEU	N-CA-C	5.41	117.25	111.36
1	B	279	LEU	N-CA-C	-5.41	102.52	110.52
1	C	25	THR	N-CA-CB	-5.40	101.61	109.82
1	D	36	HIS	CA-CB-CG	-5.40	108.40	113.80
1	D	526	ASP	CA-CB-CG	-5.40	107.20	112.60
1	D	681	PHE	CA-C-O	-5.40	115.15	120.82
1	D	50	ASP	N-CA-C	-5.40	104.81	111.40
1	C	273	GLU	CA-C-N	-5.40	113.86	122.66
1	C	273	GLU	C-N-CA	-5.40	113.86	122.66
1	D	83	TYR	N-CA-C	5.40	118.16	108.17
1	A	53	PHE	CA-C-O	5.40	125.58	119.27
1	B	387	TRP	CA-C-N	5.40	125.70	119.93
1	B	387	TRP	C-N-CA	5.40	125.70	119.93
1	B	564	ASP	CA-CB-CG	5.40	118.00	112.60
1	D	450	HIS	O-C-N	-5.39	115.44	122.39
1	B	47	THR	N-CA-CB	-5.39	100.78	110.37
1	B	378	THR	CA-C-O	5.39	126.30	120.32
1	C	825	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	D	14	SER	CA-C-N	5.39	129.56	120.29
1	D	14	SER	C-N-CA	5.39	129.56	120.29
1	A	105	GLU	CB-CG-CD	5.39	121.76	112.60
1	D	784	GLN	CG-CD-NE2	5.39	124.48	116.40
1	A	42	ASP	N-CA-CB	-5.39	103.21	111.56
1	A	766	MET	N-CA-C	5.38	117.90	111.71
1	D	549	LEU	N-CA-C	5.38	119.34	112.34
1	A	372	CYS	N-CA-CB	-5.38	101.28	110.16
1	C	309	ARG	CG-CD-NE	-5.38	100.16	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	626	ILE	N-CA-CB	-5.38	104.25	110.55
1	B	119	MET	N-CA-CB	5.38	117.81	110.01
1	A	245	SER	CA-CB-OG	5.38	121.85	111.10
1	C	714	ARG	N-CA-C	-5.38	103.52	110.19
1	A	576	GLN	O-C-N	-5.37	115.44	122.59
1	D	811	PHE	CA-CB-CG	-5.37	108.43	113.80
1	B	277	ARG	CB-CG-CD	5.37	123.65	111.30
1	B	714	ARG	CB-CG-CD	5.37	123.65	111.30
1	D	225	PRO	N-CA-C	5.37	119.73	111.57
1	D	481	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	184	ARG	O-C-N	-5.37	116.51	122.09
1	C	807	THR	CA-CB-OG1	-5.37	101.55	109.60
1	D	753	LYS	CG-CD-CE	-5.37	98.95	111.30
1	A	67	TRP	CB-CG-CD1	-5.37	118.85	126.90
1	B	97	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	B	244	TRP	CE2-CD2-CG	-5.37	100.76	107.20
1	C	119	MET	CA-CB-CG	-5.37	103.37	114.10
1	A	25	THR	CB-CA-C	5.36	119.69	110.79
1	A	416	ALA	O-C-N	5.36	128.49	122.22
1	B	237	VAL	O-C-N	-5.36	117.55	123.18
1	A	231	PRO	N-CA-CB	5.36	106.82	103.23
1	C	517	GLN	N-CA-C	-5.36	106.58	113.01
1	D	247	LYS	N-CA-C	-5.36	98.84	108.48
1	A	487	THR	N-CA-C	-5.36	103.29	109.93
1	D	343	SER	N-CA-C	5.36	118.91	112.38
1	A	266	VAL	N-CA-C	-5.35	104.36	111.05
1	D	251	ASP	CA-C-O	5.35	126.01	119.05
1	B	191	LYS	CA-CB-CG	-5.35	103.40	114.10
1	A	149	THR	CB-CA-C	5.35	119.67	110.79
1	A	507	ILE	N-CA-C	5.35	120.46	109.34
1	C	450	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	D	287	GLU	N-CA-C	-5.35	96.03	111.00
1	B	228	THR	N-CA-C	-5.35	98.80	108.85
1	C	676	THR	CB-CA-C	5.35	120.48	110.70
1	A	625	ALA	CA-C-O	5.34	126.27	120.55
1	A	579	ASN	CA-CB-CG	5.34	117.94	112.60
1	B	129	ALA	N-CA-C	-5.34	101.46	109.15
1	B	296	GLU	N-CA-C	-5.34	105.36	111.07
1	D	214	LYS	O-C-N	-5.34	116.84	123.36
1	C	365	TRP	CB-CG-CD1	-5.34	118.89	126.90
1	D	614	HIS	CB-CG-ND1	5.34	130.70	122.70
1	B	322	VAL	O-C-N	-5.33	117.55	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	SER	CA-C-O	5.33	126.79	120.66
1	D	786	ARG	N-CA-C	-5.33	105.11	111.03
1	C	453	ASN	N-CA-C	5.33	118.12	109.06
1	D	200	VAL	N-CA-C	-5.33	100.65	108.11
1	B	381	PRO	N-CA-C	5.33	123.45	112.47
1	C	390	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	B	317	GLY	CA-C-O	5.33	126.15	120.40
1	D	124	GLU	CA-C-N	5.33	129.03	120.30
1	D	124	GLU	C-N-CA	5.33	129.03	120.30
1	A	244	TRP	CE2-CD2-CG	-5.32	100.81	107.20
1	B	53	PHE	CB-CA-C	-5.32	102.52	110.88
1	C	555	VAL	CB-CA-C	-5.32	102.57	111.29
1	D	336	GLN	O-C-N	-5.32	117.26	123.27
1	C	376	ASN	CA-CB-CG	5.32	117.92	112.60
1	D	176	MET	N-CA-C	-5.32	100.23	108.90
1	D	482	LYS	CG-CD-CE	-5.32	99.08	111.30
1	D	688	THR	N-CA-C	5.32	117.93	109.96
1	A	197	THR	O-C-N	-5.31	116.74	123.12
1	C	144	LEU	O-C-N	5.31	127.75	122.12
1	A	764	MET	O-C-N	5.31	127.76	122.08
1	D	365	TRP	CB-CG-CD1	-5.31	118.93	126.90
1	C	250	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	141	ALA	N-CA-C	5.31	117.82	111.71
1	B	275	ILE	CB-CG1-CD1	-5.31	102.65	113.80
1	C	497	PRO	N-CA-C	-5.31	106.48	113.65
1	A	566	GLN	CA-CB-CG	-5.31	103.49	114.10
1	B	650	VAL	CG1-CB-CG2	-5.31	99.12	110.80
1	C	447	ALA	N-CA-C	5.31	117.07	111.28
1	C	531	ILE	CA-C-O	-5.30	115.75	121.27
1	C	560	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	C	676	THR	CA-CB-CG2	5.30	119.51	110.50
1	A	696	ASN	N-CA-C	-5.30	104.94	111.40
1	B	262	TYR	N-CA-C	5.30	117.29	108.02
1	B	726	TYR	CA-C-N	-5.30	114.68	123.37
1	B	726	TYR	C-N-CA	-5.30	114.68	123.37
1	D	336	GLN	CA-CB-CG	-5.30	103.50	114.10
1	B	414	VAL	O-C-N	-5.30	116.52	121.87
1	A	320	ASP	CA-C-N	5.29	126.46	119.84
1	A	320	ASP	C-N-CA	5.29	126.46	119.84
1	A	509	GLU	CA-C-O	-5.29	114.27	120.20
1	A	556	HIS	CB-CG-ND1	5.29	130.64	122.70
1	C	314	SER	O-C-N	5.29	129.63	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	537	VAL	CA-CB-CG1	-5.29	101.41	110.40
1	A	127	GLU	N-CA-C	-5.29	101.09	109.76
1	B	595	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	C	143	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	73	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	B	204	GLY	O-C-N	5.28	128.65	123.10
1	B	53	PHE	N-CA-CB	5.28	117.67	110.01
1	C	401	GLN	CA-C-O	-5.28	114.95	120.55
1	C	572	GLU	N-CA-C	5.28	117.72	111.33
1	C	769	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	769	ASP	CA-C-O	5.28	126.41	120.92
1	C	814	ASP	N-CA-C	-5.28	105.69	111.82
1	A	676	THR	N-CA-C	5.28	119.20	112.34
1	C	91	MET	N-CA-CB	-5.28	102.35	110.16
1	D	595	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	C	58	THR	CA-CB-OG1	-5.28	101.68	109.60
1	D	25	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	346	ILE	CA-C-O	-5.28	112.88	119.95
1	A	558	ASN	CA-C-N	5.28	125.59	119.47
1	A	558	ASN	C-N-CA	5.28	125.59	119.47
1	A	295	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	754	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	C	177	GLU	CA-CB-CG	5.27	124.64	114.10
1	C	767	HIS	CA-CB-CG	-5.27	108.53	113.80
1	D	426	ARG	CA-CB-CG	5.27	124.64	114.10
1	A	237	VAL	O-C-N	-5.27	115.94	122.52
1	A	767	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	C	81	ARG	CB-CG-CD	-5.27	99.19	111.30
1	C	481	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	C	828	GLU	CB-CA-C	5.27	116.74	108.63
1	A	537	VAL	CA-CB-CG1	5.26	119.35	110.40
1	B	522	LEU	N-CA-C	5.26	119.33	113.01
1	C	828	GLU	N-CA-C	-5.26	102.87	110.40
1	A	490	ARG	NE-CZ-NH2	-5.26	114.46	119.20
1	D	32	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	C	701	GLU	O-C-N	-5.26	116.54	122.12
1	C	808	SER	CB-CA-C	-5.26	102.39	110.81
1	A	22	GLU	O-C-N	5.26	129.58	122.59
1	C	382	GLU	N-CA-C	5.26	117.01	111.28
1	A	197	THR	N-CA-CB	-5.25	100.89	109.56
1	A	531	ILE	CA-C-O	-5.25	114.80	120.47
1	B	174	TRP	CG-CD1-NE1	-5.25	103.37	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	779	GLU	N-CA-C	-5.25	105.45	111.07
1	D	811	PHE	CA-C-N	-5.25	114.84	122.65
1	D	811	PHE	C-N-CA	-5.25	114.84	122.65
1	D	167	ASN	O-C-N	-5.24	117.19	123.06
1	A	461	GLU	N-CA-C	-5.24	105.48	111.14
1	D	36	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	208	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	C	463	LEU	CA-C-O	-5.23	114.87	120.42
1	D	633	ASP	CA-C-O	5.23	123.19	119.32
1	D	436	VAL	O-C-N	5.23	129.11	122.57
1	D	792	LYS	N-CA-CB	-5.23	101.69	110.22
1	D	820	TYR	O-C-N	5.23	128.70	122.27
1	C	301	ALA	N-CA-C	-5.23	105.66	111.36
1	A	445	CYS	CA-CB-SG	-5.22	102.38	114.40
1	C	770	ARG	CA-CB-CG	5.22	124.55	114.10
1	D	579	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	10	ARG	CB-CG-CD	5.22	123.31	111.30
1	A	207	GLU	CA-CB-CG	5.22	124.54	114.10
1	C	160	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	C	653	ALA	N-CA-C	-5.22	105.59	111.28
1	A	165	ILE	O-C-N	-5.22	116.05	122.57
1	A	332	LYS	N-CA-CB	-5.22	102.91	110.47
1	C	582	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	A	315	LYS	CA-C-N	5.21	131.50	121.54
1	A	315	LYS	C-N-CA	5.21	131.50	121.54
1	B	255	LYS	CA-C-N	5.21	131.50	121.54
1	B	255	LYS	C-N-CA	5.21	131.50	121.54
1	C	371	THR	CA-CB-OG1	-5.21	101.78	109.60
1	D	616	ALA	CA-C-O	-5.21	115.02	120.55
1	C	174	TRP	CE2-CD2-CG	-5.21	100.94	107.20
1	C	603	VAL	N-CA-CB	5.21	117.40	110.26
1	D	633	ASP	N-CA-CB	5.21	117.06	110.23
1	B	250	ASN	CA-C-O	5.21	127.49	121.34
1	D	486	ILE	N-CA-CB	-5.21	101.15	111.15
1	B	193	ARG	CA-C-O	-5.21	113.02	120.16
1	C	331	ASP	CA-C-O	-5.21	114.46	120.24
1	B	567	VAL	CA-C-O	5.21	127.29	120.78
1	C	706	GLU	N-CA-CB	5.21	119.03	110.39
1	A	374	TYR	N-CA-C	5.20	117.28	108.02
1	A	602	THR	N-CA-C	-5.20	99.93	108.41
1	A	121	GLU	CB-CA-C	-5.20	102.49	110.81
1	A	771	PHE	N-CA-C	5.20	120.26	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	ASP	N-CA-C	-5.20	104.68	111.02
1	C	395	LEU	N-CA-C	5.20	119.33	112.89
1	B	50	ASP	O-C-N	-5.19	116.72	122.07
1	B	333	VAL	CA-C-O	-5.19	115.25	121.28
1	C	482	LYS	N-CA-C	-5.19	99.87	108.75
1	D	351	ARG	CA-C-O	5.19	126.00	120.24
1	D	679	MET	CG-SD-CE	-5.19	89.48	100.90
1	D	735	ILE	N-CA-CB	-5.19	103.94	111.21
1	C	200	VAL	N-CA-CB	-5.19	104.19	111.25
1	C	567	VAL	CA-C-N	5.19	130.62	122.21
1	C	567	VAL	C-N-CA	5.19	130.62	122.21
1	C	770	ARG	N-CA-CB	-5.19	101.78	110.39
1	D	713	MET	CG-SD-CE	-5.19	89.49	100.90
1	A	280	TYR	N-CA-C	5.19	118.60	108.85
1	B	455	VAL	N-CA-C	5.19	118.18	113.20
1	C	556	HIS	CA-CB-CG	5.19	118.99	113.80
1	B	614	HIS	CB-CG-ND1	5.18	130.48	122.70
1	B	800	MET	N-CA-C	-5.18	105.54	111.14
1	A	429	SER	N-CA-C	5.18	116.98	110.24
1	B	576	GLN	N-CA-C	-5.18	105.63	111.28
1	C	44	ASN	CB-CG-ND2	5.18	124.17	116.40
1	C	298	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	714	ARG	CA-CB-CG	5.18	124.45	114.10
1	D	42	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	394	THR	CA-CB-OG1	-5.17	101.84	109.60
1	B	214	LYS	CG-CD-CE	5.17	123.20	111.30
1	B	68	ILE	N-CA-C	-5.17	105.28	110.30
1	B	193	ARG	O-C-N	-5.17	115.37	121.32
1	D	11	LYS	CA-CB-CG	5.17	124.44	114.10
1	A	797	TRP	CD2-CE2-CZ2	-5.17	117.23	122.40
1	B	369	VAL	CA-C-O	-5.17	115.76	121.29
1	D	219	GLN	N-CA-C	-5.17	103.57	110.55
1	D	381	PRO	N-CA-C	5.17	120.56	113.84
1	B	492	LEU	N-CA-C	-5.17	99.80	110.80
1	C	74	TYR	CA-C-O	-5.17	115.07	120.55
1	D	792	LYS	CB-CG-CD	-5.17	99.42	111.30
1	D	584	ILE	N-CA-C	-5.16	105.47	110.42
1	B	62	HIS	CB-CG-ND1	5.16	130.43	122.70
1	A	73	HIS	CA-CB-CG	-5.15	108.65	113.80
1	A	635	VAL	CA-C-O	-5.15	115.59	120.95
1	C	485	GLY	O-C-N	-5.15	118.77	123.56
1	B	431	VAL	CB-CA-C	-5.15	105.24	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	807	THR	CA-CB-OG1	-5.15	101.88	109.60
1	C	321	PRO	N-CA-C	5.15	123.07	112.47
1	D	233	TYR	CB-CA-C	-5.15	100.18	110.42
1	A	195	GLU	CA-CB-CG	5.15	124.39	114.10
1	C	289	LYS	CA-C-O	5.15	126.51	120.80
1	A	16	ARG	CA-CB-CG	5.14	124.39	114.10
1	A	808	SER	N-CA-C	5.14	117.56	111.33
1	A	665	GLN	CG-CD-NE2	5.14	124.11	116.40
1	B	361	TRP	NE1-CE2-CZ2	-5.14	122.39	130.10
1	B	211	GLN	CG-CD-NE2	5.14	124.11	116.40
1	B	822	ARG	N-CA-C	5.14	118.01	111.69
1	D	273	GLU	O-C-N	-5.14	115.65	122.33
1	A	376	ASN	O-C-N	-5.14	116.47	123.10
1	B	47	THR	CA-CB-OG1	-5.14	101.90	109.60
1	C	32	ASN	CA-C-O	-5.14	115.42	121.07
1	C	823	GLU	N-CA-C	5.13	119.63	112.90
1	D	19	ALA	CA-C-O	-5.13	114.37	120.89
1	D	416	ALA	N-CA-C	-5.13	105.68	111.28
1	D	514	ASP	N-CA-C	-5.13	98.20	107.60
1	D	828	GLU	N-CA-C	-5.13	103.30	109.72
1	B	702	GLU	O-C-N	5.13	128.00	122.15
1	C	136	LEU	CA-CB-CG	5.13	134.25	116.30
1	A	197	THR	CA-CB-OG1	-5.13	101.91	109.60
1	B	763	ASN	N-CA-C	5.13	117.77	111.82
1	C	336	GLN	N-CA-C	5.13	116.67	108.41
1	D	248	ALA	O-C-N	-5.13	115.81	121.66
1	A	45	VAL	N-CA-CB	-5.13	102.77	111.23
1	A	96	GLN	O-C-N	-5.13	116.55	122.09
1	B	424	ARG	N-CA-CB	5.12	117.44	110.01
1	C	761	ILE	CB-CA-C	-5.12	105.33	112.04
1	A	405	GLU	CB-CG-CD	5.12	121.31	112.60
1	B	182	TRP	O-C-N	-5.12	116.76	122.09
1	B	128	ASP	N-CA-C	-5.12	103.28	110.50
1	C	76	GLU	CB-CG-CD	5.12	121.30	112.60
1	C	391	LEU	N-CA-CB	5.12	118.12	110.19
1	D	263	ILE	CA-CB-CG1	5.12	119.10	110.40
1	B	174	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	B	698	GLU	CA-CB-CG	-5.12	103.87	114.10
1	D	266	VAL	N-CA-CB	5.12	116.87	110.47
1	D	273	GLU	CA-C-N	-5.12	114.53	122.67
1	D	273	GLU	C-N-CA	-5.12	114.53	122.67
1	D	808	SER	CA-C-N	5.12	125.76	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	808	SER	C-N-CA	5.12	125.76	120.03
1	A	636	VAL	N-CA-C	5.12	115.89	110.72
1	C	421	ASP	O-C-N	5.12	129.47	122.82
1	C	205	ARG	N-CA-CB	-5.11	101.85	110.49
1	B	379	VAL	O-C-N	-5.11	116.57	121.83
1	C	583	VAL	N-CA-C	-5.11	104.70	111.09
1	A	469	LYS	CA-CB-CG	5.11	124.32	114.10
1	D	262	TYR	N-CA-C	5.11	116.70	108.32
1	A	770	ARG	CA-CB-CG	5.11	124.31	114.10
1	C	491	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	C	764	MET	O-C-N	5.11	127.40	122.09
1	D	146	SER	CA-C-O	-5.11	115.14	120.55
1	D	669	ALA	CA-C-O	5.11	126.51	120.69
1	C	374	TYR	N-CA-CB	-5.10	102.53	110.29
1	D	683	LEU	O-C-N	-5.10	115.76	122.39
1	D	733	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	604	MET	CA-C-O	-5.10	113.98	120.20
1	A	67	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	C	69	ARG	CA-C-N	5.10	127.88	120.79
1	C	69	ARG	C-N-CA	5.10	127.88	120.79
1	A	491	TRP	N-CA-CB	-5.10	103.41	110.65
1	A	622	LEU	CB-CA-C	-5.10	102.88	110.88
1	C	310	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	A	182	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	814	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	633	ASP	CA-C-N	5.09	124.89	119.28
1	B	633	ASP	C-N-CA	5.09	124.89	119.28
1	A	407	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	511	TYR	CA-CB-CG	5.09	123.06	113.90
1	A	541	ASN	N-CA-C	-5.09	105.64	111.14
1	A	556	HIS	CA-CB-CG	-5.09	108.71	113.80
1	A	628	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	436	VAL	CA-C-N	5.09	128.08	120.95
1	D	436	VAL	C-N-CA	5.09	128.08	120.95
1	D	236	ASN	CA-C-N	-5.09	116.50	123.12
1	D	236	ASN	C-N-CA	-5.09	116.50	123.12
1	A	51	TYR	O-C-N	-5.09	115.78	122.39
1	A	746	SER	O-C-N	-5.09	116.74	122.03
1	A	746	SER	N-CA-CB	-5.09	102.48	109.91
1	B	440	ASN	CB-CG-ND2	5.09	124.03	116.40
1	D	573	TYR	CA-CB-CG	5.09	123.06	113.90
1	A	352	VAL	N-CA-C	-5.08	105.58	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	VAL	N-CA-C	5.08	116.31	108.44
1	A	277	ARG	CD-NE-CZ	5.08	131.51	124.40
1	C	154	ALA	CA-C-O	-5.08	115.37	121.11
1	A	97	ASN	CB-CA-C	-5.08	100.61	110.46
1	B	293	LEU	CA-C-O	-5.08	115.04	120.42
1	C	597	PHE	O-C-N	5.08	129.11	122.87
1	D	241	MET	O-C-N	-5.08	117.10	123.04
1	C	83	TYR	CA-CB-CG	-5.07	104.77	113.90
1	D	641	ARG	O-C-N	-5.07	117.33	123.27
1	D	649	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	B	306	ASP	N-CA-C	-5.07	105.94	111.82
1	D	833	ARG	N-CA-C	-5.07	101.44	109.96
1	B	49	ARG	CA-C-O	-5.07	115.50	120.82
1	B	61	ASP	CA-C-N	5.07	127.58	120.28
1	B	61	ASP	C-N-CA	5.07	127.58	120.28
1	B	239	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	586	LEU	CB-CA-C	-5.07	102.24	110.85
1	B	501	GLU	N-CA-CB	-5.07	102.52	109.91
1	B	644	PHE	O-C-N	-5.07	117.30	123.13
1	C	811	PHE	N-CA-CB	-5.07	103.16	110.56
1	D	387	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	B	348	GLU	O-C-N	-5.06	116.04	122.27
1	D	176	MET	CA-C-O	5.06	125.82	120.36
1	A	386	ARG	NE-CZ-NH2	-5.06	114.65	119.20
1	A	325	ASN	CA-C-O	5.05	126.68	120.92
1	A	205	ARG	N-CA-CB	-5.05	102.55	111.39
1	B	623	ILE	N-CA-C	-5.05	105.57	110.42
1	D	281	PRO	N-CA-C	5.05	124.73	112.10
1	A	378	THR	CA-C-N	-5.05	117.81	123.16
1	A	378	THR	C-N-CA	-5.05	117.81	123.16
1	B	32	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	B	561	SER	N-CA-C	5.05	121.56	110.80
1	D	365	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	B	292	ARG	CA-C-O	-5.05	115.50	120.90
1	B	457	ARG	CA-C-O	-5.05	115.52	120.82
1	C	40	VAL	CA-CB-CG2	5.05	118.98	110.40
1	C	251	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	387	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	B	105	GLU	CB-CG-CD	5.04	121.18	112.60
1	C	410	PHE	O-C-N	-5.04	116.87	122.07
1	A	596	LYS	CG-CD-CE	5.04	122.90	111.30
1	D	240	THR	N-CA-C	5.04	117.55	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	663	SER	CA-CB-OG	5.04	121.18	111.10
1	A	477	HIS	CB-CG-ND1	5.04	130.26	122.70
1	C	207	GLU	CA-CB-CG	5.04	124.18	114.10
1	C	807	THR	O-C-N	5.04	128.14	122.20
1	D	709	PHE	N-CA-C	5.04	118.57	112.93
1	A	311	PHE	CA-C-O	-5.03	115.21	120.55
1	A	678	ASN	CA-C-O	5.03	126.56	120.92
1	C	294	LYS	N-CA-C	-5.03	105.98	111.82
1	C	350	MET	CA-C-N	5.03	127.29	120.65
1	C	350	MET	C-N-CA	5.03	127.29	120.65
1	A	784	GLN	CG-CD-NE2	5.03	123.95	116.40
1	A	302	ALA	N-CA-C	-5.03	105.92	111.71
1	D	769	ASP	CA-C-O	5.03	125.74	120.36
1	A	672	GLU	CA-C-O	5.03	126.59	120.81
1	A	556	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	B	306	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	457	ARG	O-C-N	5.03	127.46	122.08
1	A	348	GLU	N-CA-C	-5.02	105.88	111.36
1	C	509	GLU	CB-CG-CD	5.02	121.14	112.60
1	A	684	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	375	THR	CA-C-O	-5.02	115.54	121.16
1	B	794	PRO	CA-N-CD	-5.02	104.97	112.00
1	C	691	THR	N-CA-CB	-5.02	102.66	110.04
1	D	125	ILE	CA-C-N	5.02	128.00	120.87
1	D	125	ILE	C-N-CA	5.02	128.00	120.87
1	A	40	VAL	CA-CB-CG1	-5.02	101.87	110.40
1	B	676	THR	N-CA-CB	-5.02	102.01	110.49
1	C	259	VAL	N-CA-C	-5.02	102.47	109.45
1	D	138	ARG	CG-CD-NE	5.02	123.04	112.00
1	D	342	PRO	N-CA-C	5.02	120.22	114.20
1	A	714	ARG	CB-CG-CD	5.02	122.84	111.30
1	A	718	VAL	CA-C-O	-5.02	115.48	121.05
1	C	742	ILE	N-CA-C	-5.02	105.81	110.53
1	D	277	ARG	CB-CG-CD	5.02	122.84	111.30
1	D	367	VAL	O-C-N	-5.01	116.14	121.80
1	A	523	SER	CA-C-O	5.01	126.08	120.82
1	D	446	ILE	N-CA-CB	-5.01	102.08	110.65
1	D	564	ASP	N-CA-C	-5.01	100.90	108.67
1	D	485	GLY	O-C-N	5.01	127.29	123.23
1	C	34	HIS	CA-C-O	-5.01	115.19	120.55
1	C	215	TRP	CD1-CG-CD2	5.01	114.31	106.30
1	A	583	VAL	N-CA-CB	5.01	117.35	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	814	ASP	O-C-N	-5.01	116.81	122.12
1	A	99	MET	CG-SD-CE	-5.00	89.89	100.90
1	A	318	CYS	CA-C-N	-5.00	115.10	122.06
1	A	318	CYS	C-N-CA	-5.00	115.10	122.06
1	A	333	VAL	O-C-N	-5.00	117.37	123.02
1	B	180	ASP	O-C-N	-5.00	116.90	122.55
1	C	331	ASP	CA-C-N	-5.00	114.68	122.73
1	C	331	ASP	C-N-CA	-5.00	114.68	122.73
1	C	811	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	277	ARG	Sidechain
1	A	280	TYR	Peptide
1	A	320	ASP	Peptide
1	A	47	THR	Peptide
1	A	49	ARG	Sidechain
1	B	262	TYR	Sidechain
1	B	320	ASP	Peptide
1	B	52	TYR	Sidechain
1	B	524	TYR	Sidechain
1	B	751	SER	Peptide
1	B	793	ASN	Peptide
1	C	280	TYR	Peptide
1	C	320	ASP	Peptide
1	C	751	SER	Peptide
1	C	820	TYR	Sidechain
1	C	84	TYR	Sidechain
1	D	155	TYR	Sidechain
1	D	280	TYR	Peptide
1	D	320	ASP	Peptide
1	D	52	TYR	Sidechain
1	D	569	ARG	Sidechain
1	D	610	ALA	Peptide
1	D	836	ALA	Peptide
1	D	84	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6692	0	6653	261	1
1	B	6692	0	6653	249	0
1	C	6692	0	6653	263	0
1	D	6692	0	6653	347	1
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
3	A	15	0	6	1	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	7	2	0
4	A	23	0	12	3	0
4	B	23	0	12	1	0
4	C	23	0	12	1	0
4	D	23	0	12	2	0
All	All	26955	0	26687	1101	1

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 21.

All (1101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:HD21	1:D:303:THR:HG21	1.43	1.00
1:D:251:ASP:HB3	1:D:255:LYS:HB3	1.46	0.98
1:D:707:ASN:HA	1:D:800:MET:SD	2.04	0.97
1:A:45:VAL:HG21	4:B:920:AMP:H3'	1.44	0.97
1:D:91:MET:HE1	1:D:144:LEU:HD12	1.48	0.94
1:A:682:MET:SD	1:A:699:MET:HG2	2.09	0.92
1:D:428:MET:SD	1:D:470:ASP:HB3	2.09	0.92
1:B:85:LEU:HD21	1:B:303:THR:HG21	1.50	0.92
1:A:677:GLY:HA2	1:A:680:LYS:HG3	1.52	0.89
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.53	0.88
1:A:103:ALA:HB2	1:A:234:ARG:HH11	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:HD22	1:B:99:MET:HE2	1.58	0.86
1:C:96:GLN:HA	1:C:99:MET:HE3	1.56	0.85
1:D:326:PHE:HA	1:D:329:PHE:HB2	1.58	0.85
1:D:91:MET:SD	1:D:241:MET:HE1	2.16	0.84
1:B:550:GLU:HA	1:B:554:LYS:HA	1.60	0.84
1:C:486:ILE:HD11	1:C:676:THR:HG23	1.56	0.84
1:D:597:PHE:HE2	1:D:792:LYS:HD2	1.43	0.83
1:C:85:LEU:HD12	1:C:342:PRO:HB3	1.61	0.82
1:A:208:HIS:HA	1:A:213:ALA:HA	1.61	0.81
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.64	0.80
1:A:799:ARG:HA	1:A:802:ILE:HD12	1.64	0.79
1:A:99:MET:HE1	1:A:119:MET:SD	2.21	0.79
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.65	0.79
1:A:337:LEU:HD23	1:A:445:CYS:SG	2.23	0.78
1:D:663:SER:HB3	1:D:688:THR:HA	1.66	0.78
1:D:315:LYS:HA	1:D:318:CYS:SG	2.25	0.77
1:A:336:GLN:HE21	1:A:825:TRP:HE1	1.33	0.77
1:A:389:VAL:HG12	1:A:439:ILE:HG13	1.65	0.77
1:C:251:ASP:HB3	1:C:255:LYS:HB3	1.65	0.76
1:A:490:ARG:HA	1:A:494:LEU:HD13	1.67	0.76
1:C:165:ILE:HD11	1:C:281:PRO:HA	1.67	0.76
1:A:337:LEU:HB2	1:A:374:TYR:HB2	1.67	0.76
1:A:492:LEU:HG	1:A:683:LEU:HD22	1.68	0.76
1:A:326:PHE:HA	1:A:329:PHE:HB2	1.69	0.75
1:D:522:LEU:O	1:D:525:VAL:HG23	1.87	0.75
1:D:692:MET:SD	1:D:710:ILE:HG21	2.26	0.74
1:D:326:PHE:HD1	1:D:329:PHE:CD2	2.05	0.74
1:A:423:ASP:HA	1:A:426:ARG:HG2	1.69	0.74
1:C:733:ASP:HA	1:C:739:ARG:HH12	1.53	0.73
1:A:459:HIS:O	1:A:462:ILE:HG12	1.88	0.73
1:D:323:ARG:HG2	1:D:325:ASN:HB2	1.69	0.73
1:A:738:LEU:O	1:A:741:ILE:HG12	1.89	0.73
1:C:486:ILE:HG12	1:C:680:LYS:HG3	1.71	0.73
1:A:738:LEU:HD12	1:A:741:ILE:HD11	1.71	0.72
1:B:316:PHE:HD2	1:B:324:THR:HG23	1.54	0.72
1:B:99:MET:HE1	1:B:119:MET:SD	2.30	0.72
1:C:163:PHE:HE1	1:C:277:ARG:HH11	1.38	0.72
1:C:224:MET:SD	1:C:247:LYS:NZ	2.62	0.72
1:D:143:PHE:O	1:D:147:MET:HG3	1.90	0.72
1:B:755:PRO:HD2	1:C:426:ARG:NH1	2.05	0.71
1:A:783:CYS:O	1:A:787:VAL:HG23	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:ILE:HB	1:C:609:ALA:HA	1.72	0.71
1:B:93:ARG:HG2	1:B:126:GLU:HB3	1.73	0.71
1:D:692:MET:HG3	1:D:697:VAL:HG22	1.71	0.71
1:A:157:TYR:HE1	1:A:242:ARG:HG2	1.56	0.70
1:B:274:ASN:ND2	1:B:291:LEU:HD21	2.07	0.70
1:D:263:ILE:O	1:D:266:VAL:HG23	1.92	0.70
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.73	0.70
1:B:458:ILE:HD11	1:B:694:GLY:H	1.55	0.70
1:B:766:MET:HE3	1:B:774:PHE:HE2	1.56	0.70
1:C:692:MET:SD	1:C:710:ILE:HG21	2.32	0.70
1:B:346:ILE:HG23	1:B:368:THR:HG21	1.74	0.69
1:D:597:PHE:CE2	1:D:792:LYS:HD2	2.26	0.69
1:A:727:ASN:HD21	1:D:725:GLY:HA3	1.58	0.69
1:D:80:LYS:HE2	1:D:331:ASP:O	1.92	0.69
1:D:474:LEU:HD13	1:D:475:GLU:HG3	1.73	0.69
1:A:34:HIS:CD2	1:A:57:HIS:HB3	2.28	0.69
1:B:678:ASN:ND2	1:B:695:ALA:HB3	2.08	0.69
1:C:91:MET:HB3	1:C:129:ALA:HB3	1.76	0.69
1:D:557:ILE:HG22	1:D:558:ASN:H	1.58	0.69
1:D:170:ILE:HG12	1:D:646:GLU:HG3	1.75	0.68
1:A:157:TYR:CE1	1:A:242:ARG:HG2	2.28	0.68
1:B:678:ASN:HD22	1:B:695:ALA:HB3	1.59	0.68
1:B:353:LEU:HB3	1:B:359:LEU:HD12	1.74	0.68
1:D:253:ASN:OD1	1:D:254:LEU:HD22	1.94	0.68
1:C:369:VAL:HA	1:C:448:GLY:O	1.94	0.67
1:C:568:LYS:HD2	1:C:574:LYS:HE3	1.76	0.67
1:A:426:ARG:NH2	1:D:754:GLN:HA	2.10	0.67
1:A:629:VAL:HG11	1:A:750:PHE:HE1	1.59	0.67
1:D:64:VAL:HA	1:D:67:TRP:HB3	1.77	0.67
1:C:346:ILE:HD13	1:C:448:GLY:HA3	1.77	0.67
1:A:396:LEU:HB3	1:A:399:HIS:HB2	1.77	0.67
1:A:49:ARG:HH21	1:A:125:ILE:HG22	1.57	0.67
1:A:692:MET:HE2	1:A:710:ILE:HG21	1.77	0.67
1:D:813:SER:O	1:D:817:ILE:HG12	1.95	0.67
1:B:562:LEU:HG	1:B:791:TYR:CD2	2.29	0.67
1:C:62:HIS:ND1	1:C:104:LEU:HD21	2.11	0.67
1:D:165:ILE:HG12	1:D:279:LEU:HB3	1.75	0.67
1:D:657:ILE:HD13	1:D:680:LYS:HB3	1.76	0.67
1:A:235:ASN:HD21	1:A:237:VAL:HG22	1.60	0.66
1:D:326:PHE:HD1	1:D:329:PHE:HD2	1.42	0.66
1:A:119:MET:O	1:A:123:GLU:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:GLU:HA	1:D:554:LYS:HA	1.76	0.66
1:C:326:PHE:HA	1:C:329:PHE:HB2	1.76	0.66
1:C:678:ASN:ND2	1:C:695:ALA:HB3	2.11	0.66
1:C:168:GLN:OE1	1:C:608:LYS:HA	1.96	0.66
1:D:732:TYR:HA	1:D:738:LEU:HD22	1.78	0.66
1:D:791:TYR:HA	1:D:797:TRP:CD1	2.30	0.66
1:A:783:CYS:SG	1:A:786:ARG:NH2	2.69	0.66
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.77	0.65
1:D:519:ARG:O	1:D:522:LEU:HB2	1.96	0.65
1:D:682:MET:HE3	1:D:808:SER:HA	1.77	0.65
1:C:85:LEU:HD12	1:C:342:PRO:CB	2.26	0.65
1:D:488:PRO:O	1:D:492:LEU:HB3	1.95	0.65
1:C:365:TRP:O	1:C:369:VAL:HG23	1.96	0.65
1:D:522:LEU:HD11	1:D:803:ARG:HH11	1.60	0.65
1:A:258:ASN:OD1	1:A:259:VAL:HG22	1.97	0.65
1:C:600:PRO:HA	1:C:639:ARG:O	1.97	0.65
1:D:312:LYS:HA	1:D:324:THR:HG21	1.79	0.64
1:D:75:TYR:HE1	1:D:314:SER:HA	1.61	0.64
1:D:235:ASN:HA	1:D:833:ARG:HG3	1.80	0.64
1:B:615:MET:CE	1:B:761:ILE:HG12	2.27	0.64
1:D:424:ARG:HG3	1:D:427:ARG:NH2	2.11	0.64
1:D:804:ASN:O	1:D:807:THR:HB	1.97	0.64
1:B:305:GLN:O	1:B:309:ARG:HB2	1.98	0.64
1:B:738:LEU:HD12	1:B:741:ILE:HD11	1.80	0.64
1:D:225:PRO:HB2	1:D:242:ARG:HD2	1.80	0.64
1:D:63:LEU:HD21	1:D:231:PRO:HB3	1.79	0.64
1:A:732:TYR:CE1	1:A:739:ARG:HA	2.33	0.63
1:A:795:ARG:O	1:A:799:ARG:HG3	1.99	0.63
1:B:581:LEU:HD22	1:B:741:ILE:HD12	1.81	0.63
1:D:60:ARG:HD3	1:D:188:PRO:O	1.99	0.63
1:D:578:LEU:HD23	1:D:666:ILE:HD12	1.79	0.63
1:C:315:LYS:HA	1:C:318:CYS:SG	2.37	0.63
1:D:198:LEU:HD22	1:D:305:GLN:HB3	1.81	0.63
1:A:599:VAL:HG11	1:A:791:TYR:HD2	1.62	0.63
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.81	0.63
1:B:790:LEU:HD23	1:B:797:TRP:CD1	2.34	0.63
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.80	0.63
1:D:530:PHE:HA	1:D:533:ASP:HB2	1.80	0.63
1:D:316:PHE:HB3	1:D:324:THR:HG23	1.81	0.62
1:D:688:THR:HG22	1:D:689:ILE:O	1.98	0.62
1:B:28:LYS:HB3	1:B:115:LEU:HD21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:615:MET:HE2	1:D:764:MET:HE3	1.80	0.62
1:A:472:TYR:CD1	1:A:476:PRO:HA	2.34	0.62
1:A:516:ASP:HA	1:A:809:GLY:HA3	1.81	0.62
1:A:110:GLU:O	1:A:114:GLN:HG3	1.99	0.62
1:A:215:TRP:CE2	1:A:218:THR:HG21	2.35	0.62
1:B:791:TYR:HA	1:B:797:TRP:CD1	2.35	0.62
1:D:567:VAL:HA	1:D:606:GLY:O	2.00	0.62
1:B:234:ARG:O	1:B:833:ARG:HG3	2.00	0.62
1:D:293:LEU:HD23	1:D:391:LEU:HD22	1.82	0.62
1:D:588:ASN:HD21	1:D:741:ILE:HG22	1.65	0.61
1:A:103:ALA:HB2	1:A:234:ARG:HD2	1.82	0.61
1:C:340:THR:O	1:C:343:SER:HB3	2.00	0.61
1:D:627:GLY:O	1:D:631:ASN:HB2	1.99	0.61
1:D:692:MET:SD	1:D:710:ILE:CG2	2.87	0.61
1:A:441:MET:HE3	1:A:444:LEU:HD12	1.81	0.61
1:A:733:ASP:HA	1:A:739:ARG:HH12	1.64	0.61
1:B:87:LEU:HD11	1:B:296:GLU:HA	1.82	0.61
1:D:85:LEU:HD13	1:D:300:VAL:HG23	1.82	0.61
1:B:502:ILE:O	1:B:506:ARG:HG2	2.00	0.61
1:D:499:LEU:N	1:D:537:VAL:HG11	2.14	0.61
1:B:666:ILE:HG22	1:B:711:PHE:CE1	2.36	0.61
1:D:498:GLY:O	1:D:501:GLU:HB3	2.01	0.61
1:A:255:LYS:O	1:A:256:ASP:HB2	2.00	0.61
1:D:396:LEU:HB3	1:D:399:HIS:HB2	1.82	0.61
1:A:91:MET:SD	1:A:241:MET:HE1	2.41	0.61
1:D:42:ASP:OD1	1:D:43:ARG:N	2.34	0.61
1:C:565:VAL:HG12	1:C:604:MET:HE3	1.83	0.60
1:D:699:MET:HE2	1:D:708:PHE:HZ	1.65	0.60
1:B:166:PHE:HB2	1:B:178:GLU:O	2.00	0.60
1:D:702:GLU:HB2	1:D:807:THR:HG23	1.82	0.60
1:B:316:PHE:HA	1:B:319:ARG:HB3	1.83	0.60
1:C:606:GLY:HA3	1:C:645:LEU:HB2	1.83	0.60
1:B:600:PRO:HA	1:B:639:ARG:O	2.01	0.60
1:D:576:GLN:O	1:D:580:CYS:SG	2.58	0.60
1:C:690:GLY:O	1:C:710:ILE:HA	2.01	0.60
1:D:748:GLY:HA3	1:D:755:PRO:HB3	1.83	0.60
1:A:395:LEU:HG	1:A:396:LEU:HD22	1.84	0.60
1:A:197:THR:O	1:A:198:LEU:HD23	2.02	0.60
1:D:64:VAL:O	1:D:68:ILE:HG12	2.01	0.60
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.01	0.60
1:A:585:THR:O	1:A:589:ARG:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:VAL:HG21	1:D:298:PHE:CD1	2.36	0.60
1:C:503:ILE:HG12	1:C:521:LEU:HD21	1.84	0.59
1:A:446:ILE:HG21	1:A:471:PHE:CD2	2.37	0.59
1:C:694:GLY:O	1:C:697:VAL:HB	2.01	0.59
1:D:341:HIS:HB2	1:D:342:PRO:HD3	1.84	0.59
1:D:507:ILE:HB	1:D:520:LYS:NZ	2.16	0.59
1:A:525:VAL:O	1:A:531:ILE:HD11	2.03	0.59
1:A:733:ASP:HA	1:A:739:ARG:NH1	2.17	0.59
1:C:716:GLU:O	1:C:720:ARG:HG2	2.02	0.59
1:D:593:GLU:HB3	1:D:596:LYS:HB2	1.83	0.59
1:D:521:LEU:HA	1:D:524:TYR:CD1	2.37	0.59
1:D:357:GLU:O	1:D:358:ARG:HB2	2.01	0.59
1:D:795:ARG:O	1:D:799:ARG:HG3	2.02	0.59
1:A:455:VAL:H	1:A:459:HIS:HD2	1.51	0.59
1:B:290:GLU:HG3	1:B:391:LEU:CD2	2.33	0.59
1:D:18:LEU:HD22	1:D:18:LEU:H	1.68	0.59
1:C:781:VAL:HG23	1:C:782:LYS:HE3	1.85	0.59
1:A:150:LEU:HD13	1:A:829:PRO:HB3	1.85	0.58
1:B:778:GLU:O	1:B:782:LYS:HG2	2.03	0.58
1:D:588:ASN:HD21	1:D:744:GLN:HE22	1.50	0.58
1:A:348:GLU:O	1:A:352:VAL:HG23	2.03	0.58
1:A:392:LEU:HB3	1:A:400:LEU:HB2	1.85	0.58
1:C:316:PHE:O	1:C:324:THR:HG23	2.03	0.58
1:C:336:GLN:HG2	1:C:825:TRP:HE1	1.68	0.58
1:D:703:ALA:HB2	1:D:807:THR:HG21	1.85	0.58
1:A:528:GLU:HB3	1:A:532:ARG:NH2	2.19	0.58
1:A:629:VAL:HG11	1:A:750:PHE:CE1	2.38	0.58
1:C:642:VAL:O	1:C:643:ILE:HG13	2.03	0.58
1:D:511:TYR:HA	1:D:514:ASP:O	2.03	0.58
1:B:573:TYR:HD2	1:B:671:THR:HB	1.69	0.58
1:C:692:MET:SD	1:C:710:ILE:HG13	2.44	0.58
1:D:642:VAL:O	1:D:643:ILE:HG13	2.02	0.58
1:D:350:MET:SD	1:D:365:TRP:HE3	2.26	0.58
1:C:68:ILE:O	1:C:72:GLN:HG3	2.04	0.58
1:B:82:ILE:HB	1:B:334:ALA:HB3	1.86	0.58
1:C:711:PHE:CZ	1:C:780:TYR:HD1	2.21	0.58
1:D:98:THR:O	1:D:102:LEU:HB2	2.04	0.58
1:D:336:GLN:HG3	1:D:825:TRP:HE1	1.67	0.58
1:B:458:ILE:HD11	1:B:694:GLY:N	2.19	0.58
1:B:184:ARG:HD2	1:B:185:TYR:CE2	2.39	0.58
1:B:293:LEU:HD23	1:B:395:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:GLN:O	1:B:543:LEU:HB2	2.04	0.57
1:C:322:VAL:O	1:C:325:ASN:HB2	2.03	0.57
1:D:675:GLY:HA3	1:D:678:ASN:HD21	1.68	0.57
1:D:721:LEU:HG	1:D:726:TYR:HB2	1.85	0.57
1:A:421:ASP:O	1:A:425:LEU:HD23	2.04	0.57
1:A:600:PRO:HB3	1:A:639:ARG:HA	1.86	0.57
1:B:211:GLN:HG2	1:B:358:ARG:HD2	1.85	0.57
1:C:85:LEU:HD22	1:C:303:THR:HG21	1.84	0.57
1:D:459:HIS:CD2	1:D:673:ALA:HB1	2.39	0.57
1:B:707:ASN:HA	1:B:800:MET:SD	2.44	0.57
1:A:74:TYR:CE2	1:A:153:ALA:HA	2.40	0.57
1:B:319:ARG:HE	1:B:319:ARG:C	2.13	0.57
1:C:150:LEU:HB3	1:C:829:PRO:HB3	1.85	0.57
1:D:97:ASN:HA	1:D:494:LEU:HD11	1.87	0.57
1:D:410:PHE:O	1:D:414:VAL:HG23	2.05	0.57
1:A:30:ASN:HB2	1:A:58:THR:HG23	1.84	0.57
1:A:651:SER:HA	1:A:654:GLU:HG2	1.86	0.57
1:C:96:GLN:O	1:C:100:VAL:HG13	2.05	0.57
1:C:224:MET:HB2	1:C:247:LYS:HE2	1.85	0.57
1:A:336:GLN:NE2	1:A:825:TRP:HE1	2.02	0.57
1:C:129:ALA:HB1	1:C:131:LEU:HD23	1.86	0.57
1:C:751:SER:HB2	1:C:754:GLN:O	2.04	0.57
1:D:661:ASP:HB3	1:D:797:TRP:CH2	2.40	0.57
1:B:90:TYR:HB3	1:B:137:GLY:C	2.30	0.56
1:D:456:ALA:HB3	1:D:459:HIS:HB3	1.87	0.56
1:A:181:ASP:O	1:A:184:ARG:HB2	2.05	0.56
1:B:727:ASN:O	1:B:730:GLU:HG2	2.05	0.56
1:C:322:VAL:HG13	1:C:325:ASN:HB2	1.87	0.56
1:D:224:MET:HE3	1:D:226:TYR:CE1	2.40	0.56
1:A:583:VAL:HG11	1:A:642:VAL:HG22	1.88	0.56
1:B:320:ASP:HA	1:B:324:THR:HA	1.87	0.56
1:B:459:HIS:CD2	1:B:673:ALA:HB1	2.39	0.56
1:D:28:LYS:HZ2	1:D:114:GLN:HB3	1.70	0.56
1:D:764:MET:HA	1:D:768:HIS:CE1	2.41	0.56
1:A:411:LEU:HD11	1:A:429:SER:HB2	1.87	0.56
1:B:781:VAL:HG23	1:B:782:LYS:HE3	1.87	0.56
1:D:798:THR:O	1:D:802:ILE:HG13	2.06	0.56
1:B:181:ASP:O	1:B:184:ARG:HB2	2.06	0.56
1:D:316:PHE:HD2	1:D:324:THR:HG23	1.71	0.56
1:A:661:ASP:HB3	1:A:797:TRP:CZ2	2.41	0.56
1:A:590:ILE:HG12	1:A:598:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASN:O	1:B:254:LEU:HD12	2.05	0.56
1:B:290:GLU:O	1:B:294:LYS:HG3	2.06	0.56
1:C:678:ASN:HD22	1:C:695:ALA:HB3	1.71	0.56
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.41	0.56
1:B:319:ARG:NE	1:B:321:PRO:HD2	2.21	0.56
1:C:609:ALA:HB2	1:C:620:ILE:HD11	1.87	0.56
1:C:615:MET:HE2	1:C:761:ILE:HG23	1.88	0.56
1:C:726:TYR:OH	1:C:774:PHE:HB2	2.05	0.56
1:D:73:HIS:CD2	1:D:834:LEU:HD11	2.40	0.56
1:B:599:VAL:HG21	1:B:788:SER:O	2.05	0.55
1:C:129:ALA:HB1	1:C:131:LEU:CD2	2.35	0.55
1:B:677:GLY:HA2	1:B:680:LYS:HD2	1.88	0.55
1:C:626:ILE:O	1:C:630:VAL:HG13	2.06	0.55
1:D:235:ASN:HB2	1:D:833:ARG:HA	1.87	0.55
1:B:511:TYR:HA	1:B:514:ASP:O	2.07	0.55
1:A:565:VAL:HG12	1:A:604:MET:HE3	1.88	0.55
1:C:235:ASN:OD1	1:C:237:VAL:HG22	2.07	0.55
1:C:695:ALA:O	1:C:699:MET:SD	2.65	0.55
1:B:459:HIS:HB2	1:B:673:ALA:O	2.06	0.55
1:A:14:SER:OG	1:A:16:ARG:NH1	2.39	0.55
1:A:468:PHE:HB3	1:A:479:PHE:CZ	2.41	0.55
1:A:322:VAL:HG13	1:A:325:ASN:HD22	1.71	0.55
1:A:492:LEU:HG	1:A:683:LEU:CD2	2.35	0.55
1:A:583:VAL:HG11	1:A:642:VAL:CG2	2.36	0.55
1:C:147:MET:O	1:C:152:LEU:HB2	2.07	0.55
1:C:665:GLN:HE21	1:C:678:ASN:HA	1.72	0.55
1:C:692:MET:SD	1:C:710:ILE:CG2	2.94	0.55
1:D:143:PHE:CD1	1:D:817:ILE:HD11	2.41	0.55
1:D:613:TYR:HE1	1:D:615:MET:HB3	1.71	0.55
1:A:204:GLY:HA3	1:A:218:THR:HG22	1.89	0.55
1:A:689:ILE:HA	1:A:709:PHE:HB2	1.89	0.55
1:D:507:ILE:HB	1:D:520:LYS:HZ2	1.71	0.55
1:D:721:LEU:HD21	1:D:726:TYR:HD1	1.71	0.55
1:A:540:GLU:O	1:A:544:LYS:HD3	2.06	0.55
1:B:161:TYR:HA	1:B:276:SER:O	2.07	0.55
1:B:612:GLY:H	1:B:617:LYS:HE2	1.72	0.55
1:B:728:ALA:O	1:B:731:TYR:HB2	2.07	0.55
1:D:506:ARG:HH22	1:D:533:ASP:CG	2.14	0.55
1:B:810:LYS:HD3	1:B:811:PHE:HE1	1.72	0.55
1:D:144:LEU:HD21	1:D:156:GLY:HA3	1.89	0.55
1:A:503:ILE:HG23	1:A:521:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:ARG:O	1:B:799:ARG:HG3	2.07	0.54
1:C:323:ARG:HB2	1:C:325:ASN:CG	2.32	0.54
1:C:343:SER:HB2	1:C:445:CYS:SG	2.47	0.54
1:C:834:LEU:HD12	1:C:835:PRO:HD2	1.89	0.54
1:A:458:ILE:HG21	1:A:697:VAL:HG21	1.90	0.54
1:D:486:ILE:HG12	1:D:680:LYS:HG3	1.88	0.54
1:B:355:ASP:OD2	1:B:398:ARG:HD3	2.08	0.54
1:B:204:GLY:HA3	1:B:215:TRP:HE1	1.73	0.54
1:B:391:LEU:O	1:B:395:LEU:HD23	2.07	0.54
1:D:818:ALA:O	1:D:821:ALA:HB3	2.08	0.54
1:A:797:TRP:CZ3	1:A:801:VAL:HG21	2.43	0.54
1:C:204:GLY:HA3	1:C:218:THR:HG22	1.90	0.54
1:C:742:ILE:HD11	1:C:774:PHE:CZ	2.43	0.54
1:B:341:HIS:HB2	1:B:342:PRO:HD3	1.89	0.54
1:C:492:LEU:HG	1:C:683:LEU:HD22	1.90	0.54
1:D:138:ARG:HD3	1:D:491:TRP:HZ2	1.72	0.54
1:B:67:TRP:O	1:B:71:GLN:HG2	2.08	0.54
1:C:727:ASN:O	1:C:730:GLU:HG2	2.08	0.54
1:D:707:ASN:CA	1:D:800:MET:SD	2.90	0.54
1:A:482:LYS:HE3	1:A:819:GLN:O	2.06	0.54
1:D:351:ARG:HG2	1:D:398:ARG:HG2	1.89	0.54
1:D:424:ARG:HA	1:D:427:ARG:NH2	2.23	0.54
1:D:527:ASP:OD2	1:D:529:ALA:HB3	2.07	0.54
1:A:336:GLN:HE21	1:A:825:TRP:NE1	2.05	0.54
1:D:665:GLN:HE22	1:D:678:ASN:HA	1.73	0.54
1:B:82:ILE:HD11	1:B:147:MET:SD	2.47	0.53
1:B:456:ALA:HB2	1:B:674:SER:HB2	1.89	0.53
1:B:746:SER:OG	1:B:762:VAL:HG11	2.07	0.53
1:C:340:THR:HB	1:C:385:GLU:OE1	2.08	0.53
1:C:707:ASN:HA	1:C:800:MET:SD	2.48	0.53
1:A:21:VAL:O	1:A:23:ASN:N	2.41	0.53
1:A:129:ALA:HA	1:A:182:TRP:CE3	2.43	0.53
1:A:191:LYS:HD2	1:A:193:ARG:HH11	1.73	0.53
1:A:39:LEU:HD21	1:A:53:PHE:HB2	1.90	0.53
1:A:49:ARG:HG3	1:A:53:PHE:HE2	1.73	0.53
1:C:250:ASN:HD21	1:C:269:ARG:HE	1.56	0.53
1:A:42:ASP:OD2	1:A:44:ASN:HB2	2.08	0.53
1:B:423:ASP:HA	1:B:426:ARG:HG3	1.89	0.53
1:B:574:LYS:NZ	2:B:901:SO4:O2	2.41	0.53
1:B:577:LEU:HD13	1:B:765:LEU:HD13	1.89	0.53
1:B:735:ILE:O	1:B:739:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:VAL:HB	1:D:438:ARG:NH2	2.24	0.53
1:B:573:TYR:CD2	1:B:671:THR:HB	2.43	0.53
1:B:590:ILE:HD11	1:B:598:VAL:HG21	1.91	0.53
1:C:363:LYS:O	1:C:367:VAL:HG23	2.07	0.53
1:D:390:HIS:HA	1:D:393:GLU:OE1	2.09	0.53
1:C:224:MET:SD	1:C:247:LYS:CE	2.96	0.53
1:D:322:VAL:O	1:D:325:ASN:N	2.41	0.53
1:D:575:ARG:NH2	1:D:776:ASP:HB2	2.24	0.53
1:B:322:VAL:O	1:B:325:ASN:HB2	2.09	0.53
1:B:350:MET:O	1:B:354:VAL:HG23	2.08	0.53
1:A:426:ARG:NH1	1:D:755:PRO:HD2	2.24	0.53
1:C:395:LEU:H	1:C:395:LEU:HD23	1.74	0.53
1:D:91:MET:SD	1:D:241:MET:CE	2.92	0.53
1:D:231:PRO:HA	1:D:238:VAL:HG22	1.91	0.53
1:C:665:GLN:NE2	1:C:678:ASN:HA	2.24	0.53
1:D:507:ILE:HG21	1:D:520:LYS:HB2	1.89	0.53
1:D:561:SER:HA	1:D:600:PRO:HG2	1.90	0.53
1:D:603:VAL:HG23	1:D:642:VAL:HA	1.91	0.53
1:A:361:TRP:CZ3	1:A:409:ARG:HD2	2.44	0.53
1:B:580:CYS:SG	1:B:622:LEU:HD12	2.49	0.53
1:B:347:PRO:HG3	1:B:403:ILE:HD11	1.91	0.52
1:D:661:ASP:HB3	1:D:797:TRP:HH2	1.72	0.52
1:C:168:GLN:HB2	1:C:608:LYS:HG2	1.91	0.52
1:D:528:GLU:HG2	1:D:532:ARG:HH21	1.73	0.52
1:D:664:GLU:HA	1:D:689:ILE:HG22	1.91	0.52
1:D:675:GLY:HA3	1:D:678:ASN:ND2	2.24	0.52
1:D:677:GLY:HA2	1:D:680:LYS:HD2	1.92	0.52
1:A:264:GLN:NE2	1:C:267:LEU:HD22	2.24	0.52
1:B:157:TYR:CE2	1:B:242:ARG:HG2	2.44	0.52
1:B:183:LEU:HD23	1:B:187:ASN:HB2	1.91	0.52
1:B:783:CYS:SG	1:B:786:ARG:NH2	2.83	0.52
1:C:689:ILE:HA	1:C:709:PHE:HB2	1.90	0.52
1:D:167:ASN:HD22	1:D:180:ASP:HB2	1.72	0.52
1:A:670:GLY:H	1:A:693:ASP:CG	2.17	0.52
1:B:361:TRP:HH2	1:B:406:ILE:HG12	1.74	0.52
1:D:569:ARG:HG2	1:D:574:LYS:HD3	1.92	0.52
1:D:699:MET:HB3	1:D:708:PHE:HE2	1.73	0.52
1:A:682:MET:SD	1:A:699:MET:HE3	2.49	0.52
1:D:274:ASN:HA	1:D:277:ARG:HG3	1.91	0.52
1:B:82:ILE:HA	1:B:334:ALA:HB3	1.91	0.52
1:D:503:ILE:HG12	1:D:521:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:ILE:O	1:C:594:PRO:HA	2.10	0.52
1:C:699:MET:HB3	1:C:708:PHE:HZ	1.74	0.52
1:D:75:TYR:CE1	1:D:314:SER:HA	2.44	0.52
1:D:491:TRP:HA	1:D:495:CYS:SG	2.50	0.52
1:D:735:ILE:HG22	1:D:738:LEU:HB2	1.92	0.52
1:C:63:LEU:HD13	1:C:229:PRO:HG2	1.92	0.52
1:C:253:ASN:H	1:C:259:VAL:HG21	1.74	0.52
1:D:171:CYS:O	1:D:174:TRP:HB2	2.09	0.52
1:A:676:THR:HG22	3:A:999:PLP:C4A	2.40	0.52
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.10	0.51
1:C:579:ASN:O	1:C:583:VAL:HG23	2.09	0.51
1:A:577:LEU:O	1:A:581:LEU:HG	2.11	0.51
1:B:810:LYS:HD3	1:B:811:PHE:CE1	2.45	0.51
1:C:182:TRP:H	1:C:182:TRP:CD1	2.29	0.51
1:C:378:THR:O	1:C:459:HIS:CE1	2.63	0.51
1:D:326:PHE:CA	1:D:329:PHE:HB2	2.36	0.51
1:D:567:VAL:HB	1:D:648:TYR:CZ	2.45	0.51
1:B:255:LYS:O	1:B:256:ASP:HB2	2.09	0.51
1:B:571:HIS:CE1	1:B:613:TYR:HH	2.27	0.51
1:B:798:THR:O	1:B:802:ILE:HG13	2.11	0.51
1:C:348:GLU:OE1	1:C:399:HIS:HE1	1.93	0.51
1:C:258:ASN:OD1	1:C:259:VAL:HG22	2.10	0.51
1:C:591:LYS:HZ2	1:C:633:ASP:CG	2.18	0.51
1:B:112:THR:HG22	1:B:117:LEU:HB2	1.92	0.51
1:B:315:LYS:O	1:B:319:ARG:HB2	2.10	0.51
1:C:250:ASN:HD21	1:C:269:ARG:NE	2.08	0.51
1:A:369:VAL:HG22	1:A:448:GLY:HA2	1.92	0.51
1:A:538:LYS:O	1:A:538:LYS:HG3	2.10	0.51
1:B:402:ILE:O	1:B:406:ILE:HG13	2.10	0.51
1:A:149:THR:HA	1:A:235:ASN:OD1	2.10	0.51
1:B:290:GLU:HG3	1:B:391:LEU:HD21	1.92	0.51
1:C:676:THR:HG22	3:C:999:PLP:C4A	2.40	0.51
1:D:168:GLN:HE22	1:D:644:PHE:HE2	1.59	0.51
1:A:203:TYR:O	1:A:218:THR:HG22	2.11	0.51
1:A:353:LEU:O	1:A:357:GLU:HB2	2.11	0.51
1:C:91:MET:HB3	1:C:129:ALA:CB	2.40	0.51
1:C:472:TYR:CE1	1:C:476:PRO:HA	2.46	0.51
1:A:88:GLU:HG3	1:A:279:LEU:HD11	1.93	0.51
1:A:703:ALA:CA	1:A:807:THR:HG21	2.40	0.51
1:B:280:TYR:OH	1:B:291:LEU:HD12	2.11	0.51
1:B:433:GLU:CD	1:B:437:LYS:HZ1	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:TRP:C	1:B:495:CYS:SG	2.95	0.50
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.10	0.50
1:B:426:ARG:NH2	1:B:427:ARG:HG2	2.27	0.50
1:B:738:LEU:O	1:B:742:ILE:HG12	2.11	0.50
1:C:446:ILE:HG12	1:C:452:VAL:HG21	1.93	0.50
1:D:138:ARG:HD3	1:D:491:TRP:CZ2	2.45	0.50
1:D:637:GLY:O	1:D:641:ARG:NH2	2.44	0.50
1:A:274:ASN:HA	1:A:277:ARG:HB2	1.93	0.50
1:C:315:LYS:CA	1:C:318:CYS:SG	2.99	0.50
1:D:211:GLN:HG3	1:D:358:ARG:HD2	1.92	0.50
1:D:252:PHE:HZ	1:D:268:ASP:OD2	1.94	0.50
1:B:99:MET:HB3	1:B:105:GLU:HA	1.93	0.50
1:B:279:LEU:HD23	1:B:280:TYR:H	1.76	0.50
1:C:341:HIS:HB2	1:C:342:PRO:HD3	1.93	0.50
1:D:224:MET:HE3	1:D:226:TYR:HE1	1.77	0.50
1:D:575:ARG:HH22	1:D:776:ASP:HB2	1.76	0.50
1:D:810:LYS:O	1:D:815:ARG:NH2	2.43	0.50
1:C:357:GLU:O	1:C:358:ARG:HB2	2.11	0.50
1:C:589:ARG:HH11	1:C:737:GLU:HG2	1.77	0.50
1:D:346:ILE:HD13	1:D:445:CYS:HA	1.93	0.50
1:A:529:ALA:O	1:A:532:ARG:HG2	2.12	0.50
1:D:70:THR:O	1:D:73:HIS:HB3	2.11	0.50
1:D:455:VAL:HG12	1:D:459:HIS:HD2	1.76	0.50
1:D:677:GLY:O	1:D:681:PHE:HD1	1.95	0.50
1:B:263:ILE:O	1:B:266:VAL:HG23	2.12	0.50
1:A:330:PRO:HG3	1:A:370:LYS:HE3	1.93	0.50
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.47	0.50
1:B:207:GLU:OE2	1:B:214:LYS:NZ	2.45	0.50
1:C:13:ILE:O	1:D:43:ARG:HD3	2.11	0.50
1:A:687:LEU:HD22	1:A:800:MET:HG2	1.94	0.50
1:C:699:MET:HB3	1:C:708:PHE:CZ	2.46	0.50
1:D:373:ALA:HA	1:D:449:SER:HB3	1.93	0.50
1:A:449:SER:O	1:A:478:LYS:HD3	2.12	0.49
1:B:47:THR:H	1:B:50:ASP:HB2	1.77	0.49
1:C:34:HIS:HA	1:C:38:THR:HB	1.93	0.49
1:C:764:MET:SD	1:C:769:ASP:HA	2.52	0.49
1:D:562:LEU:HB2	1:D:600:PRO:O	2.12	0.49
1:A:456:ALA:HA	1:A:483:THR:HG23	1.93	0.49
1:A:601:ARG:NH2	1:A:784:GLN:OE1	2.45	0.49
1:B:48:PRO:HB2	1:B:125:ILE:HD11	1.94	0.49
1:B:742:ILE:HG22	1:B:762:VAL:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ARG:HG3	1:D:189:TRP:CE3	2.47	0.49
1:D:82:ILE:HD13	1:D:82:ILE:O	2.12	0.49
1:D:516:ASP:HA	1:D:809:GLY:HA3	1.94	0.49
1:D:713:MET:HG2	1:D:717:ASP:HB2	1.94	0.49
1:A:526:ASP:OD2	1:A:799:ARG:NH1	2.45	0.49
1:B:601:ARG:NH2	1:B:784:GLN:OE1	2.45	0.49
1:B:267:LEU:HD23	1:B:271:LEU:HD21	1.94	0.49
1:C:70:THR:O	1:C:73:HIS:HB3	2.12	0.49
1:C:289:LYS:HG2	1:C:291:LEU:HB2	1.94	0.49
1:D:579:ASN:HB2	1:D:666:ILE:HD11	1.93	0.49
1:A:506:ARG:HB3	1:A:524:TYR:CE2	2.47	0.49
1:B:369:VAL:O	1:B:450:HIS:HB3	2.12	0.49
1:D:531:ILE:HD11	1:D:799:ARG:CD	2.43	0.49
1:B:366:GLU:O	1:B:370:LYS:HB2	2.13	0.49
1:C:605:ILE:O	1:C:644:PHE:HA	2.12	0.49
1:D:507:ILE:CG2	1:D:520:LYS:HD2	2.42	0.49
1:B:93:ARG:HA	1:B:126:GLU:OE2	2.13	0.49
1:B:558:ASN:OD1	1:B:560:ASN:HB2	2.13	0.49
1:C:392:LEU:HB3	1:C:400:LEU:HG	1.94	0.49
1:D:24:VAL:O	1:D:28:LYS:HG3	2.13	0.49
1:D:92:GLY:H	1:D:129:ALA:HB3	1.78	0.49
1:A:614:HIS:O	1:A:618:MET:HG2	2.12	0.49
1:B:91:MET:SD	1:B:141:ALA:CB	3.00	0.49
1:B:538:LYS:HG3	1:B:542:LYS:HD3	1.95	0.49
1:C:487:THR:O	1:C:491:TRP:HB2	2.13	0.49
1:C:711:PHE:CZ	1:C:780:TYR:CD1	3.00	0.49
1:C:784:GLN:HA	1:C:787:VAL:HB	1.93	0.49
1:D:163:PHE:CD1	1:D:181:ASP:HB3	2.48	0.49
1:D:352:VAL:HA	1:D:356:LEU:HD12	1.95	0.49
1:A:169:LYS:HB2	1:A:178:GLU:OE1	2.13	0.49
1:A:310:ARG:O	1:A:314:SER:HB2	2.13	0.49
1:D:293:LEU:CD2	1:D:391:LEU:HD22	2.43	0.49
1:D:568:LYS:HE2	1:D:665:GLN:OE1	2.11	0.49
1:D:587:TYR:HE2	1:D:749:PHE:CZ	2.31	0.49
1:D:665:GLN:HG2	1:D:696:ASN:OD1	2.13	0.49
1:A:80:LYS:HE3	1:A:825:TRP:O	2.12	0.48
1:A:486:ILE:HD11	1:A:676:THR:HG23	1.95	0.48
1:B:571:HIS:ND1	1:B:613:TYR:OH	2.44	0.48
1:C:455:VAL:O	1:C:674:SER:HB2	2.12	0.48
1:C:726:TYR:CE2	1:C:728:ALA:HB2	2.48	0.48
1:D:486:ILE:HD13	1:D:679:MET:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:ARG:HD3	1:D:489:ARG:N	2.27	0.48
1:A:665:GLN:HE21	1:A:678:ASN:HA	1.76	0.48
1:C:313:SER:O	1:C:315:LYS:N	2.46	0.48
1:C:522:LEU:HD13	1:C:806:ALA:CB	2.43	0.48
1:D:170:ILE:O	1:D:170:ILE:HG22	2.13	0.48
1:D:352:VAL:O	1:D:356:LEU:HB2	2.14	0.48
1:B:64:VAL:O	1:B:68:ILE:HG12	2.13	0.48
1:C:323:ARG:HB2	1:C:325:ASN:HA	1.96	0.48
1:D:558:ASN:OD1	1:D:560:ASN:HB2	2.13	0.48
1:D:699:MET:HB3	1:D:708:PHE:CE2	2.47	0.48
1:D:816:THR:O	1:D:820:TYR:HD1	1.95	0.48
1:A:55:LEU:HD13	1:A:112:THR:HG21	1.95	0.48
1:A:336:GLN:HG3	1:A:825:TRP:CZ2	2.49	0.48
1:A:712:GLY:H	1:A:779:GLU:HG2	1.78	0.48
1:B:582:HIS:HD2	1:B:781:VAL:HG12	1.79	0.48
1:B:742:ILE:CG2	1:B:762:VAL:HG13	2.43	0.48
1:C:766:MET:HE3	1:C:774:PHE:HE2	1.78	0.48
1:D:36:HIS:O	1:D:40:VAL:HA	2.14	0.48
1:D:80:LYS:HA	1:D:332:LYS:O	2.13	0.48
1:B:506:ARG:HB3	1:B:524:TYR:CE2	2.49	0.48
1:B:665:GLN:NE2	1:B:678:ASN:HA	2.29	0.48
1:D:713:MET:SD	1:D:718:VAL:HG22	2.53	0.48
1:D:759:LYS:NZ	1:D:763:ASN:OD1	2.38	0.48
1:A:235:ASN:ND2	1:A:237:VAL:HG13	2.29	0.48
1:B:615:MET:HE2	1:B:761:ILE:HG12	1.95	0.48
1:B:720:ARG:O	1:B:723:GLN:HB3	2.13	0.48
1:A:636:VAL:O	1:A:639:ARG:HD3	2.13	0.48
1:B:506:ARG:HB3	1:B:524:TYR:HE2	1.79	0.48
1:C:43:ARG:HD3	1:D:13:ILE:O	2.12	0.48
1:D:27:LEU:HD11	1:D:107:ALA:HB1	1.96	0.48
1:D:200:VAL:HG11	1:D:298:PHE:HA	1.94	0.48
1:D:374:TYR:OH	1:D:376:ASN:ND2	2.45	0.48
1:A:665:GLN:HG2	1:A:678:ASN:ND2	2.28	0.48
1:C:60:ARG:O	1:C:64:VAL:HG13	2.13	0.48
1:D:27:LEU:CD1	1:D:107:ALA:HB1	2.44	0.48
1:B:202:PHE:CE1	1:B:297:TYR:HD2	2.32	0.48
1:D:253:ASN:C	1:D:254:LEU:HD13	2.39	0.48
1:C:458:ILE:HD11	1:C:694:GLY:H	1.78	0.48
1:C:562:LEU:HB3	1:C:601:ARG:HG2	1.96	0.48
1:C:601:ARG:NH2	1:C:784:GLN:OE1	2.47	0.48
1:D:147:MET:SD	1:D:154:ALA:HB1	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:LEU:HG	1:D:396:LEU:HD13	1.95	0.48
1:D:651:SER:O	1:D:655:LYS:HG3	2.14	0.48
1:B:403:ILE:HG21	1:B:439:ILE:HD13	1.95	0.47
1:B:821:ALA:HB1	1:B:827:VAL:O	2.14	0.47
1:C:55:LEU:HG	1:C:95:LEU:HD11	1.95	0.47
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.67	0.47
1:D:492:LEU:HD11	1:D:511:TYR:OH	2.14	0.47
1:D:765:LEU:HG	1:D:774:PHE:CE1	2.48	0.47
1:C:49:ARG:HA	1:C:125:ILE:HG21	1.96	0.47
1:C:103:ALA:HA	1:C:234:ARG:NH1	2.29	0.47
1:D:19:ALA:C	1:D:21:VAL:H	2.20	0.47
1:D:615:MET:O	1:D:619:ILE:HG13	2.13	0.47
1:A:128:ASP:OD2	1:A:649:ARG:HG3	2.14	0.47
1:B:224:MET:HE3	1:B:226:TYR:CE1	2.49	0.47
1:C:204:GLY:HA2	1:C:217:ASP:O	2.13	0.47
1:C:589:ARG:NH1	1:C:737:GLU:HG2	2.29	0.47
1:D:163:PHE:CE1	1:D:181:ASP:HB3	2.49	0.47
1:A:40:VAL:HG11	1:B:67:TRP:CZ3	2.49	0.47
1:A:49:ARG:NH2	1:A:125:ILE:HG22	2.27	0.47
1:B:24:VAL:O	1:B:28:LYS:HG3	2.15	0.47
1:B:252:PHE:CE2	1:B:269:ARG:HB2	2.49	0.47
1:C:614:HIS:HE1	1:C:760:ASP:OD2	1.98	0.47
1:A:346:ILE:HG23	1:A:368:THR:CG2	2.44	0.47
1:A:519:ARG:O	1:A:522:LEU:HB2	2.14	0.47
1:C:536:LYS:HG3	1:C:540:GLU:OE1	2.14	0.47
1:C:798:THR:O	1:C:802:ILE:HG13	2.13	0.47
1:D:536:LYS:O	1:D:539:GLN:HB3	2.15	0.47
1:A:499:LEU:HD12	1:A:537:VAL:HG11	1.97	0.47
1:A:536:LYS:HG3	1:A:540:GLU:OE1	2.15	0.47
1:A:574:LYS:NZ	2:A:901:SO4:O4	2.48	0.47
1:B:35:LEU:O	1:B:39:LEU:HB2	2.14	0.47
1:B:325:ASN:C	1:B:327:ASP:H	2.23	0.47
1:C:235:ASN:ND2	1:C:237:VAL:H	2.13	0.47
1:C:389:VAL:HG22	1:C:437:LYS:O	2.14	0.47
1:C:468:PHE:HB3	1:C:471:PHE:HB2	1.95	0.47
1:A:253:ASN:H	1:A:259:VAL:HG21	1.79	0.47
1:B:491:TRP:HA	1:B:495:CYS:SG	2.54	0.47
1:C:99:MET:HE1	1:C:119:MET:HE3	1.96	0.47
1:C:430:LEU:O	1:C:439:ILE:HA	2.13	0.47
1:D:30:ASN:O	1:D:34:HIS:ND1	2.47	0.47
1:D:67:TRP:HB2	1:D:238:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:PHE:CD1	1:D:329:PHE:HD2	2.28	0.47
1:D:489:ARG:HD3	1:D:489:ARG:H	1.80	0.47
1:A:55:LEU:HD23	1:A:95:LEU:HD11	1.97	0.47
1:A:133:ASN:OD1	1:A:165:ILE:HG21	2.14	0.47
1:A:151:GLY:HA2	1:A:237:VAL:HG11	1.96	0.47
1:C:193:ARG:HB2	1:C:225:PRO:HG2	1.97	0.47
1:C:251:ASP:HB3	1:C:255:LYS:CB	2.41	0.47
1:C:536:LYS:HD2	1:C:536:LYS:HA	1.74	0.47
1:D:207:GLU:OE1	1:D:214:LYS:NZ	2.47	0.47
1:A:80:LYS:HA	1:A:332:LYS:HA	1.97	0.47
1:A:235:ASN:C	1:A:235:ASN:HD22	2.23	0.47
1:B:29:LYS:NZ	1:B:29:LYS:HB3	2.29	0.47
1:B:564:ASP:OD1	1:B:662:LEU:HD12	2.15	0.47
1:A:103:ALA:CB	1:A:234:ARG:HH11	2.18	0.47
1:A:487:THR:HA	1:A:813:SER:OG	2.15	0.47
1:B:47:THR:HG22	1:B:49:ARG:H	1.80	0.47
1:B:91:MET:SD	1:B:141:ALA:HB2	2.55	0.47
1:B:241:MET:HG2	1:B:243:LEU:CD1	2.45	0.47
1:B:319:ARG:HH21	1:B:320:ASP:C	2.23	0.47
1:D:456:ALA:HB3	1:D:459:HIS:CB	2.45	0.47
1:D:754:GLN:HB2	1:D:757:LEU:HB2	1.97	0.47
1:A:369:VAL:O	1:A:450:HIS:HB3	2.16	0.46
1:A:378:THR:O	1:A:459:HIS:HE1	1.97	0.46
1:C:486:ILE:CD1	1:C:676:THR:HG23	2.37	0.46
1:B:70:THR:O	1:B:73:HIS:HB3	2.15	0.46
1:B:206:VAL:HG23	1:B:397:PRO:HB2	1.97	0.46
1:B:426:ARG:NH1	1:C:755:PRO:HD2	2.31	0.46
1:B:698:GLU:O	1:B:702:GLU:HG2	2.14	0.46
1:C:455:VAL:HA	1:C:482:LYS:O	2.16	0.46
1:C:506:ARG:HH22	1:C:533:ASP:CG	2.23	0.46
1:D:502:ILE:HD12	1:D:533:ASP:HB3	1.97	0.46
1:D:529:ALA:O	1:D:532:ARG:HG2	2.15	0.46
1:D:549:LEU:HD23	1:D:557:ILE:HD11	1.98	0.46
1:D:550:GLU:HA	1:D:553:TYR:O	2.15	0.46
1:D:587:TYR:HE2	1:D:749:PHE:HZ	1.62	0.46
1:A:71:GLN:HB3	4:A:920:AMP:O4'	2.15	0.46
1:A:688:THR:HB	1:A:708:PHE:CE2	2.50	0.46
1:C:575:ARG:HD3	1:C:666:ILE:O	2.16	0.46
1:D:525:VAL:HG12	1:D:799:ARG:NH1	2.30	0.46
1:A:91:MET:HE3	1:A:141:ALA:HB1	1.97	0.46
1:B:90:TYR:HB3	1:B:138:ARG:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLY:HA3	1:B:215:TRP:NE1	2.30	0.46
1:B:322:VAL:HG22	1:B:323:ARG:HG2	1.96	0.46
1:B:380:ILE:HA	1:B:381:PRO:HD3	1.90	0.46
1:C:235:ASN:HD21	1:C:237:VAL:HG22	1.81	0.46
1:D:366:GLU:O	1:D:370:LYS:HB2	2.14	0.46
1:A:129:ALA:HA	1:A:182:TRP:CZ3	2.51	0.46
1:A:485:GLY:C	1:A:486:ILE:HD12	2.41	0.46
1:A:648:TYR:HA	1:A:652:LEU:HD12	1.97	0.46
1:B:442:ALA:O	1:B:446:ILE:HG13	2.16	0.46
1:C:91:MET:SD	1:C:241:MET:HE1	2.56	0.46
1:C:96:GLN:HA	1:C:99:MET:CE	2.37	0.46
1:C:799:ARG:O	1:C:803:ARG:HG3	2.16	0.46
1:D:37:PHE:CD1	1:D:37:PHE:N	2.80	0.46
1:D:316:PHE:CD2	1:D:324:THR:HG23	2.48	0.46
1:A:89:PHE:CE1	1:A:140:ALA:HB1	2.50	0.46
1:A:440:ASN:OD1	1:A:442:ALA:HB3	2.15	0.46
1:D:302:ALA:O	1:D:305:GLN:HB2	2.15	0.46
1:D:815:ARG:HD2	1:D:819:GLN:OE1	2.15	0.46
1:A:115:LEU:HD22	1:B:13:ILE:HG12	1.97	0.46
1:A:698:GLU:O	1:A:702:GLU:HG2	2.16	0.46
1:A:707:ASN:HA	1:A:800:MET:SD	2.55	0.46
1:B:703:ALA:HA	1:B:807:THR:HG21	1.97	0.46
1:C:71:GLN:HB3	4:C:920:AMP:O4'	2.16	0.46
1:C:166:PHE:HB2	1:C:178:GLU:O	2.16	0.46
1:C:727:ASN:ND2	1:C:729:GLN:HB3	2.31	0.46
1:D:81:ARG:NH1	1:D:314:SER:OG	2.48	0.46
1:D:783:CYS:SG	1:D:786:ARG:CZ	3.04	0.46
1:D:791:TYR:HD1	1:D:797:TRP:CE2	2.33	0.46
1:A:311:PHE:O	1:A:316:PHE:HB3	2.16	0.46
1:C:314:SER:O	1:C:316:PHE:N	2.49	0.46
1:A:596:LYS:HD3	1:A:597:PHE:N	2.31	0.46
1:B:566:GLN:O	1:B:605:ILE:HA	2.16	0.46
1:C:163:PHE:HE1	1:C:277:ARG:NH1	2.11	0.46
1:C:198:LEU:HD13	1:C:305:GLN:HB2	1.98	0.46
1:C:495:CYS:HB2	1:C:654:GLU:O	2.16	0.46
1:C:603:VAL:HG23	1:C:642:VAL:HG13	1.97	0.46
1:D:80:LYS:HD3	1:D:334:ALA:HB2	1.98	0.46
1:D:170:ILE:HG22	1:D:173:GLY:HA2	1.98	0.46
1:A:95:LEU:O	1:A:99:MET:HG3	2.16	0.46
1:A:189:TRP:O	1:A:228:THR:HG23	2.15	0.46
1:B:60:ARG:O	1:B:64:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:ILE:HD13	1:B:680:LYS:HB3	1.98	0.46
1:B:713:MET:SD	1:B:775:ALA:HB1	2.56	0.46
1:C:325:ASN:HB3	1:C:327:ASP:HB2	1.98	0.46
1:C:381:PRO:HG3	1:C:467:ILE:HG13	1.97	0.46
1:C:542:LYS:HE2	1:C:559:PRO:O	2.16	0.46
1:A:78:ASP:O	1:A:332:LYS:NZ	2.49	0.45
1:B:104:LEU:HB3	1:B:108:CYS:SG	2.56	0.45
1:B:575:ARG:HH22	1:B:776:ASP:CG	2.24	0.45
1:C:70:THR:HG21	1:C:238:VAL:O	2.16	0.45
1:C:253:ASN:N	1:C:259:VAL:HG21	2.31	0.45
1:C:519:ARG:O	1:C:522:LEU:HB2	2.16	0.45
1:D:599:VAL:HG22	1:D:792:LYS:HD3	1.97	0.45
1:D:687:LEU:HD23	1:D:804:ASN:ND2	2.31	0.45
1:C:738:LEU:HD11	1:C:774:PHE:CE1	2.51	0.45
1:C:778:GLU:O	1:C:782:LYS:HG2	2.16	0.45
1:C:822:ARG:NH1	1:C:828:GLU:OE1	2.50	0.45
1:D:28:LYS:HZ2	1:D:114:GLN:CB	2.29	0.45
1:D:575:ARG:HG3	1:D:773:VAL:HG22	1.98	0.45
1:A:91:MET:SD	1:A:241:MET:CE	3.04	0.45
1:D:648:TYR:HA	1:D:652:LEU:HD12	1.98	0.45
1:A:428:MET:HE1	1:A:474:LEU:HG	1.98	0.45
1:A:724:ARG:HH22	1:A:730:GLU:CD	2.24	0.45
1:C:355:ASP:OD1	1:C:398:ARG:NH1	2.49	0.45
1:C:600:PRO:C	1:C:601:ARG:HG3	2.40	0.45
1:D:522:LEU:HD13	1:D:522:LEU:HA	1.77	0.45
1:A:165:ILE:HD13	1:A:166:PHE:CD1	2.51	0.45
1:B:376:ASN:HD22	1:B:468:PHE:HE2	1.65	0.45
1:B:735:ILE:HG22	1:B:738:LEU:H	1.81	0.45
1:C:308:ILE:HD12	1:C:352:VAL:HG11	1.99	0.45
1:C:657:ILE:HD13	1:C:680:LYS:HB3	1.98	0.45
1:D:136:LEU:HD21	1:D:339:ASP:HB2	1.98	0.45
1:A:555:VAL:HG21	1:A:643:ILE:HD13	1.99	0.45
1:B:99:MET:CE	1:B:119:MET:SD	3.03	0.45
1:B:631:ASN:O	1:B:641:ARG:NH1	2.50	0.45
1:A:817:ILE:HD13	1:A:817:ILE:HA	1.80	0.45
1:B:567:VAL:HB	1:B:648:TYR:CZ	2.52	0.45
1:B:715:VAL:HA	1:B:718:VAL:HG23	1.97	0.45
1:C:502:ILE:HG13	1:C:503:ILE:N	2.31	0.45
1:B:454:GLY:HA3	1:B:460:SER:OG	2.16	0.45
1:B:571:HIS:ND1	1:B:572:GLU:N	2.65	0.45
1:B:793:ASN:N	1:B:794:PRO:HD2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:TRP:CH2	1:C:448:GLY:HA2	2.52	0.45
1:D:550:GLU:HG2	1:D:555:VAL:H	1.82	0.45
1:D:631:ASN:OD1	1:D:641:ARG:HD3	2.17	0.45
1:A:206:VAL:HG12	1:A:208:HIS:CD2	2.52	0.45
1:B:630:VAL:O	1:B:636:VAL:HG11	2.17	0.45
1:B:799:ARG:O	1:B:803:ARG:HG3	2.16	0.45
1:C:555:VAL:HG11	1:C:643:ILE:HG12	1.99	0.45
1:C:657:ILE:HD13	1:C:680:LYS:CB	2.46	0.45
1:D:122:LEU:O	1:D:125:ILE:HB	2.17	0.45
1:D:563:PHE:HD2	1:D:659:ALA:O	1.99	0.45
1:D:592:LYS:NZ	1:D:593:GLU:OE2	2.50	0.45
1:A:615:MET:HE3	1:A:615:MET:O	2.17	0.45
1:B:292:ARG:NH1	1:B:385:GLU:OE2	2.50	0.45
1:B:605:ILE:O	1:B:644:PHE:HA	2.17	0.45
1:B:815:ARG:O	1:B:819:GLN:HG3	2.17	0.45
1:C:44:ASN:ND2	4:D:920:AMP:C2	2.84	0.45
1:C:355:ASP:O	1:C:358:ARG:NH1	2.50	0.45
1:C:400:LEU:HD23	1:C:400:LEU:HA	1.83	0.45
1:C:819:GLN:O	1:C:823:GLU:HB2	2.16	0.45
1:A:706:GLU:H	1:A:706:GLU:CD	2.25	0.44
1:B:515:LEU:HD21	1:B:683:LEU:HD11	1.99	0.44
1:C:565:VAL:CG1	1:C:604:MET:HE3	2.47	0.44
1:C:703:ALA:HA	1:C:807:THR:HG21	1.98	0.44
1:D:309:ARG:NH2	4:D:920:AMP:P	2.91	0.44
1:A:157:TYR:HA	1:A:242:ARG:O	2.16	0.44
1:A:207:GLU:OE1	1:A:214:LYS:NZ	2.50	0.44
1:A:482:LYS:HD2	1:A:819:GLN:HB3	1.99	0.44
1:A:700:ALA:HB2	1:A:710:ILE:HD11	2.00	0.44
1:C:162:GLU:HB3	1:C:163:PHE:CD1	2.53	0.44
1:D:314:SER:O	1:D:316:PHE:N	2.51	0.44
1:A:81:ARG:O	1:A:334:ALA:N	2.50	0.44
1:A:143:PHE:HB3	1:A:147:MET:HE2	2.00	0.44
1:A:452:VAL:HB	1:A:479:PHE:CD1	2.52	0.44
1:A:576:GLN:H	1:A:576:GLN:NE2	2.15	0.44
1:A:773:VAL:O	1:A:774:PHE:C	2.61	0.44
1:B:26:GLU:OE1	1:B:29:LYS:NZ	2.50	0.44
1:B:206:VAL:HB	1:B:401:GLN:HE22	1.82	0.44
1:D:252:PHE:N	1:D:252:PHE:CD1	2.85	0.44
1:A:398:ARG:O	1:A:402:ILE:HG13	2.18	0.44
1:A:727:ASN:O	1:A:729:GLN:N	2.51	0.44
1:B:53:PHE:HE1	1:B:188:PRO:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:PHE:HA	1:B:329:PHE:HB2	1.98	0.44
1:C:456:ALA:H	1:C:481:ASN:ND2	2.16	0.44
1:C:528:GLU:O	1:C:532:ARG:HG2	2.16	0.44
1:A:721:LEU:HD21	1:A:726:TYR:CD1	2.53	0.44
4:A:920:AMP:C2	1:B:44:ASN:ND2	2.85	0.44
1:B:83:TYR:CD1	1:B:155:TYR:HB2	2.53	0.44
1:D:187:ASN:ND2	1:D:190:GLU:HB3	2.32	0.44
1:D:466:THR:OG1	1:D:467:ILE:HG13	2.17	0.44
1:A:80:LYS:HG3	1:A:331:ASP:O	2.18	0.44
1:A:85:LEU:HD12	1:A:335:ILE:HG23	1.99	0.44
1:A:235:ASN:ND2	1:A:237:VAL:HG22	2.30	0.44
1:A:499:LEU:O	1:A:503:ILE:HG13	2.18	0.44
1:B:53:PHE:CE1	1:B:188:PRO:HD3	2.52	0.44
1:B:481:ASN:O	1:B:482:LYS:HG2	2.17	0.44
1:B:666:ILE:HG22	1:B:711:PHE:HE1	1.81	0.44
1:D:571:HIS:H	1:D:576:GLN:HE21	1.65	0.44
1:C:289:LYS:HG2	1:C:291:LEU:H	1.81	0.44
1:D:728:ALA:HB3	1:D:766:MET:O	2.18	0.44
1:A:548:TYR:C	1:A:550:GLU:H	2.25	0.44
1:B:152:LEU:HD22	1:B:827:VAL:HG21	1.99	0.44
1:C:162:GLU:HA	1:C:183:LEU:HD12	2.00	0.44
1:C:764:MET:SD	1:C:764:MET:C	3.01	0.44
1:D:88:GLU:CD	1:D:133:ASN:H	2.25	0.44
1:D:205:ARG:HB3	1:D:216:VAL:HG23	1.98	0.44
1:D:235:ASN:OD1	1:D:237:VAL:HG22	2.18	0.44
1:D:531:ILE:HG22	1:D:532:ARG:N	2.33	0.44
1:A:31:PHE:HA	1:A:58:THR:OG1	2.17	0.44
1:A:395:LEU:O	1:A:396:LEU:HD13	2.18	0.44
1:A:455:VAL:O	1:A:483:THR:HA	2.18	0.44
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.82	0.44
1:B:292:ARG:O	1:B:296:GLU:HG3	2.18	0.44
1:B:316:PHE:HA	1:B:319:ARG:CB	2.47	0.44
1:B:319:ARG:NH2	1:B:320:ASP:O	2.49	0.44
1:B:456:ALA:C	1:B:481:ASN:HD21	2.25	0.44
1:C:88:GLU:HG2	1:C:132:GLY:HA2	2.00	0.44
1:C:338:ASN:OD1	1:C:377:HIS:CE1	2.70	0.44
1:C:482:LYS:HE3	1:C:819:GLN:O	2.17	0.44
1:C:609:ALA:HB2	1:C:620:ILE:CD1	2.47	0.44
1:C:803:ARG:HG3	1:C:803:ARG:HH11	1.82	0.44
1:D:277:ARG:NH1	1:D:277:ARG:HG2	2.32	0.44
1:D:446:ILE:O	1:D:478:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:HB3	1:A:255:LYS:NZ	2.33	0.43
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.18	0.43
1:B:52:TYR:OH	1:B:126:GLU:HG3	2.18	0.43
1:C:144:LEU:HA	1:C:147:MET:HG3	1.99	0.43
1:C:487:THR:HG23	1:C:490:ARG:H	1.82	0.43
1:C:539:GLN:O	1:C:543:LEU:HB2	2.18	0.43
1:C:544:LYS:O	1:C:547:ALA:HB3	2.17	0.43
1:C:574:LYS:NZ	2:C:901:SO4:O2	2.51	0.43
1:C:614:HIS:O	1:C:618:MET:HB2	2.18	0.43
1:D:163:PHE:HE2	1:D:277:ARG:HH11	1.65	0.43
1:D:304:LEU:HD21	1:D:349:LEU:HB2	1.99	0.43
1:A:162:GLU:HA	1:A:183:LEU:HD12	2.01	0.43
1:A:322:VAL:O	1:A:325:ASN:HB2	2.17	0.43
1:A:524:TYR:CD1	1:A:524:TYR:N	2.85	0.43
1:A:703:ALA:HA	1:A:807:THR:HG21	1.99	0.43
1:B:150:LEU:HB3	1:B:829:PRO:HB3	1.99	0.43
1:B:290:GLU:OE1	1:B:294:LYS:NZ	2.51	0.43
1:B:721:LEU:CD1	1:B:726:TYR:HA	2.49	0.43
1:C:523:SER:HB2	1:C:524:TYR:CE1	2.52	0.43
1:C:524:TYR:CD1	1:C:524:TYR:N	2.86	0.43
1:D:297:TYR:CD2	1:D:396:LEU:HD11	2.52	0.43
1:D:713:MET:CE	1:D:775:ALA:HB1	2.48	0.43
1:A:398:ARG:HG3	1:A:402:ILE:HD11	2.00	0.43
1:C:281:PRO:HB2	1:C:611:PRO:CD	2.49	0.43
1:C:456:ALA:H	1:C:481:ASN:HD21	1.66	0.43
1:D:170:ILE:CG2	1:D:173:GLY:HA2	2.49	0.43
1:D:571:HIS:H	1:D:576:GLN:NE2	2.17	0.43
1:D:816:THR:HG22	1:D:820:TYR:CE1	2.53	0.43
1:C:37:PHE:CD2	1:D:61:ASP:HB3	2.53	0.43
1:C:37:PHE:CE1	1:D:18:LEU:HD23	2.53	0.43
1:C:692:MET:HE3	1:C:697:VAL:HA	2.00	0.43
1:D:822:ARG:NH1	1:D:828:GLU:OE1	2.51	0.43
1:B:379:VAL:HG11	1:B:671:THR:O	2.19	0.43
1:B:657:ILE:CD1	1:B:680:LYS:HD3	2.49	0.43
1:C:165:ILE:HG12	1:C:279:LEU:HB3	2.00	0.43
1:C:454:GLY:HA3	1:C:460:SER:OG	2.18	0.43
1:D:24:VAL:O	1:D:24:VAL:HG12	2.17	0.43
1:D:348:GLU:CD	1:D:351:ARG:HH21	2.26	0.43
1:D:380:ILE:HG13	1:D:382:GLU:OE1	2.19	0.43
1:D:528:GLU:HG2	1:D:532:ARG:NH2	2.31	0.43
1:D:633:ASP:OD2	1:D:636:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:753:LYS:HB2	1:D:754:GLN:OE1	2.18	0.43
1:D:797:TRP:O	1:D:801:VAL:HG23	2.18	0.43
1:A:269:ARG:HH11	1:A:269:ARG:HD3	1.71	0.43
1:B:56:ALA:HB1	1:B:189:TRP:CZ2	2.54	0.43
1:B:730:GLU:HG3	1:B:734:ARG:HH12	1.84	0.43
1:B:822:ARG:HD3	1:B:828:GLU:OE2	2.18	0.43
1:C:280:TYR:HB3	1:C:281:PRO:HD3	1.99	0.43
1:C:679:MET:HE2	1:C:811:PHE:CD1	2.54	0.43
1:D:603:VAL:HG22	1:D:641:ARG:O	2.18	0.43
1:D:631:ASN:OD1	1:D:641:ARG:HA	2.19	0.43
1:D:677:GLY:CA	3:D:999:PLP:H5A1	2.48	0.43
1:B:455:VAL:HG12	1:B:674:SER:HB3	1.99	0.43
1:C:224:MET:SD	1:C:247:LYS:HE2	2.59	0.43
1:C:311:PHE:CE1	1:C:329:PHE:HA	2.54	0.43
1:D:66:ARG:HH12	1:D:837:PRO:HG3	1.84	0.43
1:D:530:PHE:CA	1:D:533:ASP:HB2	2.47	0.43
1:D:555:VAL:HG23	1:D:556:HIS:H	1.84	0.43
1:D:689:ILE:HG12	1:D:690:GLY:N	2.34	0.43
1:A:727:ASN:ND2	1:D:725:GLY:HA3	2.28	0.43
1:B:78:ASP:O	1:B:332:LYS:NZ	2.51	0.43
1:B:202:PHE:O	1:B:218:THR:HB	2.18	0.43
1:B:433:GLU:OE2	1:B:437:LYS:NZ	2.50	0.43
1:C:570:ILE:HG21	1:C:620:ILE:HG13	2.01	0.43
1:C:603:VAL:CG2	1:C:642:VAL:HG13	2.49	0.43
1:C:746:SER:OG	1:C:762:VAL:HG21	2.18	0.43
1:D:380:ILE:HA	1:D:381:PRO:HD3	1.61	0.43
1:A:94:THR:HB	1:A:189:TRP:NE1	2.33	0.43
1:A:509:GLU:OE2	1:A:512:ILE:HD12	2.19	0.43
1:A:544:LYS:O	1:A:547:ALA:HB3	2.19	0.43
1:B:545:PHE:HZ	1:B:645:LEU:HD21	1.84	0.43
1:D:152:LEU:HD22	1:D:827:VAL:HG21	2.01	0.43
1:D:312:LYS:HA	1:D:324:THR:CG2	2.46	0.43
1:D:689:ILE:HA	1:D:709:PHE:HB2	2.01	0.43
1:A:531:ILE:HG12	1:A:802:ILE:HD11	2.01	0.43
1:B:435:ALA:HB2	1:C:174:TRP:CD2	2.54	0.43
1:B:735:ILE:HA	1:B:736:PRO:HD3	1.83	0.43
1:D:338:ASN:OD1	1:D:377:HIS:CE1	2.72	0.43
1:A:55:LEU:HD13	1:A:112:THR:CG2	2.48	0.42
1:B:790:LEU:HD23	1:B:797:TRP:HD1	1.83	0.42
1:C:526:ASP:OD2	1:C:799:ARG:NH1	2.52	0.42
1:C:626:ILE:HG22	1:C:642:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LYS:HD3	1:D:45:VAL:HG12	2.01	0.42
1:D:562:LEU:HD13	1:D:601:ARG:CZ	2.49	0.42
1:D:591:LYS:NZ	1:D:633:ASP:CG	2.77	0.42
1:A:293:LEU:HD23	1:A:395:LEU:HD21	2.02	0.42
1:A:485:GLY:O	1:A:486:ILE:HD12	2.18	0.42
1:B:182:TRP:CE2	1:B:183:LEU:HG	2.54	0.42
1:C:36:HIS:O	1:C:40:VAL:HA	2.19	0.42
1:C:592:LYS:HZ3	1:C:593:GLU:CD	2.27	0.42
1:C:678:ASN:HB3	1:C:699:MET:HE1	2.00	0.42
1:C:734:ARG:O	1:C:736:PRO:HD3	2.19	0.42
1:D:291:LEU:HA	1:D:294:LYS:HB2	2.01	0.42
1:D:316:PHE:HB3	1:D:324:THR:CG2	2.49	0.42
1:D:455:VAL:HG22	1:D:484:ASN:OD1	2.20	0.42
1:A:47:THR:HG22	1:A:49:ARG:N	2.34	0.42
1:A:450:HIS:O	1:A:450:HIS:ND1	2.52	0.42
1:B:31:PHE:HA	1:B:58:THR:OG1	2.19	0.42
1:B:423:ASP:O	1:B:427:ARG:N	2.53	0.42
1:C:366:GLU:HG2	1:C:370:LYS:HE3	2.01	0.42
1:C:610:ALA:HA	1:C:611:PRO:HD3	1.83	0.42
1:C:795:ARG:O	1:C:799:ARG:HG3	2.20	0.42
1:D:62:HIS:O	1:D:66:ARG:HG3	2.19	0.42
1:A:21:VAL:HG13	1:A:22:GLU:H	1.84	0.42
1:A:22:GLU:OE1	1:A:104:LEU:HA	2.19	0.42
1:B:253:ASN:H	1:B:259:VAL:HG21	1.84	0.42
1:C:730:GLU:HB2	1:C:734:ARG:NH2	2.34	0.42
1:D:407:ASN:HB2	1:D:430:LEU:HD12	2.01	0.42
1:D:453:ASN:ND2	1:D:482:LYS:HB2	2.33	0.42
1:D:632:HIS:O	1:D:634:PRO:HD3	2.19	0.42
1:D:688:THR:HB	1:D:708:PHE:CE1	2.55	0.42
1:A:75:TYR:CE2	4:A:920:AMP:N7	2.87	0.42
1:A:225:PRO:HB3	1:A:244:TRP:CE3	2.54	0.42
1:A:346:ILE:HG23	1:A:368:THR:HG21	2.02	0.42
1:A:536:LYS:NZ	1:A:540:GLU:CD	2.77	0.42
1:B:314:SER:O	1:B:316:PHE:N	2.52	0.42
1:C:102:LEU:O	1:C:104:LEU:HD12	2.20	0.42
1:C:144:LEU:HA	1:C:144:LEU:HD23	1.90	0.42
1:C:474:LEU:HD22	1:C:474:LEU:O	2.19	0.42
1:A:233:TYR:OH	1:A:234:ARG:NH2	2.53	0.42
1:A:338:ASN:OD1	1:A:377:HIS:CE1	2.72	0.42
1:A:573:TYR:CZ	1:A:574:LYS:HD2	2.54	0.42
1:A:703:ALA:HB2	1:A:807:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:PHE:HE2	1:B:604:MET:SD	2.42	0.42
1:C:551:ARG:O	1:C:551:ARG:NH1	2.53	0.42
1:C:590:ILE:HG12	1:C:598:VAL:HG11	2.01	0.42
1:D:82:ILE:CD1	1:D:147:MET:SD	3.07	0.42
1:D:423:ASP:O	1:D:426:ARG:HD3	2.19	0.42
1:D:649:ARG:HH11	1:D:649:ARG:HD2	1.61	0.42
1:B:379:VAL:HG23	1:B:462:ILE:HD12	2.01	0.42
1:C:64:VAL:O	1:C:68:ILE:HG12	2.20	0.42
1:C:187:ASN:HB3	1:C:190:GLU:OE2	2.19	0.42
1:C:281:PRO:HB2	1:C:611:PRO:HD2	2.01	0.42
1:C:502:ILE:HD13	1:C:534:VAL:HA	2.01	0.42
1:D:60:ARG:HG3	1:D:189:TRP:HE3	1.81	0.42
1:D:110:GLU:O	1:D:113:TYR:HB3	2.19	0.42
1:D:290:GLU:HG3	1:D:391:LEU:HD21	2.00	0.42
1:D:486:ILE:HD11	1:D:680:LYS:HE3	2.01	0.42
1:D:588:ASN:HD21	1:D:744:GLN:NE2	2.18	0.42
1:B:481:ASN:OD1	1:B:482:LYS:N	2.53	0.42
1:B:629:VAL:HG12	1:B:630:VAL:N	2.33	0.42
1:B:680:LYS:NZ	3:B:999:PLP:O3	2.53	0.42
1:B:783:CYS:HA	1:B:786:ARG:NH1	2.35	0.42
1:D:119:MET:O	1:D:123:GLU:HG3	2.20	0.42
1:D:152:LEU:HD22	1:D:827:VAL:CG2	2.50	0.42
1:D:490:ARG:HG2	1:D:491:TRP:CE2	2.55	0.42
1:D:588:ASN:ND2	1:D:741:ILE:HG22	2.31	0.42
1:A:94:THR:HG21	1:A:189:TRP:CD2	2.55	0.42
1:A:460:SER:OG	1:A:481:ASN:HB2	2.20	0.42
1:A:735:ILE:HA	1:A:736:PRO:HD3	1.79	0.42
1:B:97:ASN:OD1	1:B:490:ARG:NH1	2.53	0.42
1:B:492:LEU:HB3	1:B:493:VAL:H	1.59	0.42
1:C:700:ALA:O	1:C:704:GLY:N	2.53	0.42
1:D:206:VAL:HG22	1:D:398:ARG:HD2	2.01	0.42
1:D:461:GLU:OE1	1:D:465:LYS:NZ	2.53	0.42
1:B:375:THR:HG22	1:B:377:HIS:CE1	2.55	0.42
1:B:379:VAL:HG23	1:B:462:ILE:CD1	2.50	0.42
1:C:475:GLU:CD	1:C:478:LYS:HE2	2.45	0.42
1:C:730:GLU:HG3	1:C:734:ARG:NH1	2.35	0.42
1:A:32:ASN:OD1	1:B:13:ILE:HA	2.20	0.41
1:A:538:LYS:HD2	1:A:658:PRO:O	2.19	0.41
1:A:540:GLU:HA	1:A:543:LEU:HB2	2.01	0.41
1:A:665:GLN:NE2	1:A:678:ASN:HA	2.35	0.41
1:B:160:ARG:HH21	1:B:190:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:THR:HA	1:B:488:PRO:HD2	1.92	0.41
1:B:515:LEU:O	1:B:518:LEU:HG	2.20	0.41
1:C:37:PHE:N	1:C:37:PHE:CD1	2.88	0.41
1:C:379:VAL:HG11	1:C:671:THR:O	2.20	0.41
1:C:738:LEU:HA	1:C:741:ILE:HG12	2.01	0.41
1:C:817:ILE:HD13	1:C:817:ILE:HA	1.74	0.41
1:D:456:ALA:C	1:D:481:ASN:HD21	2.28	0.41
1:D:484:ASN:O	1:D:679:MET:SD	2.78	0.41
1:A:509:GLU:CD	1:A:512:ILE:HD12	2.45	0.41
1:A:575:ARG:HG2	1:A:773:VAL:CG2	2.50	0.41
1:B:49:ARG:O	1:B:52:TYR:HB3	2.20	0.41
1:B:565:VAL:HG11	1:B:656:VAL:HG21	2.02	0.41
1:B:622:LEU:HA	1:B:758:PHE:CZ	2.55	0.41
1:D:83:TYR:CZ	1:D:307:ILE:HG12	2.55	0.41
1:D:198:LEU:HB3	1:D:305:GLN:OE1	2.20	0.41
1:D:522:LEU:O	1:D:524:TYR:N	2.53	0.41
1:D:613:TYR:CE1	1:D:615:MET:HB3	2.52	0.41
1:D:778:GLU:OE1	1:D:782:LYS:NZ	2.53	0.41
1:A:271:LEU:HA	1:A:274:ASN:ND2	2.34	0.41
1:A:610:ALA:HA	1:A:611:PRO:HD3	1.84	0.41
1:A:678:ASN:ND2	1:A:696:ASN:OD1	2.52	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.80	0.41
1:B:224:MET:HE3	1:B:226:TYR:HE1	1.85	0.41
1:B:469:LYS:HE2	1:B:469:LYS:HB2	1.84	0.41
1:B:583:VAL:HG11	1:B:642:VAL:CG2	2.50	0.41
1:C:453:ASN:HB3	1:C:480:GLN:HB2	2.03	0.41
1:C:567:VAL:HA	1:C:606:GLY:O	2.20	0.41
1:C:622:LEU:O	1:C:625:ALA:HB3	2.20	0.41
1:D:28:LYS:NZ	1:D:114:GLN:HB3	2.33	0.41
1:D:128:ASP:O	1:D:130:GLY:N	2.53	0.41
1:D:209:THR:O	1:D:211:GLN:N	2.53	0.41
1:D:571:HIS:ND1	1:D:572:GLU:N	2.68	0.41
1:C:13:ILE:HG23	1:D:32:ASN:OD1	2.21	0.41
1:C:432:GLU:HB3	1:C:438:ARG:HB2	2.03	0.41
1:C:482:LYS:HE3	1:C:819:GLN:C	2.45	0.41
1:D:344:LEU:HD22	1:D:347:PRO:HG3	2.02	0.41
1:D:622:LEU:HG	1:D:761:ILE:HD12	2.01	0.41
1:D:711:PHE:CG	1:D:712:GLY:N	2.87	0.41
1:B:460:SER:OG	1:B:481:ASN:ND2	2.54	0.41
1:D:206:VAL:HG11	1:D:401:GLN:OE1	2.20	0.41
1:D:463:LEU:O	1:D:468:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:816:THR:HG22	1:D:820:TYR:HE1	1.85	0.41
1:A:482:LYS:CD	1:A:819:GLN:HB3	2.50	0.41
1:A:591:LYS:O	1:A:594:PRO:HD3	2.20	0.41
1:A:738:LEU:O	1:A:741:ILE:N	2.54	0.41
1:B:688:THR:O	1:B:709:PHE:HB2	2.21	0.41
1:B:789:ALA:O	1:B:792:LYS:NZ	2.53	0.41
1:C:663:SER:HB3	1:C:688:THR:HA	2.02	0.41
1:D:677:GLY:HA3	3:D:999:PLP:H5A1	2.02	0.41
1:A:306:ASP:OD1	1:A:309:ARG:NH1	2.54	0.41
1:A:389:VAL:HG23	1:A:390:HIS:N	2.36	0.41
1:B:78:ASP:HA	1:B:79:PRO:HD3	1.76	0.41
1:B:566:GLN:HG3	1:B:664:GLU:HB2	2.02	0.41
1:B:764:MET:HA	1:B:768:HIS:CE1	2.55	0.41
1:C:588:ASN:HD21	1:C:744:GLN:NE2	2.18	0.41
1:C:830:SER:OG	1:C:832:GLN:HG2	2.20	0.41
1:D:166:PHE:CD1	1:D:177:GLU:HB3	2.56	0.41
1:D:815:ARG:O	1:D:818:ALA:HB3	2.21	0.41
1:A:575:ARG:HG2	1:A:773:VAL:HG22	2.02	0.41
1:A:627:GLY:HA2	1:A:642:VAL:HB	2.02	0.41
1:B:67:TRP:CD1	1:B:71:GLN:HE21	2.38	0.41
1:C:433:GLU:OE2	1:C:437:LYS:NZ	2.54	0.41
1:C:446:ILE:O	1:C:478:LYS:HE3	2.21	0.41
1:D:162:GLU:HA	1:D:183:LEU:HD12	2.02	0.41
1:D:322:VAL:HG13	1:D:325:ASN:HB3	2.03	0.41
1:D:366:GLU:O	1:D:370:LYS:HE3	2.21	0.41
1:A:13:ILE:HA	1:B:32:ASN:OD1	2.21	0.41
1:A:27:LEU:HD21	1:A:104:LEU:HD22	2.02	0.41
1:A:41:LYS:HD3	1:A:41:LYS:HA	1.74	0.41
1:A:89:PHE:O	1:A:131:LEU:HB2	2.21	0.41
1:A:267:LEU:O	1:A:268:ASP:C	2.64	0.41
1:A:290:GLU:HG2	1:A:391:LEU:HD21	2.02	0.41
1:A:539:GLN:O	1:A:543:LEU:HD23	2.21	0.41
1:A:569:ARG:HB2	2:A:901:SO4:O2	2.21	0.41
1:A:665:GLN:HG2	1:A:678:ASN:CG	2.46	0.41
1:B:241:MET:HE3	1:B:243:LEU:HD11	2.03	0.41
1:B:395:LEU:HG	1:B:396:LEU:HD13	2.02	0.41
1:B:446:ILE:O	1:B:478:LYS:HE3	2.21	0.41
1:B:490:ARG:HA	1:B:494:LEU:HD23	2.03	0.41
1:C:361:TRP:CZ3	1:C:409:ARG:HD2	2.55	0.41
1:C:746:SER:C	1:C:748:GLY:N	2.79	0.41
1:D:255:LYS:HZ1	1:D:256:ASP:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:SER:O	1:D:314:SER:C	2.63	0.41
1:D:457:ARG:HH22	1:D:701:GLU:CD	2.29	0.41
1:D:602:THR:HA	1:D:641:ARG:HB2	2.03	0.41
1:D:655:LYS:O	1:D:658:PRO:HB2	2.21	0.41
1:D:733:ASP:O	1:D:739:ARG:NH1	2.54	0.41
1:D:791:TYR:HA	1:D:797:TRP:NE1	2.35	0.41
1:A:264:GLN:O	1:A:267:LEU:HD12	2.21	0.41
1:B:88:GLU:HG2	1:B:132:GLY:HA2	2.02	0.41
1:B:222:LEU:O	1:B:247:LYS:N	2.49	0.41
1:B:232:GLY:HA3	1:B:235:ASN:ND2	2.36	0.41
1:B:355:ASP:O	1:B:358:ARG:NH1	2.54	0.41
1:C:44:ASN:OD1	1:D:72:GLN:NE2	2.54	0.41
1:C:150:LEU:HA	1:C:830:SER:O	2.21	0.41
1:C:163:PHE:HA	1:C:181:ASP:HA	2.02	0.41
1:C:320:ASP:HA	1:C:324:THR:HA	2.02	0.41
1:C:548:TYR:HE2	1:C:655:LYS:NZ	2.19	0.41
1:D:23:ASN:OD1	1:D:25:THR:HB	2.20	0.41
1:D:95:LEU:HD23	1:D:95:LEU:HA	1.84	0.41
1:D:338:ASN:OD1	1:D:377:HIS:HE1	2.03	0.41
1:D:706:GLU:CD	1:D:706:GLU:H	2.29	0.41
1:A:230:VAL:O	1:A:230:VAL:HG23	2.21	0.40
1:A:426:ARG:NE	1:D:753:LYS:O	2.54	0.40
1:A:509:GLU:O	1:A:510:GLU:C	2.63	0.40
1:B:822:ARG:HD3	1:B:822:ARG:HH11	1.63	0.40
1:C:290:GLU:O	1:C:294:LYS:HG3	2.21	0.40
1:D:386:ARG:HA	1:D:439:ILE:O	2.21	0.40
1:D:466:THR:OG1	1:D:467:ILE:N	2.54	0.40
1:D:622:LEU:O	1:D:625:ALA:HB3	2.22	0.40
1:B:63:LEU:HD23	1:B:63:LEU:HA	1.95	0.40
1:B:738:LEU:HA	1:B:741:ILE:HG12	2.02	0.40
1:B:799:ARG:HH11	1:B:799:ARG:HD2	1.67	0.40
1:C:530:PHE:HA	1:C:533:ASP:OD2	2.21	0.40
1:C:548:TYR:HE2	1:C:655:LYS:HZ2	1.68	0.40
1:C:733:ASP:HA	1:C:739:ARG:NH1	2.27	0.40
1:D:161:TYR:HA	1:D:276:SER:O	2.21	0.40
1:D:424:ARG:HA	1:D:427:ARG:CZ	2.51	0.40
1:A:47:THR:HG22	1:A:49:ARG:H	1.86	0.40
1:A:143:PHE:O	1:A:147:MET:HG3	2.21	0.40
1:A:168:GLN:HE21	1:A:646:GLU:HA	1.87	0.40
1:A:249:PRO:HD2	1:A:252:PHE:CZ	2.57	0.40
1:A:748:GLY:HA3	1:A:755:PRO:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:GLU:N	1:C:438:ARG:O	2.55	0.40
1:C:758:PHE:HD1	1:C:761:ILE:CD1	2.34	0.40
1:D:369:VAL:O	1:D:450:HIS:HB3	2.21	0.40
1:D:518:LEU:HB3	1:D:806:ALA:HA	2.04	0.40
1:D:682:MET:CE	1:D:808:SER:HA	2.49	0.40
1:A:682:MET:CE	1:A:808:SER:HA	2.51	0.40
1:B:656:VAL:O	1:B:657:ILE:C	2.65	0.40
1:C:142:CYS:O	1:C:143:PHE:C	2.63	0.40
1:C:598:VAL:HG12	1:C:639:ARG:HH21	1.86	0.40
1:D:295:GLN:O	1:D:298:PHE:HB3	2.22	0.40
1:A:409:ARG:O	1:A:412:ASN:N	2.55	0.40
1:B:14:SER:OG	1:B:15:VAL:N	2.52	0.40
1:B:272:ALA:O	1:B:274:ASN:N	2.55	0.40
1:B:524:TYR:CD1	1:B:524:TYR:N	2.89	0.40
1:B:718:VAL:HG13	1:B:772:LYS:HD2	2.02	0.40
1:C:452:VAL:O	1:C:479:PHE:HA	2.21	0.40
1:C:522:LEU:HD13	1:C:806:ALA:HB3	2.03	0.40
1:C:550:GLU:HA	1:C:554:LYS:HA	2.03	0.40
1:C:591:LYS:NZ	1:C:633:ASP:CG	2.79	0.40
1:C:647:ASN:O	1:C:649:ARG:HG2	2.21	0.40
1:D:63:LEU:CD2	1:D:231:PRO:HB3	2.48	0.40
1:D:73:HIS:NE2	1:D:834:LEU:HD11	2.36	0.40
1:D:522:LEU:HD11	1:D:803:ARG:HD3	2.04	0.40
1:D:795:ARG:C	1:D:799:ARG:HG3	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLU:N	1:D:321:PRO:O[2_646]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	820/842 (97%)	669 (82%)	116 (14%)	35 (4%)	2	8
1	B	820/842 (97%)	687 (84%)	92 (11%)	41 (5%)	1	6
1	C	820/842 (97%)	708 (86%)	82 (10%)	30 (4%)	2	11
1	D	820/842 (97%)	669 (82%)	100 (12%)	51 (6%)	1	3
All	All	3280/3368 (97%)	2733 (83%)	390 (12%)	157 (5%)	2	7

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	A	321	PRO
1	A	358	ARG
1	A	553	TYR
1	A	674	SER
1	A	728	ALA
1	A	793	ASN
1	A	835	PRO
1	B	16	ARG
1	B	93	ARG
1	B	166	PHE
1	B	253	ASN
1	B	281	PRO
1	B	321	PRO
1	B	610	ALA
1	B	752	PRO
1	B	794	PRO
1	B	835	PRO
1	C	210	SER
1	C	253	ASN
1	C	314	SER
1	C	315	LYS
1	C	321	PRO
1	C	323	ARG
1	C	358	ARG
1	C	555	VAL
1	C	556	HIS
1	C	609	ALA
1	C	836	ALA
1	D	129	ALA
1	D	210	SER

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Mol	Chain	Res	Type
1	D	314	SER
1	D	321	PRO
1	D	358	ARG
1	D	609	ALA
1	D	674	SER
1	D	829	PRO
1	A	21	VAL
1	A	91	MET
1	A	253	ASN
1	A	256	ASP
1	A	281	PRO
1	A	451	ALA
1	A	477	HIS
1	A	555	VAL
1	A	610	ALA
1	A	836	ALA
1	B	21	VAL
1	B	22	GLU
1	B	95	LEU
1	B	252	PHE
1	B	256	ASP
1	B	436	VAL
1	C	21	VAL
1	C	256	ASP
1	C	694	GLY
1	C	809	GLY
1	D	16	ARG
1	D	103	ALA
1	D	104	LEU
1	D	151	GLY
1	D	183	LEU
1	D	217	ASP
1	D	234	ARG
1	D	256	ASP
1	D	323	ARG
1	D	429	SER
1	D	489	ARG
1	D	523	SER
1	D	531	ILE
1	D	556	HIS
1	D	561	SER
1	D	610	ALA

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Mol	Chain	Res	Type
1	D	694	GLY
1	A	93	ARG
1	A	210	SER
1	A	316	PHE
1	A	492	LEU
1	A	556	HIS
1	B	19	ALA
1	B	273	GLU
1	B	314	SER
1	B	381	PRO
1	B	555	VAL
1	C	92	GLY
1	C	93	ARG
1	C	436	VAL
1	C	625	ALA
1	D	21	VAL
1	D	95	LEU
1	D	252	PHE
1	D	253	ASN
1	D	555	VAL
1	D	658	PRO
1	A	22	GLU
1	A	88	GLU
1	A	357	GLU
1	B	203	TYR
1	B	272	ALA
1	B	674	SER
1	C	456	ALA
1	C	484	ASN
1	C	778	GLU
1	D	91	MET
1	D	166	PHE
1	D	637	GLY
1	A	129	ALA
1	A	259	VAL
1	A	436	VAL
1	A	483	THR
1	B	254	LEU
1	B	315	LYS
1	B	344	LEU
1	B	728	ALA
1	B	836	ALA

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Mol	Chain	Res	Type
1	C	257	PHE
1	C	394	THR
1	C	835	PRO
1	D	93	ARG
1	D	96	GLN
1	D	254	LEU
1	D	259	VAL
1	D	298	PHE
1	D	315	LYS
1	D	436	VAL
1	D	557	ILE
1	D	751	SER
1	D	830	SER
1	D	835	PRO
1	B	45	VAL
1	B	326	PHE
1	B	625	ALA
1	B	666	ILE
1	B	756	ASP
1	C	357	GLU
1	D	229	PRO
1	D	625	ALA
1	A	263	ILE
1	B	263	ILE
1	B	629	VAL
1	C	697	VAL
1	A	685	GLY
1	B	493	VAL
1	C	263	ILE
1	C	666	ILE
1	A	594	PRO
1	A	704	GLY
1	B	79	PRO
1	B	231	PRO
1	D	263	ILE
1	B	736	PRO
1	C	751	SER
1	D	17	GLY
1	D	710	ILE
1	D	725	GLY
1	A	342	PRO
1	B	751	SER

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	712/731 (97%)	563 (79%)	149 (21%)	1	4
1	B	712/731 (97%)	571 (80%)	141 (20%)	1	5
1	C	712/731 (97%)	583 (82%)	129 (18%)	2	6
1	D	712/731 (97%)	574 (81%)	138 (19%)	1	5
All	All	2848/2924 (97%)	2291 (80%)	557 (20%)	1	5

All (557) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	12	GLN
1	A	15	VAL
1	A	16	ARG
1	A	18	LEU
1	A	25	THR
1	A	40	VAL
1	A	49	ARG
1	A	63	LEU
1	A	82	ILE
1	A	87	LEU
1	A	90	TYR
1	A	95	LEU
1	A	97	ASN
1	A	100	VAL
1	A	117	LEU
1	A	118	ASP
1	A	127	GLU
1	A	131	LEU
1	A	150	LEU
1	A	165	ILE
1	A	167	ASN
1	A	169	LYS
1	A	171	CYS

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Mol	Chain	Res	Type
1	A	176	MET
1	A	177	GLU
1	A	184	ARG
1	A	187	ASN
1	A	195	GLU
1	A	197	THR
1	A	214	LYS
1	A	216	VAL
1	A	234	ARG
1	A	235	ASN
1	A	237	VAL
1	A	242	ARG
1	A	243	LEU
1	A	247	LYS
1	A	252	PHE
1	A	255	LYS
1	A	256	ASP
1	A	262	TYR
1	A	266	VAL
1	A	269	ARG
1	A	270	ASN
1	A	274	ASN
1	A	277	ARG
1	A	279	LEU
1	A	287	GLU
1	A	290	GLU
1	A	291	LEU
1	A	292	ARG
1	A	299	VAL
1	A	303	THR
1	A	308	ILE
1	A	315	LYS
1	A	319	ARG
1	A	321	PRO
1	A	324	THR
1	A	327	ASP
1	A	333	VAL
1	A	337	LEU
1	A	340	THR
1	A	358	ARG
1	A	359	LEU
1	A	363	LYS

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Mol	Chain	Res	Type
1	A	377	HIS
1	A	378	THR
1	A	380	ILE
1	A	391	LEU
1	A	392	LEU
1	A	398	ARG
1	A	400	LEU
1	A	412	ASN
1	A	429	SER
1	A	430	LEU
1	A	439	ILE
1	A	441	MET
1	A	444	LEU
1	A	455	VAL
1	A	462	ILE
1	A	467	ILE
1	A	473	GLU
1	A	474	LEU
1	A	478	LYS
1	A	480	GLN
1	A	483	THR
1	A	486	ILE
1	A	492	LEU
1	A	495	CYS
1	A	501	GLU
1	A	506	ARG
1	A	510	GLU
1	A	516	ASP
1	A	522	LEU
1	A	530	PHE
1	A	537	VAL
1	A	543	LEU
1	A	548	TYR
1	A	549	LEU
1	A	554	LYS
1	A	555	VAL
1	A	562	LEU
1	A	565	VAL
1	A	576	GLN
1	A	583	VAL
1	A	586	LEU
1	A	589	ARG

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Mol	Chain	Res	Type
1	A	603	VAL
1	A	622	LEU
1	A	624	THR
1	A	630	VAL
1	A	640	LEU
1	A	649	ARG
1	A	652	LEU
1	A	662	LEU
1	A	665	GLN
1	A	676	THR
1	A	683	LEU
1	A	689	ILE
1	A	699	MET
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	714	ARG
1	A	717	ASP
1	A	724	ARG
1	A	727	ASN
1	A	734	ARG
1	A	741	ILE
1	A	751	SER
1	A	753	LYS
1	A	756	ASP
1	A	759	LYS
1	A	760	ASP
1	A	765	LEU
1	A	766	MET
1	A	779	GLU
1	A	782	LYS
1	A	788	SER
1	A	790	LEU
1	A	792	LYS
1	A	794	PRO
1	A	800	MET
1	A	807	THR
1	A	808	SER
1	A	810	LYS
1	A	832	GLN
1	A	833	ARG
1	B	15	VAL

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Mol	Chain	Res	Type
1	B	18	LEU
1	B	21	VAL
1	B	29	LYS
1	B	42	ASP
1	B	45	VAL
1	B	47	THR
1	B	63	LEU
1	B	64	VAL
1	B	70	THR
1	B	72	GLN
1	B	80	LYS
1	B	82	ILE
1	B	85	LEU
1	B	87	LEU
1	B	100	VAL
1	B	112	THR
1	B	121	GLU
1	B	127	GLU
1	B	136	LEU
1	B	165	ILE
1	B	167	ASN
1	B	169	LYS
1	B	177	GLU
1	B	191	LYS
1	B	195	GLU
1	B	210	SER
1	B	221	VAL
1	B	228	THR
1	B	234	ARG
1	B	235	ASN
1	B	237	VAL
1	B	243	LEU
1	B	245	SER
1	B	250	ASN
1	B	254	LEU
1	B	255	LYS
1	B	256	ASP
1	B	262	TYR
1	B	267	LEU
1	B	274	ASN
1	B	287	GLU
1	B	292	ARG

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Mol	Chain	Res	Type
1	B	299	VAL
1	B	304	LEU
1	B	313	SER
1	B	315	LYS
1	B	316	PHE
1	B	318	CYS
1	B	319	ARG
1	B	321	PRO
1	B	323	ARG
1	B	356	LEU
1	B	361	TRP
1	B	366	GLU
1	B	380	ILE
1	B	381	PRO
1	B	384	LEU
1	B	391	LEU
1	B	392	LEU
1	B	395	LEU
1	B	400	LEU
1	B	422	VAL
1	B	423	ASP
1	B	425	LEU
1	B	426	ARG
1	B	430	LEU
1	B	444	LEU
1	B	455	VAL
1	B	457	ARG
1	B	458	ILE
1	B	459	HIS
1	B	462	ILE
1	B	474	LEU
1	B	486	ILE
1	B	492	LEU
1	B	499	LEU
1	B	505	GLU
1	B	506	ARG
1	B	509	GLU
1	B	510	GLU
1	B	516	ASP
1	B	521	LEU
1	B	531	ILE
1	B	536	LYS

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Mol	Chain	Res	Type
1	B	540	GLU
1	B	543	LEU
1	B	552	GLU
1	B	553	TYR
1	B	554	LYS
1	B	555	VAL
1	B	562	LEU
1	B	564	ASP
1	B	565	VAL
1	B	569	ARG
1	B	586	LEU
1	B	589	ARG
1	B	591	LYS
1	B	592	LYS
1	B	596	LYS
1	B	602	THR
1	B	613	TYR
1	B	621	LYS
1	B	630	VAL
1	B	636	VAL
1	B	640	LEU
1	B	649	ARG
1	B	651	SER
1	B	652	LEU
1	B	655	LYS
1	B	658	PRO
1	B	662	LEU
1	B	665	GLN
1	B	666	ILE
1	B	674	SER
1	B	676	THR
1	B	678	ASN
1	B	698	GLU
1	B	705	GLU
1	B	706	GLU
1	B	714	ARG
1	B	717	ASP
1	B	724	ARG
1	B	733	ASP
1	B	751	SER
1	B	753	LYS
1	B	754	GLN

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Mol	Chain	Res	Type
1	B	756	ASP
1	B	760	ASP
1	B	764	MET
1	B	766	MET
1	B	782	LYS
1	B	787	VAL
1	B	790	LEU
1	B	792	LYS
1	B	795	ARG
1	B	807	THR
1	B	813	SER
1	B	830	SER
1	B	833	ARG
1	B	834	LEU
1	C	12	GLN
1	C	15	VAL
1	C	18	LEU
1	C	21	VAL
1	C	25	THR
1	C	27	LEU
1	C	37	PHE
1	C	42	ASP
1	C	45	VAL
1	C	47	THR
1	C	64	VAL
1	C	66	ARG
1	C	77	LYS
1	C	82	ILE
1	C	85	LEU
1	C	90	TYR
1	C	95	LEU
1	C	100	VAL
1	C	102	LEU
1	C	121	GLU
1	C	128	ASP
1	C	131	LEU
1	C	147	MET
1	C	165	ILE
1	C	167	ASN
1	C	169	LYS
1	C	177	GLU
1	C	206	VAL

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Mol	Chain	Res	Type
1	C	219	GLN
1	C	229	PRO
1	C	230	VAL
1	C	231	PRO
1	C	234	ARG
1	C	235	ASN
1	C	242	ARG
1	C	243	LEU
1	C	250	ASN
1	C	254	LEU
1	C	255	LYS
1	C	256	ASP
1	C	266	VAL
1	C	267	LEU
1	C	274	ASN
1	C	275	ILE
1	C	276	SER
1	C	279	LEU
1	C	281	PRO
1	C	287	GLU
1	C	291	LEU
1	C	292	ARG
1	C	300	VAL
1	C	304	LEU
1	C	306	ASP
1	C	309	ARG
1	C	314	SER
1	C	318	CYS
1	C	320	ASP
1	C	336	GLN
1	C	337	LEU
1	C	339	ASP
1	C	340	THR
1	C	358	ARG
1	C	359	LEU
1	C	360	ASP
1	C	361	TRP
1	C	378	THR
1	C	380	ILE
1	C	381	PRO
1	C	384	LEU
1	C	395	LEU

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Mol	Chain	Res	Type
1	C	396	LEU
1	C	398	ARG
1	C	400	LEU
1	C	422	VAL
1	C	426	ARG
1	C	432	GLU
1	C	438	ARG
1	C	444	LEU
1	C	455	VAL
1	C	464	LYS
1	C	474	LEU
1	C	486	ILE
1	C	492	LEU
1	C	494	LEU
1	C	499	LEU
1	C	506	ARG
1	C	509	GLU
1	C	510	GLU
1	C	521	LEU
1	C	522	LEU
1	C	527	ASP
1	C	532	ARG
1	C	537	VAL
1	C	540	GLU
1	C	543	LEU
1	C	549	LEU
1	C	553	TYR
1	C	554	LYS
1	C	555	VAL
1	C	574	LYS
1	C	575	ARG
1	C	576	GLN
1	C	586	LEU
1	C	589	ARG
1	C	592	LYS
1	C	618	MET
1	C	624	THR
1	C	630	VAL
1	C	638	ASP
1	C	652	LEU
1	C	658	PRO
1	C	665	GLN

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Mol	Chain	Res	Type
1	C	676	THR
1	C	705	GLU
1	C	706	GLU
1	C	714	ARG
1	C	727	ASN
1	C	734	ARG
1	C	751	SER
1	C	753	LYS
1	C	759	LYS
1	C	761	ILE
1	C	764	MET
1	C	766	MET
1	C	782	LYS
1	C	787	VAL
1	C	807	THR
1	C	812	SER
1	C	833	ARG
1	D	18	LEU
1	D	22	GLU
1	D	39	LEU
1	D	42	ASP
1	D	45	VAL
1	D	47	THR
1	D	64	VAL
1	D	82	ILE
1	D	88	GLU
1	D	91	MET
1	D	94	THR
1	D	95	LEU
1	D	100	VAL
1	D	104	LEU
1	D	131	LEU
1	D	136	LEU
1	D	145	ASP
1	D	150	LEU
1	D	165	ILE
1	D	167	ASN
1	D	169	LYS
1	D	176	MET
1	D	177	GLU
1	D	184	ARG
1	D	197	THR

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Mol	Chain	Res	Type
1	D	198	LEU
1	D	209	THR
1	D	210	SER
1	D	214	LYS
1	D	217	ASP
1	D	220	VAL
1	D	229	PRO
1	D	231	PRO
1	D	234	ARG
1	D	236	ASN
1	D	242	ARG
1	D	243	LEU
1	D	245	SER
1	D	250	ASN
1	D	254	LEU
1	D	255	LYS
1	D	259	VAL
1	D	262	TYR
1	D	274	ASN
1	D	281	PRO
1	D	287	GLU
1	D	289	LYS
1	D	291	LEU
1	D	300	VAL
1	D	304	LEU
1	D	306	ASP
1	D	315	LYS
1	D	318	CYS
1	D	319	ARG
1	D	321	PRO
1	D	323	ARG
1	D	336	GLN
1	D	337	LEU
1	D	340	THR
1	D	344	LEU
1	D	360	ASP
1	D	363	LYS
1	D	370	LYS
1	D	380	ILE
1	D	388	PRO
1	D	391	LEU
1	D	392	LEU

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Mol	Chain	Res	Type
1	D	393	GLU
1	D	394	THR
1	D	395	LEU
1	D	396	LEU
1	D	398	ARG
1	D	400	LEU
1	D	401	GLN
1	D	402	ILE
1	D	425	LEU
1	D	426	ARG
1	D	429	SER
1	D	455	VAL
1	D	458	ILE
1	D	459	HIS
1	D	461	GLU
1	D	474	LEU
1	D	477	HIS
1	D	478	LYS
1	D	480	GLN
1	D	486	ILE
1	D	492	LEU
1	D	494	LEU
1	D	499	LEU
1	D	511	TYR
1	D	516	ASP
1	D	522	LEU
1	D	526	ASP
1	D	530	PHE
1	D	533	ASP
1	D	543	LEU
1	D	549	LEU
1	D	562	LEU
1	D	565	VAL
1	D	573	TYR
1	D	575	ARG
1	D	576	GLN
1	D	578	LEU
1	D	591	LYS
1	D	592	LYS
1	D	613	TYR
1	D	618	MET
1	D	622	LEU

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Mol	Chain	Res	Type
1	D	640	LEU
1	D	649	ARG
1	D	652	LEU
1	D	658	PRO
1	D	662	LEU
1	D	665	GLN
1	D	676	THR
1	D	678	ASN
1	D	683	LEU
1	D	688	THR
1	D	705	GLU
1	D	706	GLU
1	D	714	ARG
1	D	717	ASP
1	D	724	ARG
1	D	727	ASN
1	D	756	ASP
1	D	759	LYS
1	D	760	ASP
1	D	765	LEU
1	D	787	VAL
1	D	792	LYS
1	D	798	THR
1	D	803	ARG
1	D	813	SER
1	D	816	THR
1	D	823	GLU
1	D	828	GLU
1	D	833	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	168	GLN
1	A	235	ASN
1	A	270	ASN
1	A	295	GLN
1	A	336	GLN
1	A	341	HIS
1	A	399	HIS
1	A	459	HIS

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Mol	Chain	Res	Type
1	A	560	ASN
1	A	576	GLN
1	A	614	HIS
1	A	665	GLN
1	A	727	ASN
1	A	744	GLN
1	A	832	GLN
1	B	72	GLN
1	B	187	ASN
1	B	211	GLN
1	B	219	GLN
1	B	235	ASN
1	B	239	ASN
1	B	341	HIS
1	B	377	HIS
1	B	412	ASN
1	B	443	HIS
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	566	GLN
1	B	582	HIS
1	B	588	ASN
1	B	595	ASN
1	B	614	HIS
1	B	665	GLN
1	B	740	GLN
1	C	36	HIS
1	C	71	GLN
1	C	235	ASN
1	C	264	GLN
1	C	336	GLN
1	C	377	HIS
1	C	399	HIS
1	C	453	ASN
1	C	459	HIS
1	C	477	HIS
1	C	481	ASN
1	C	566	GLN
1	C	579	ASN
1	C	614	HIS
1	C	727	ASN

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Mol	Chain	Res	Type
1	C	744	GLN
1	C	793	ASN
1	D	72	GLN
1	D	133	ASN
1	D	168	GLN
1	D	187	ASN
1	D	274	ASN
1	D	336	GLN
1	D	376	ASN
1	D	377	HIS
1	D	412	ASN
1	D	450	HIS
1	D	453	ASN
1	D	481	ASN
1	D	576	GLN
1	D	582	HIS
1	D	588	ASN
1	D	595	ASN
1	D	665	GLN
1	D	727	ASN
1	D	744	GLN
1	D	767	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	A	999	1	15,15,16	1.87	5 (33%)	21,22,23	1.07	2 (9%)
3	PLP	D	999	1	15,15,16	1.12	1 (6%)	21,22,23	1.87	2 (9%)
3	PLP	B	999	1	15,15,16	1.60	1 (6%)	21,22,23	1.09	1 (4%)
3	PLP	C	999	1	15,15,16	1.14	1 (6%)	21,22,23	0.98	1 (4%)
2	SO4	B	900	-	4,4,4	0.46	0	6,6,6	0.44	0
2	SO4	A	901	-	4,4,4	0.34	0	6,6,6	0.33	0
4	AMP	C	920	-	25,25,25	0.75	0	37,38,38	0.73	0
2	SO4	D	900	-	4,4,4	0.24	0	6,6,6	0.32	0
2	SO4	A	900	-	4,4,4	0.24	0	6,6,6	0.37	0
4	AMP	D	920	-	25,25,25	0.75	0	37,38,38	0.67	0
4	AMP	A	920	-	25,25,25	0.74	0	37,38,38	0.78	0
4	AMP	B	920	-	25,25,25	0.73	0	37,38,38	0.72	0
2	SO4	C	901	-	4,4,4	0.32	0	6,6,6	0.41	0
2	SO4	C	900	-	4,4,4	0.36	0	6,6,6	0.34	0
2	SO4	B	901	-	4,4,4	0.41	0	6,6,6	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1
3	PLP	D	999	1	-	0/6/6/8	0/1/1/1
3	PLP	B	999	1	-	0/6/6/8	0/1/1/1
3	PLP	C	999	1	-	0/6/6/8	0/1/1/1
4	AMP	D	920	-	-	3/10/26/26	0/3/3/3
4	AMP	A	920	-	-	3/10/26/26	0/3/3/3
4	AMP	B	920	-	-	2/10/26/26	0/3/3/3
4	AMP	C	920	-	-	3/10/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	PLP	C3-C2	-3.98	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C3-C2	-3.92	1.36	1.41
3	A	999	PLP	P-O2P	-2.57	1.45	1.54
3	C	999	PLP	C3-C2	-2.55	1.38	1.41
3	A	999	PLP	C5-C4	-2.41	1.37	1.40
3	A	999	PLP	C5A-C5	-2.26	1.45	1.50
3	A	999	PLP	C4A-C4	-2.12	1.47	1.51
3	D	999	PLP	P-O3P	-2.05	1.47	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	999	PLP	O4P-C5A-C5	7.49	123.39	109.36
3	C	999	PLP	C6-C5-C4	2.34	120.01	118.10
3	A	999	PLP	C5-C6-N1	-2.28	120.12	123.83
3	D	999	PLP	C5-C6-N1	-2.26	120.16	123.83
3	B	999	PLP	O4P-C5A-C5	2.22	113.52	109.36
3	A	999	PLP	O2P-P-O4P	-2.00	101.44	106.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	920	AMP	C5'-O5'-P-O2P
4	A	920	AMP	C5'-O5'-P-O3P
4	B	920	AMP	C5'-O5'-P-O2P
4	B	920	AMP	C5'-O5'-P-O3P
4	C	920	AMP	C5'-O5'-P-O2P
4	C	920	AMP	C5'-O5'-P-O3P
4	D	920	AMP	C5'-O5'-P-O2P
4	A	920	AMP	C5'-O5'-P-O1P
4	C	920	AMP	C5'-O5'-P-O1P
4	D	920	AMP	C5'-O5'-P-O3P
4	D	920	AMP	C5'-O5'-P-O1P

There are no ring outliers.

11 monomers are involved in 16 short contacts:

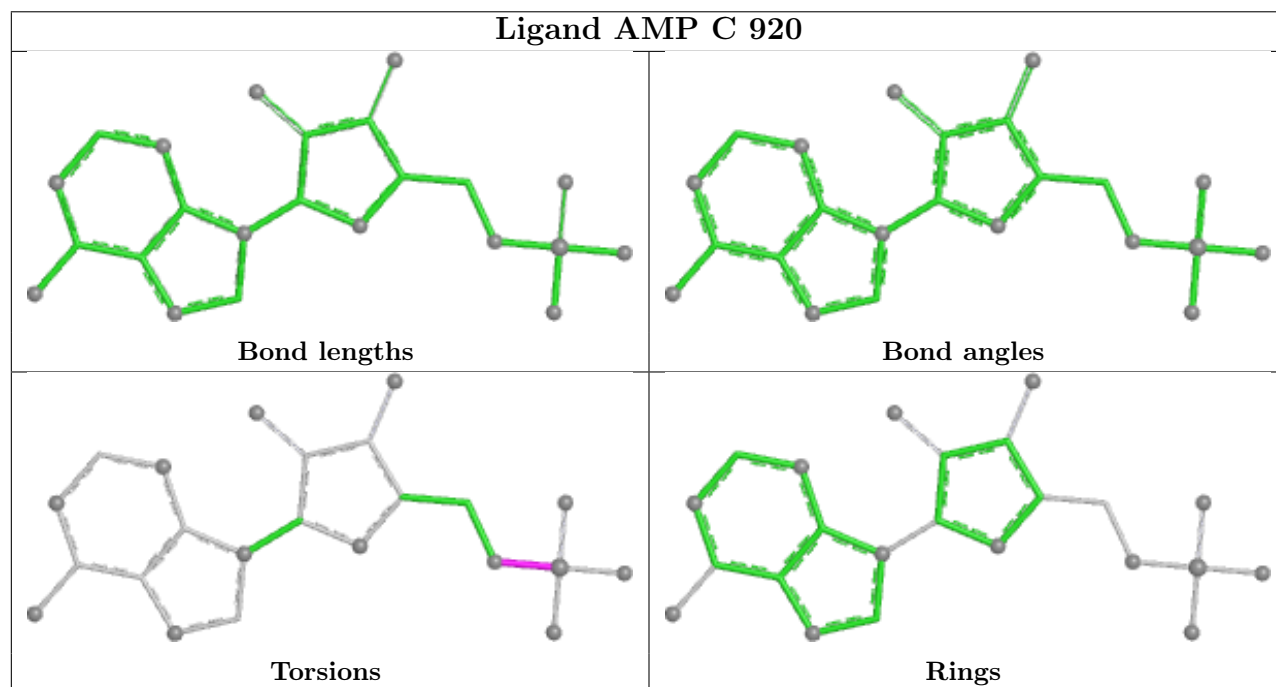
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	PLP	1	0
3	D	999	PLP	2	0
3	B	999	PLP	1	0

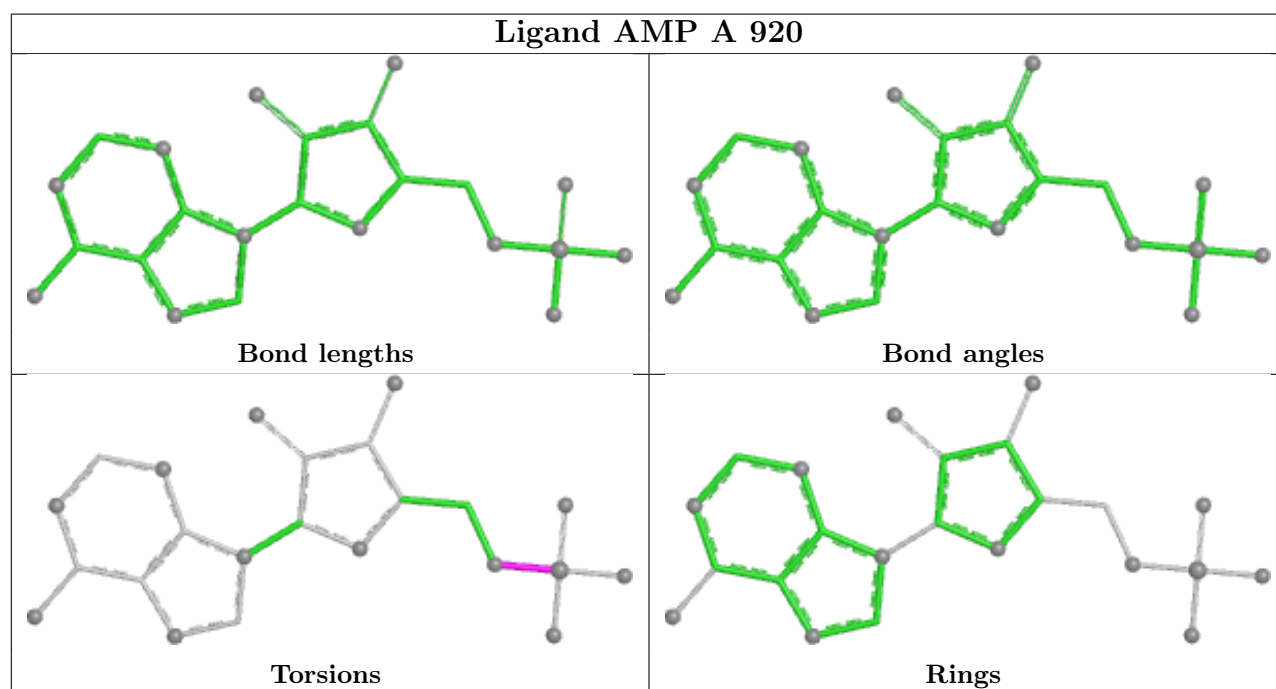
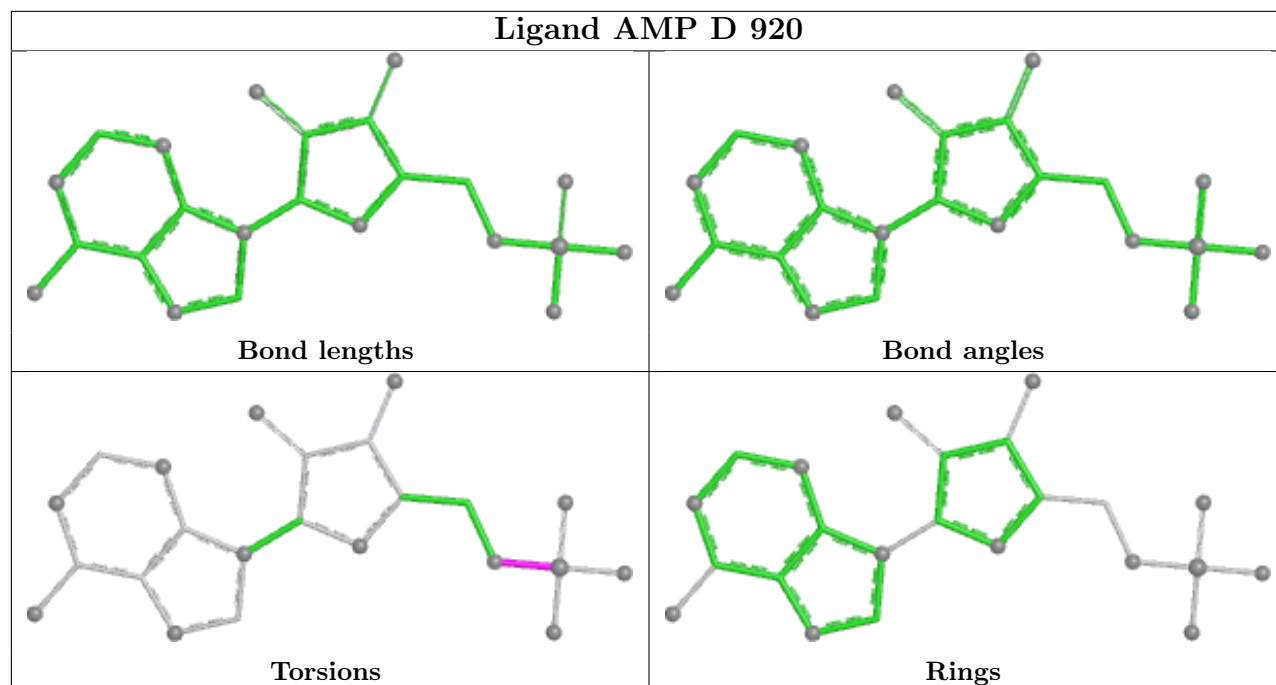
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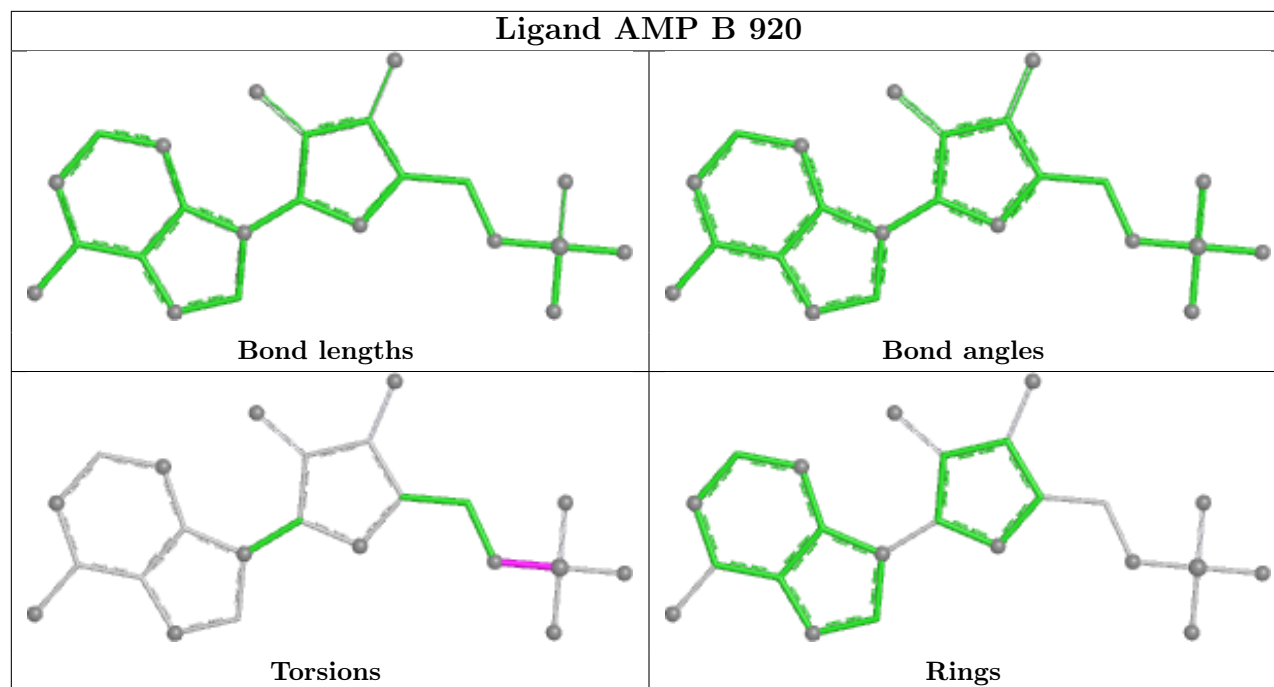
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	999	PLP	1	0
2	A	901	SO4	2	0
4	C	920	AMP	1	0
4	D	920	AMP	2	0
4	A	920	AMP	3	0
4	B	920	AMP	1	0
2	C	901	SO4	1	0
2	B	901	SO4	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.