



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:25 PM UTC

PDB ID : 1SZP / pdb_00001szp
Title : A Crystal Structure of the Rad51 Filament
Authors : Conway, A.B.; Lynch, T.W.; Zhang, Y.; Fortin, G.S.; Symington, L.S.; Rice, P.A.
Deposited on : 2004-04-06
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

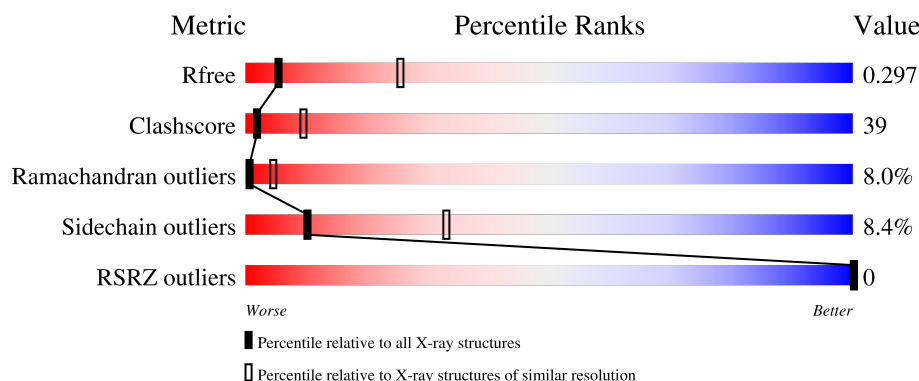
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	321	
1	B	321	
1	C	321	
1	D	321	
1	E	321	

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Mol	Chain	Length	Quality of chain
1	F	321	

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	B	502	-	-	X	-
2	SO4	C	503	-	-	X	-
2	SO4	D	504	-	-	X	-
2	SO4	E	505	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

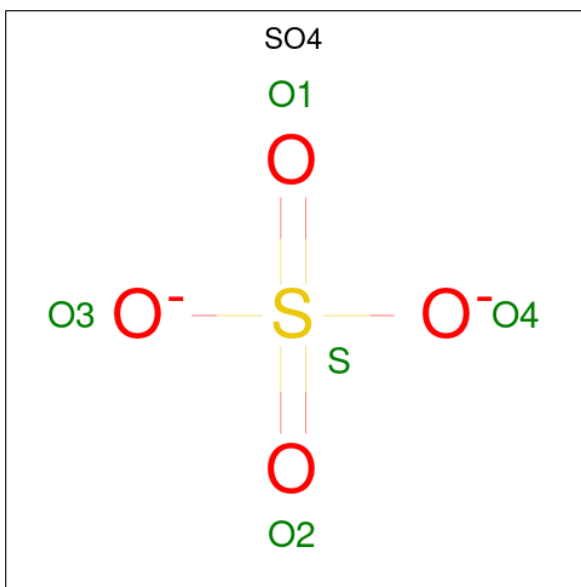
- Molecule 1 is a protein called DNA repair protein RAD51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2148	1349	376	408	15			
1	B	274	Total	C	N	O	S	0	0	0
			1985	1245	351	376	13			
1	C	274	Total	C	N	O	S	0	0	0
			1995	1249	354	378	14			
1	D	293	Total	C	N	O	S	0	0	0
			2143	1344	377	406	16			
1	E	294	Total	C	N	O	S	0	0	0
			2147	1346	378	407	16			
1	F	294	Total	C	N	O	S	0	0	0
			2135	1341	372	407	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	MET	-	initiating methionine	UNP P25454
A	345	THR	ILE	engineered mutation	UNP P25454
B	80	MET	-	initiating methionine	UNP P25454
B	345	THR	ILE	engineered mutation	UNP P25454
C	80	MET	-	initiating methionine	UNP P25454
C	345	THR	ILE	engineered mutation	UNP P25454
D	80	MET	-	initiating methionine	UNP P25454
D	345	THR	ILE	engineered mutation	UNP P25454
E	80	MET	-	initiating methionine	UNP P25454
E	345	THR	ILE	engineered mutation	UNP P25454
F	80	MET	-	initiating methionine	UNP P25454
F	345	THR	ILE	engineered mutation	UNP P25454

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

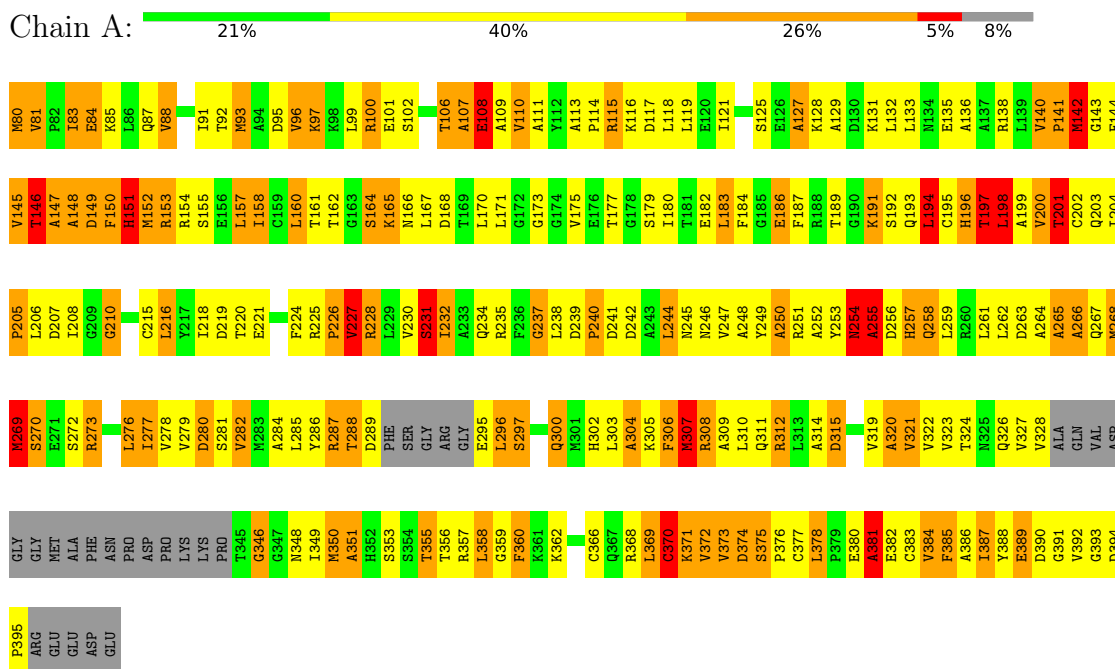


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

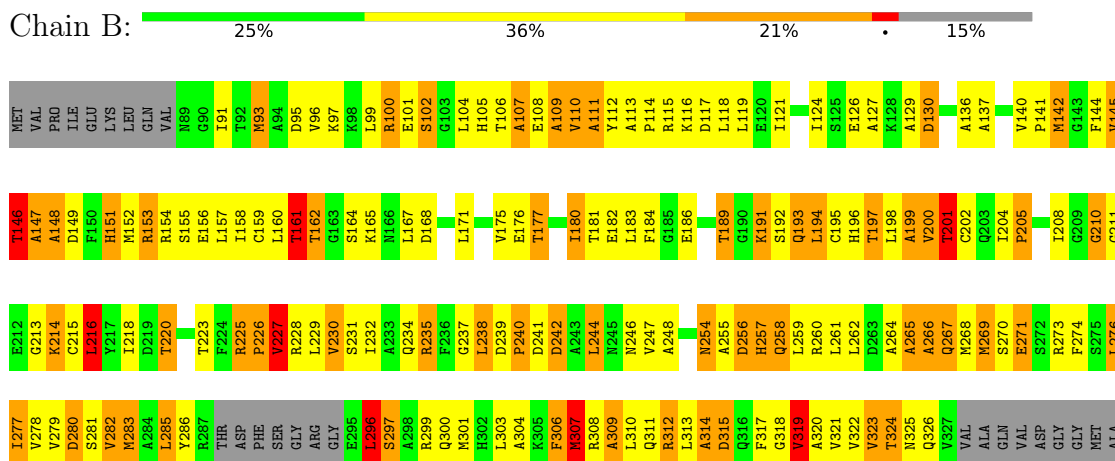
3 Residue-property plots

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

• Molecule 1: DNA repair protein RAD51



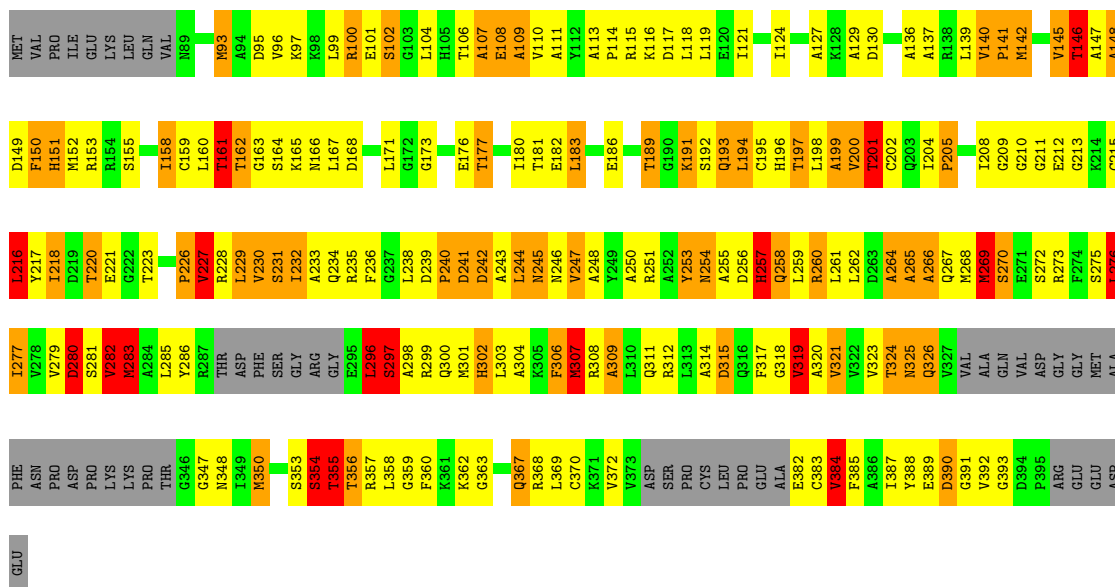
• Molecule 1: DNA repair protein RAD51





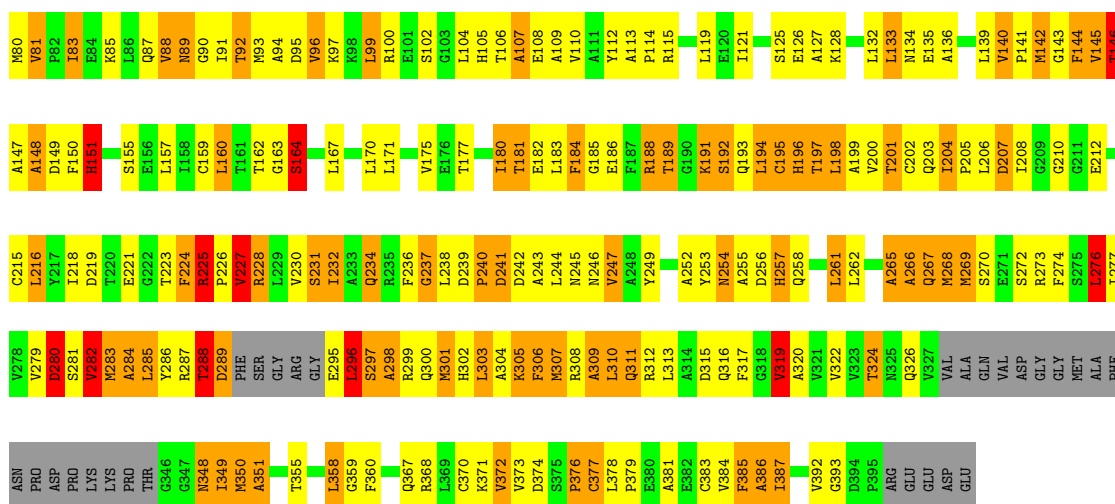
• Molecule 1: DNA repair protein RAD51

Chain C: 23% 38% 18% 6% 15%



• Molecule 1: DNA repair protein RAD51

Chain D: 27% 38% 23% 9%



• Molecule 1: DNA repair protein RAD51

Chain E: 29% 36% 22% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	135.26Å 135.26Å 128.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.25 40.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	88.4 (40.00-3.25) 99.1 (40.00-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.268 , 0.320 0.250 , 0.297	Depositor DCC
R_{free} test set	4063 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å ²)	85.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 101.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.408 for -h,-k,l 0.046 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12583	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.90	179/2177 (8.2%)	1.85	49/2951 (1.7%)
1	B	2.44	94/2009 (4.7%)	1.69	37/2719 (1.4%)
1	C	2.43	94/2019 (4.7%)	1.70	40/2730 (1.5%)
1	D	2.55	120/2172 (5.5%)	1.74	35/2942 (1.2%)
1	E	2.51	113/2176 (5.2%)	1.72	36/2947 (1.2%)
1	F	2.88	169/2164 (7.8%)	1.86	51/2934 (1.7%)
All	All	2.63	769/12717 (6.0%)	1.76	248/17223 (1.4%)

All (769) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	386	ALA	CA-CB	-15.24	1.28	1.53
1	D	283	MET	SD-CE	14.66	2.16	1.79
1	F	307	MET	SD-CE	-14.60	1.43	1.79
1	B	279	VAL	CA-C	-13.74	1.35	1.52
1	E	110	VAL	CA-CB	-13.44	1.40	1.54
1	C	279	VAL	CA-C	-13.43	1.36	1.52
1	A	386	ALA	CA-CB	-12.77	1.32	1.53
1	A	147	ALA	C-O	-12.56	1.09	1.24
1	B	279	VAL	CA-CB	-12.29	1.39	1.54
1	F	314	ALA	CA-CB	-12.21	1.33	1.53
1	D	96	VAL	C-O	-12.20	1.10	1.24
1	A	110	VAL	CA-CB	-11.96	1.41	1.54
1	D	310	LEU	C-O	-11.96	1.10	1.24
1	D	113	ALA	CA-CB	-11.90	1.37	1.53
1	C	283	MET	SD-CE	11.89	2.09	1.79
1	A	375	SER	C-O	-11.88	1.09	1.24
1	F	191	LYS	C-O	-11.68	1.11	1.24
1	C	280	ASP	CA-C	11.63	1.66	1.52
1	D	115	ARG	C-O	-11.54	1.10	1.24
1	C	307	MET	SD-CE	-11.30	1.51	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	219	ASP	C-O	-11.29	1.10	1.24
1	E	115	ARG	C-O	-11.23	1.11	1.24
1	D	282	VAL	CA-CB	-11.21	1.37	1.54
1	E	96	VAL	C-O	-11.20	1.11	1.24
1	A	278	VAL	C-O	-11.19	1.12	1.24
1	F	373	VAL	CA-CB	-10.99	1.41	1.54
1	A	219	ASP	C-O	-10.95	1.11	1.24
1	D	255	ALA	CA-CB	-10.92	1.35	1.53
1	B	280	ASP	CA-C	10.85	1.65	1.52
1	A	391	GLY	C-O	-10.77	1.13	1.24
1	F	375	SER	C-O	-10.69	1.10	1.24
1	E	80	MET	SD-CE	10.57	2.06	1.79
1	A	218	ILE	C-O	-10.55	1.12	1.24
1	F	308	ARG	CG-CD	10.55	1.84	1.52
1	D	218	ILE	C-O	-10.53	1.12	1.24
1	A	108	GLU	CA-C	-10.49	1.39	1.52
1	F	93	MET	SD-CE	10.45	2.05	1.79
1	A	304	ALA	CA-CB	-10.41	1.37	1.53
1	A	191	LYS	C-O	-10.41	1.12	1.24
1	D	115	ARG	CA-C	-10.36	1.39	1.52
1	A	145	VAL	CA-CB	-10.33	1.48	1.55
1	F	373	VAL	C-O	-10.21	1.12	1.24
1	E	269	MET	SD-CE	-10.17	1.54	1.79
1	F	184	PHE	C-O	-10.10	1.11	1.23
1	E	310	LEU	C-O	-10.10	1.12	1.24
1	D	110	VAL	CA-CB	-10.07	1.43	1.54
1	B	320	ALA	C-O	-10.02	1.12	1.24
1	F	300	GLN	C-O	-9.99	1.11	1.24
1	A	322	VAL	C-O	-9.94	1.13	1.24
1	A	110	VAL	N-CA	-9.88	1.35	1.46
1	F	110	VAL	N-CA	-9.85	1.35	1.46
1	B	145	VAL	CA-CB	-9.85	1.44	1.55
1	E	218	ILE	C-O	-9.76	1.13	1.24
1	E	282	VAL	CA-CB	-9.74	1.40	1.54
1	C	279	VAL	CA-CB	-9.71	1.42	1.54
1	B	355	THR	CA-C	-9.59	1.40	1.52
1	D	145	VAL	CA-CB	-9.57	1.45	1.55
1	E	303	LEU	C-O	-9.56	1.13	1.24
1	E	194	LEU	C-O	-9.55	1.13	1.24
1	A	382	GLU	C-O	-9.54	1.11	1.23
1	A	306	PHE	C-O	-9.46	1.16	1.23
1	F	219	ASP	CA-C	-9.43	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	234	GLN	C-O	-9.42	1.13	1.24
1	F	108	GLU	CA-C	-9.41	1.40	1.52
1	C	321	VAL	CA-CB	-9.40	1.42	1.54
1	A	373	VAL	CA-CB	-9.35	1.42	1.54
1	C	150	PHE	C-O	-9.32	1.13	1.24
1	A	93	MET	SD-CE	9.29	2.02	1.79
1	A	382	GLU	CA-C	-9.28	1.40	1.53
1	F	162	THR	C-O	-9.24	1.12	1.24
1	A	143	GLY	C-O	-9.21	1.12	1.23
1	E	180	ILE	C-O	-9.19	1.11	1.24
1	A	150	PHE	C-O	-9.19	1.13	1.24
1	C	232	ILE	CA-CB	-9.18	1.42	1.54
1	D	107	ALA	CA-CB	-9.14	1.39	1.53
1	F	303	LEU	C-O	-9.12	1.12	1.24
1	A	307	MET	SD-CE	-9.12	1.56	1.79
1	D	265	ALA	CA-C	-9.12	1.39	1.52
1	F	186	GLU	CA-C	-9.12	1.40	1.53
1	A	244	LEU	C-O	-9.10	1.13	1.24
1	F	322	VAL	C-O	-9.08	1.14	1.24
1	C	320	ALA	CA-CB	-9.04	1.39	1.53
1	D	349	ILE	CA-CB	-9.01	1.42	1.54
1	B	320	ALA	CA-CB	-8.97	1.39	1.53
1	F	191	LYS	CA-C	-8.95	1.42	1.53
1	F	136	ALA	C-O	-8.95	1.13	1.24
1	F	145	VAL	CA-CB	-8.93	1.45	1.55
1	C	306	PHE	C-O	-8.86	1.14	1.23
1	E	148	ALA	C-O	-8.86	1.13	1.24
1	C	269	MET	C-O	-8.85	1.12	1.24
1	F	308	ARG	CD-NE	8.85	1.58	1.46
1	E	115	ARG	CA-C	-8.82	1.41	1.52
1	F	321	VAL	CA-CB	-8.81	1.43	1.54
1	A	252	ALA	C-O	-8.81	1.13	1.24
1	A	136	ALA	C-O	-8.76	1.14	1.24
1	A	191	LYS	CA-C	-8.72	1.42	1.53
1	A	359	GLY	C-O	-8.71	1.13	1.23
1	F	224	PHE	CA-C	-8.70	1.42	1.52
1	F	152	MET	C-O	-8.70	1.13	1.24
1	C	220	THR	CA-CB	8.69	1.67	1.53
1	D	282	VAL	CA-C	-8.69	1.40	1.52
1	F	303	LEU	CA-C	-8.66	1.40	1.52
1	F	183	LEU	CA-C	-8.63	1.42	1.52
1	C	320	ALA	C-O	-8.62	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	PRO	CA-C	-8.59	1.40	1.52
1	D	148	ALA	C-O	-8.58	1.14	1.24
1	A	162	THR	CA-C	-8.57	1.41	1.52
1	C	244	LEU	C-O	-8.57	1.14	1.24
1	A	197	THR	C-O	-8.56	1.13	1.24
1	D	142	MET	CA-C	-8.55	1.43	1.53
1	A	303	LEU	C-O	-8.54	1.13	1.24
1	F	273	ARG	C-O	-8.48	1.13	1.24
1	E	183	LEU	CA-C	-8.48	1.42	1.52
1	D	143	GLY	C-O	-8.42	1.14	1.23
1	A	148	ALA	C-O	-8.41	1.14	1.24
1	A	83	ILE	CA-CB	-8.41	1.42	1.54
1	B	218	ILE	C-O	-8.40	1.15	1.24
1	A	321	VAL	C-O	-8.38	1.15	1.24
1	A	152	MET	C-O	-8.37	1.13	1.24
1	B	321	VAL	CA-CB	-8.37	1.44	1.54
1	B	355	THR	C-O	-8.32	1.13	1.24
1	D	191	LYS	C-O	-8.30	1.17	1.23
1	A	149	ASP	C-O	-8.29	1.14	1.24
1	A	183	LEU	CA-C	-8.26	1.42	1.52
1	A	234	GLN	C-O	-8.25	1.14	1.24
1	B	356	THR	CA-C	8.24	1.63	1.52
1	A	276	LEU	C-O	-8.21	1.13	1.23
1	F	312	ARG	C-O	-8.18	1.14	1.24
1	C	160	LEU	C-O	-8.16	1.14	1.23
1	E	113	ALA	CA-CB	-8.14	1.42	1.53
1	F	321	VAL	C-O	-8.13	1.14	1.24
1	E	265	ALA	C-O	-8.12	1.13	1.24
1	A	184	PHE	C-O	-8.11	1.13	1.23
1	A	118	LEU	C-O	-8.07	1.14	1.23
1	C	216	LEU	C-O	-8.07	1.14	1.24
1	F	264	ALA	C-O	-8.07	1.13	1.24
1	B	391	GLY	C-O	-8.04	1.14	1.23
1	B	244	LEU	C-O	-8.02	1.14	1.24
1	A	147	ALA	CA-C	-8.02	1.43	1.52
1	C	248	ALA	C-O	-8.01	1.14	1.24
1	F	226	PRO	C-O	-8.01	1.13	1.24
1	F	165	LYS	CA-C	-8.00	1.41	1.52
1	A	308	ARG	CG-CD	8.00	1.76	1.52
1	B	390	ASP	C-O	-8.00	1.17	1.24
1	E	228	ARG	NE-CZ	7.97	1.41	1.33
1	F	303	LEU	CG-CD1	-7.96	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	ILE	C-O	-7.95	1.15	1.24
1	A	320	ALA	C-O	-7.93	1.15	1.24
1	F	384	VAL	CA-CB	-7.92	1.43	1.54
1	B	306	PHE	C-O	-7.91	1.15	1.23
1	F	320	ALA	C-O	-7.91	1.15	1.24
1	F	162	THR	CA-C	-7.88	1.42	1.52
1	B	352	HIS	C-O	7.84	1.33	1.24
1	C	314	ALA	CA-CB	-7.82	1.40	1.53
1	D	192	SER	CA-C	-7.81	1.42	1.52
1	C	216	LEU	CA-C	-7.80	1.43	1.52
1	A	182	GLU	C-O	-7.80	1.14	1.24
1	F	182	GLU	C-O	-7.80	1.14	1.24
1	E	204	ILE	CA-C	-7.76	1.44	1.52
1	F	143	GLY	C-O	-7.75	1.13	1.23
1	E	265	ALA	CA-C	-7.74	1.41	1.52
1	D	225	ARG	NE-CZ	-7.73	1.24	1.33
1	D	204	ILE	CA-C	-7.71	1.44	1.52
1	E	320	ALA	C-O	-7.65	1.15	1.24
1	A	194	LEU	C-O	-7.62	1.15	1.24
1	E	349	ILE	CA-CB	-7.61	1.43	1.54
1	F	359	GLY	C-O	-7.60	1.14	1.23
1	F	248	ALA	CA-C	-7.60	1.43	1.52
1	D	267	GLN	C-O	-7.58	1.14	1.24
1	E	386	ALA	CA-CB	-7.58	1.40	1.53
1	C	199	ALA	CA-C	-7.56	1.41	1.52
1	D	184	PHE	C-O	-7.56	1.14	1.23
1	F	278	VAL	C-O	-7.56	1.16	1.24
1	A	106	THR	C-O	-7.53	1.14	1.23
1	E	186	GLU	C-O	-7.53	1.13	1.23
1	A	324	THR	C-O	-7.52	1.15	1.23
1	E	189	THR	CA-CB	-7.52	1.43	1.53
1	A	300	GLN	C-O	-7.51	1.14	1.24
1	A	226	PRO	C-O	-7.51	1.14	1.24
1	F	254	ASN	C-O	-7.50	1.15	1.23
1	A	216	LEU	C-O	-7.49	1.14	1.24
1	C	189	THR	CA-CB	-7.49	1.42	1.53
1	D	298	ALA	N-CA	7.49	1.55	1.46
1	F	288	THR	N-CA	7.47	1.55	1.46
1	F	87	GLN	CA-C	-7.47	1.44	1.53
1	D	180	ILE	CA-CB	-7.46	1.45	1.54
1	F	282	VAL	C-O	7.46	1.32	1.24
1	F	258	GLN	C-O	-7.45	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	386	ALA	CA-CB	-7.45	1.41	1.53
1	C	193	GLN	C-O	-7.44	1.15	1.24
1	C	162	THR	CA-CB	-7.44	1.42	1.53
1	B	193	GLN	C-O	-7.44	1.15	1.24
1	A	198	LEU	CG-CD1	-7.43	1.28	1.52
1	F	96	VAL	C-O	-7.43	1.15	1.24
1	C	108	GLU	CA-C	-7.43	1.43	1.52
1	F	250	ALA	C-O	-7.41	1.15	1.24
1	C	254	ASN	CA-C	-7.41	1.43	1.52
1	F	304	ALA	CA-CB	-7.40	1.43	1.53
1	F	226	PRO	CA-C	-7.40	1.41	1.52
1	B	315	ASP	CB-CG	7.39	1.70	1.52
1	F	83	ILE	CA-CB	-7.38	1.44	1.54
1	D	301	MET	C-O	-7.36	1.15	1.24
1	B	148	ALA	C-O	-7.36	1.15	1.24
1	F	152	MET	CA-C	-7.36	1.43	1.52
1	D	309	ALA	C-O	-7.35	1.15	1.24
1	D	189	THR	CA-CB	-7.34	1.43	1.53
1	A	309	ALA	C-O	-7.34	1.15	1.24
1	D	358	LEU	CA-C	-7.33	1.44	1.52
1	D	81	VAL	N-CA	-7.33	1.40	1.46
1	B	162	THR	CA-CB	-7.32	1.42	1.53
1	A	263	ASP	CA-CB	-7.32	1.42	1.53
1	B	160	LEU	C-O	-7.32	1.15	1.23
1	F	92	THR	C-O	-7.31	1.15	1.23
1	D	194	LEU	C-O	-7.31	1.15	1.24
1	C	199	ALA	C-O	-7.30	1.14	1.24
1	F	266	ALA	CA-CB	-7.30	1.42	1.53
1	B	314	ALA	CA-CB	-7.30	1.41	1.53
1	D	372	VAL	CA-CB	-7.29	1.44	1.54
1	D	92	THR	C-O	-7.27	1.15	1.23
1	F	160	LEU	CA-C	-7.26	1.43	1.53
1	E	279	VAL	CA-CB	-7.26	1.45	1.54
1	A	186	GLU	CA-C	-7.26	1.43	1.53
1	B	269	MET	C-O	-7.25	1.14	1.24
1	C	108	GLU	C-O	-7.25	1.15	1.24
1	C	319	VAL	CA-CB	7.21	1.64	1.54
1	F	175	VAL	N-CA	-7.21	1.38	1.46
1	B	277	ILE	C-O	-7.21	1.15	1.24
1	A	143	GLY	CA-C	-7.20	1.45	1.52
1	F	198	LEU	CG-CD1	-7.20	1.28	1.52
1	B	265	ALA	C-O	-7.19	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	VAL	CA-CB	-7.19	1.44	1.54
1	F	175	VAL	C-O	-7.18	1.16	1.24
1	D	159	CYS	N-CA	7.17	1.54	1.46
1	C	218	ILE	C-O	-7.16	1.16	1.24
1	B	110	VAL	CA-C	-7.16	1.44	1.52
1	A	232	ILE	C-O	-7.15	1.16	1.24
1	F	244	LEU	C-O	-7.14	1.15	1.24
1	B	323	VAL	CA-CB	-7.13	1.45	1.54
1	A	270	SER	CA-C	-7.10	1.43	1.53
1	D	247	VAL	C-O	-7.10	1.15	1.24
1	A	372	VAL	CA-CB	-7.08	1.44	1.54
1	F	324	THR	C-O	-7.07	1.15	1.23
1	A	81	VAL	CA-C	-7.07	1.45	1.52
1	F	148	ALA	C-O	-7.07	1.16	1.24
1	A	279	VAL	C-O	-7.05	1.16	1.24
1	F	129	ALA	CA-CB	-7.04	1.42	1.53
1	E	188	ARG	C-O	-7.04	1.15	1.23
1	B	227	VAL	CB-CG2	7.01	1.75	1.52
1	A	138	ARG	C-O	-7.00	1.15	1.24
1	B	160	LEU	CA-C	-7.00	1.44	1.52
1	F	99	LEU	C-O	-6.99	1.15	1.24
1	A	224	PHE	CA-C	-6.95	1.44	1.52
1	F	283	MET	CA-C	6.95	1.62	1.52
1	C	253	TYR	C-O	-6.94	1.15	1.24
1	C	209	GLY	C-O	-6.94	1.14	1.23
1	A	385	PHE	C-O	-6.94	1.15	1.24
1	F	307	MET	N-CA	-6.94	1.37	1.46
1	F	137	ALA	CA-CB	6.94	1.66	1.53
1	D	146	THR	CA-CB	6.93	1.64	1.53
1	D	134	ASN	CA-C	-6.93	1.43	1.52
1	A	253	TYR	CA-C	-6.91	1.43	1.52
1	F	223	THR	CA-CB	6.90	1.62	1.53
1	A	201	THR	N-CA	-6.90	1.37	1.46
1	B	226	PRO	C-O	-6.89	1.15	1.24
1	E	284	ALA	CA-CB	-6.89	1.41	1.53
1	B	248	ALA	CA-C	-6.87	1.44	1.52
1	F	255	ALA	C-O	-6.86	1.15	1.24
1	F	147	ALA	C-O	-6.86	1.16	1.24
1	D	306	PHE	C-O	-6.86	1.16	1.23
1	A	355	THR	CA-C	-6.84	1.43	1.52
1	D	350	MET	SD-CE	-6.83	1.62	1.79
1	E	298	ALA	N-CA	6.83	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	ALA	CA-CB	-6.82	1.42	1.53
1	E	107	ALA	CA-CB	-6.82	1.42	1.53
1	A	314	ALA	CA-CB	-6.81	1.42	1.53
1	F	231	SER	C-O	-6.81	1.15	1.24
1	D	223	THR	CA-CB	6.80	1.63	1.53
1	E	99	LEU	CA-C	-6.80	1.44	1.53
1	F	106	THR	CA-CB	-6.80	1.42	1.53
1	A	279	VAL	N-CA	-6.79	1.38	1.46
1	E	348	ASN	CA-C	-6.79	1.44	1.52
1	A	358	LEU	C-O	-6.76	1.16	1.24
1	A	273	ARG	C-O	-6.76	1.15	1.24
1	F	355	THR	C-O	-6.76	1.15	1.24
1	B	247	VAL	C-O	-6.75	1.16	1.24
1	B	254	ASN	CA-C	-6.75	1.44	1.52
1	F	319	VAL	C-O	-6.75	1.16	1.24
1	D	114	PRO	C-O	-6.74	1.15	1.23
1	A	81	VAL	CA-CB	-6.74	1.45	1.54
1	A	219	ASP	CA-C	-6.74	1.44	1.52
1	A	162	THR	C-O	-6.73	1.15	1.24
1	C	277	ILE	CA-C	-6.73	1.44	1.52
1	A	158	ILE	C-O	-6.72	1.16	1.24
1	F	101	GLU	C-O	-6.72	1.15	1.24
1	A	263	ASP	N-CA	-6.71	1.38	1.46
1	D	269	MET	SD-CE	-6.71	1.62	1.79
1	A	148	ALA	CA-CB	-6.71	1.42	1.53
1	D	180	ILE	C-O	-6.70	1.15	1.24
1	C	217	TYR	C-O	-6.70	1.16	1.24
1	A	288	THR	N-CA	6.69	1.54	1.46
1	E	255	ALA	CA-CB	-6.68	1.42	1.53
1	B	326	GLN	CA-C	-6.67	1.44	1.52
1	C	104	LEU	C-O	-6.67	1.15	1.23
1	E	385	PHE	C-O	-6.65	1.16	1.23
1	E	145	VAL	CA-CB	-6.65	1.48	1.55
1	F	106	THR	C-O	-6.65	1.15	1.23
1	A	92	THR	C-O	-6.63	1.16	1.23
1	A	201	THR	CA-CB	6.63	1.64	1.53
1	A	150	PHE	N-CA	6.63	1.54	1.46
1	A	100	ARG	NE-CZ	-6.62	1.25	1.33
1	B	216	LEU	CA-C	-6.61	1.44	1.52
1	D	193	GLN	C-O	-6.60	1.16	1.24
1	E	306	PHE	C-O	-6.60	1.16	1.24
1	A	250	ALA	C-O	-6.59	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	215	CYS	CA-CB	-6.59	1.42	1.53
1	B	109	ALA	CA-CB	-6.59	1.43	1.53
1	B	199	ALA	CA-C	-6.58	1.43	1.52
1	B	220	THR	CA-CB	6.58	1.64	1.53
1	B	201	THR	C-O	-6.58	1.15	1.24
1	F	100	ARG	NE-CZ	-6.57	1.25	1.33
1	A	127	ALA	C-O	-6.56	1.15	1.23
1	F	252	ALA	CA-CB	-6.56	1.44	1.53
1	F	96	VAL	CA-CB	-6.56	1.46	1.54
1	A	96	VAL	C-O	-6.56	1.16	1.24
1	A	307	MET	N-CA	-6.55	1.37	1.46
1	D	252	ALA	CA-CB	6.54	1.62	1.53
1	F	288	THR	CA-CB	6.54	1.64	1.53
1	F	279	VAL	C-O	-6.53	1.17	1.24
1	A	355	THR	C-O	-6.53	1.15	1.24
1	C	309	ALA	CA-CB	-6.52	1.43	1.53
1	C	391	GLY	C-O	-6.52	1.17	1.24
1	B	107	ALA	CA-C	-6.50	1.44	1.52
1	C	199	ALA	CA-CB	-6.50	1.41	1.53
1	C	227	VAL	CB-CG2	6.48	1.74	1.52
1	D	88	VAL	CA-CB	6.47	1.65	1.55
1	D	188	ARG	C-O	-6.47	1.15	1.23
1	E	282	VAL	CA-C	-6.47	1.43	1.52
1	C	183	LEU	CA-C	-6.45	1.45	1.52
1	A	87	GLN	CA-C	-6.45	1.44	1.52
1	E	359	GLY	C-O	-6.44	1.15	1.23
1	E	162	THR	CA-C	-6.44	1.44	1.52
1	A	166	ASN	C-O	-6.44	1.16	1.24
1	A	248	ALA	CA-C	-6.43	1.45	1.52
1	F	309	ALA	C-O	-6.43	1.16	1.24
1	F	268	MET	C-O	-6.43	1.16	1.24
1	F	285	LEU	CA-C	-6.43	1.43	1.52
1	F	148	ALA	CA-CB	-6.42	1.43	1.53
1	A	101	GLU	C-O	-6.42	1.15	1.24
1	D	303	LEU	C-O	-6.40	1.16	1.24
1	E	267	GLN	C-O	-6.40	1.16	1.24
1	A	96	VAL	CA-CB	-6.39	1.47	1.54
1	D	350	MET	CG-SD	-6.39	1.64	1.80
1	C	205	PRO	C-O	-6.39	1.16	1.23
1	D	283	MET	C-O	-6.39	1.16	1.24
1	F	183	LEU	C-O	-6.37	1.16	1.24
1	F	228	ARG	NE-CZ	6.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	TYR	C-O	-6.37	1.16	1.23
1	C	201	THR	C-O	-6.37	1.16	1.24
1	C	390	ASP	C-O	-6.37	1.16	1.24
1	C	148	ALA	C-O	-6.36	1.15	1.24
1	A	381	ALA	C-O	-6.36	1.16	1.24
1	B	352	HIS	CA-C	6.35	1.61	1.52
1	B	147	ALA	C-O	-6.34	1.15	1.24
1	B	276	LEU	C-O	-6.33	1.16	1.23
1	E	283	MET	CG-SD	-6.33	1.65	1.80
1	C	315	ASP	CB-CG	6.32	1.67	1.52
1	E	88	VAL	CA-CB	6.32	1.64	1.55
1	F	127	ALA	C-O	-6.31	1.16	1.23
1	F	320	ALA	CA-CB	-6.31	1.43	1.53
1	B	306	PHE	CA-C	-6.30	1.46	1.53
1	F	189	THR	CA-CB	-6.29	1.44	1.53
1	F	325	ASN	C-O	-6.29	1.16	1.23
1	C	146	THR	C-O	-6.28	1.16	1.24
1	E	143	GLY	C-O	-6.28	1.15	1.23
1	F	269	MET	SD-CE	-6.27	1.63	1.79
1	D	91	ILE	CA-CB	-6.27	1.46	1.54
1	E	319	VAL	CA-CB	6.27	1.62	1.54
1	E	321	VAL	CA-CB	-6.26	1.46	1.54
1	A	360	PHE	CD2-CE2	-6.26	1.19	1.38
1	A	135	GLU	C-O	-6.26	1.16	1.24
1	A	254	ASN	C-O	-6.26	1.16	1.23
1	A	100	ARG	C-O	-6.24	1.16	1.24
1	F	324	THR	CA-C	-6.24	1.45	1.52
1	B	110	VAL	CA-CB	-6.24	1.47	1.54
1	D	195	CYS	C-O	-6.23	1.16	1.24
1	B	319	VAL	CA-CB	6.22	1.62	1.54
1	C	142	MET	SD-CE	6.22	1.95	1.79
1	F	149	ASP	C-O	-6.22	1.16	1.24
1	B	321	VAL	C-O	-6.21	1.17	1.24
1	D	279	VAL	CA-C	-6.21	1.45	1.52
1	D	286	TYR	C-O	-6.20	1.16	1.24
1	A	183	LEU	C-O	-6.20	1.17	1.24
1	A	268	MET	C-O	-6.20	1.17	1.24
1	C	276	LEU	C-O	-6.19	1.16	1.23
1	A	115	ARG	CA-C	-6.18	1.45	1.52
1	A	231	SER	C-O	-6.17	1.16	1.24
1	C	275	SER	CA-C	6.16	1.60	1.52
1	A	215	CYS	CA-CB	-6.15	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	373	VAL	C-O	-6.15	1.16	1.23
1	D	228	ARG	NE-CZ	6.15	1.39	1.33
1	B	385	PHE	CA-C	-6.15	1.45	1.52
1	B	355	THR	CA-CB	-6.14	1.43	1.53
1	D	196	HIS	C-O	-6.14	1.16	1.24
1	B	93	MET	SD-CE	6.13	1.94	1.79
1	E	107	ALA	CA-C	-6.13	1.44	1.52
1	A	371	LYS	N-CA	-6.13	1.38	1.45
1	B	194	LEU	C-O	-6.12	1.17	1.24
1	B	220	THR	CA-C	-6.12	1.45	1.53
1	E	181	THR	CA-CB	6.11	1.63	1.53
1	F	304	ALA	C-O	-6.11	1.17	1.24
1	C	229	LEU	C-O	-6.10	1.16	1.24
1	D	85	LYS	C-O	-6.10	1.16	1.24
1	A	131	LYS	N-CA	6.10	1.53	1.46
1	B	205	PRO	C-O	-6.10	1.16	1.23
1	E	191	LYS	C-O	-6.10	1.17	1.23
1	A	268	MET	CA-C	-6.10	1.45	1.53
1	D	268	MET	CG-SD	6.09	1.96	1.80
1	D	136	ALA	C-O	-6.09	1.17	1.24
1	D	276	LEU	CA-C	6.09	1.60	1.52
1	D	110	VAL	N-CA	-6.08	1.39	1.46
1	D	160	LEU	CA-C	-6.07	1.44	1.53
1	D	265	ALA	C-O	-6.07	1.16	1.24
1	A	308	ARG	CB-CG	6.07	1.70	1.52
1	F	383	CYS	C-O	-6.07	1.16	1.23
1	F	107	ALA	N-CA	-6.06	1.38	1.46
1	E	100	ARG	CG-CD	6.06	1.70	1.52
1	F	299	ARG	CA-C	-6.05	1.45	1.52
1	B	147	ALA	CA-CB	-6.05	1.43	1.53
1	D	385	PHE	C-O	-6.04	1.17	1.24
1	F	277	ILE	C-O	-6.04	1.17	1.24
1	E	184	PHE	C-O	-6.03	1.16	1.23
1	F	311	GLN	C-O	-6.02	1.17	1.24
1	F	265	ALA	CA-C	-6.02	1.44	1.52
1	D	254	ASN	CA-C	-6.02	1.45	1.52
1	F	158	ILE	C-O	-6.01	1.16	1.24
1	C	150	PHE	CA-C	-6.01	1.45	1.52
1	C	142	MET	CA-C	-6.00	1.45	1.52
1	E	361	LYS	CA-C	-6.00	1.45	1.52
1	C	191	LYS	C-O	-6.00	1.19	1.23
1	E	298	ALA	C-O	-5.99	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ALA	C-O	-5.99	1.16	1.24
1	E	163	GLY	C-O	-5.99	1.16	1.24
1	A	279	VAL	CA-CB	-5.99	1.46	1.54
1	C	155	SER	N-CA	5.98	1.53	1.46
1	B	130	ASP	CA-C	5.98	1.61	1.52
1	B	349	ILE	CA-CB	5.98	1.62	1.54
1	A	303	LEU	C-N	-5.97	1.26	1.33
1	C	226	PRO	C-O	-5.97	1.16	1.24
1	D	280	ASP	CA-C	5.97	1.59	1.52
1	B	154	ARG	C-O	-5.96	1.17	1.24
1	F	109	ALA	C-O	-5.96	1.16	1.24
1	D	277	ILE	CA-C	-5.95	1.45	1.52
1	C	229	LEU	CA-C	-5.95	1.44	1.52
1	F	233	ALA	CA-CB	-5.94	1.44	1.53
1	F	306	PHE	CE1-CZ	-5.93	1.20	1.38
1	F	139	LEU	C-O	-5.92	1.16	1.24
1	B	384	VAL	CA-CB	-5.91	1.47	1.54
1	E	355	THR	CA-C	-5.90	1.44	1.52
1	A	160	LEU	CA-C	-5.90	1.45	1.53
1	F	355	THR	CA-CB	5.89	1.62	1.53
1	E	226	PRO	CA-C	-5.88	1.44	1.52
1	E	263	ASP	C-O	-5.88	1.17	1.24
1	D	298	ALA	CA-CB	5.87	1.63	1.53
1	F	194	LEU	C-O	-5.86	1.17	1.24
1	D	305	LYS	C-O	-5.86	1.16	1.24
1	D	351	ALA	CA-CB	-5.86	1.44	1.53
1	F	224	PHE	CA-CB	-5.85	1.45	1.53
1	B	265	ALA	CA-C	-5.85	1.44	1.52
1	C	297	SER	CA-C	5.85	1.60	1.52
1	C	354	SER	C-O	-5.85	1.16	1.23
1	A	386	ALA	C-O	-5.84	1.17	1.23
1	E	264	ALA	C-O	-5.84	1.16	1.24
1	A	248	ALA	CA-CB	-5.83	1.45	1.53
1	F	200	VAL	CB-CG1	-5.83	1.33	1.52
1	D	114	PRO	CA-CB	-5.82	1.45	1.53
1	C	158	ILE	CA-CB	5.82	1.61	1.54
1	D	311	GLN	CA-C	-5.82	1.45	1.52
1	E	196	HIS	C-O	-5.81	1.16	1.24
1	E	263	ASP	CA-C	-5.80	1.45	1.52
1	D	317	PHE	CG-CD1	-5.80	1.26	1.38
1	E	124	ILE	CA-CB	-5.80	1.47	1.53
1	A	287	ARG	CA-C	5.79	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	376	PRO	C-O	-5.79	1.16	1.24
1	A	380	GLU	CA-C	-5.79	1.45	1.52
1	F	104	LEU	CA-C	5.78	1.59	1.52
1	C	325	ASN	CA-C	-5.77	1.45	1.52
1	D	247	VAL	CA-C	-5.77	1.45	1.52
1	E	265	ALA	CA-CB	-5.77	1.44	1.53
1	A	114	PRO	CA-C	-5.77	1.45	1.52
1	D	107	ALA	CA-C	-5.77	1.44	1.52
1	A	324	THR	CB-CG2	-5.76	1.33	1.52
1	B	309	ALA	CA-CB	-5.76	1.44	1.53
1	C	277	ILE	C-O	-5.75	1.18	1.24
1	E	92	THR	CA-C	-5.75	1.45	1.52
1	A	311	GLN	CA-C	-5.74	1.45	1.52
1	C	160	LEU	CA-C	-5.73	1.45	1.52
1	D	310	LEU	C-N	-5.73	1.26	1.33
1	E	282	VAL	N-CA	-5.73	1.39	1.46
1	D	99	LEU	CA-C	-5.72	1.45	1.53
1	C	236	PHE	CA-C	-5.72	1.45	1.52
1	C	163	GLY	C-O	-5.71	1.18	1.24
1	A	387	ILE	CA-CB	-5.71	1.47	1.54
1	C	350	MET	CG-SD	-5.71	1.66	1.80
1	A	362	LYS	CA-C	-5.71	1.46	1.52
1	E	192	SER	CA-C	-5.71	1.45	1.52
1	A	196	HIS	C-O	-5.70	1.16	1.24
1	E	81	VAL	N-CA	-5.70	1.41	1.46
1	F	358	LEU	C-O	-5.69	1.17	1.24
1	E	114	PRO	CG-CD	-5.68	1.31	1.50
1	D	113	ALA	CA-C	-5.68	1.47	1.53
1	F	181	THR	C-O	-5.68	1.17	1.23
1	A	99	LEU	C-O	-5.68	1.16	1.24
1	B	368	ARG	CA-C	-5.68	1.45	1.52
1	E	311	GLN	CA-C	-5.67	1.45	1.52
1	F	391	GLY	C-O	-5.67	1.16	1.23
1	F	382	GLU	CA-C	-5.66	1.45	1.53
1	E	175	VAL	CA-CB	5.66	1.60	1.53
1	F	100	ARG	C-O	-5.66	1.16	1.24
1	D	139	LEU	N-CA	5.66	1.53	1.46
1	F	267	GLN	CA-C	-5.66	1.44	1.52
1	E	220	THR	CA-C	-5.65	1.45	1.52
1	F	358	LEU	C-N	-5.65	1.29	1.33
1	F	197	THR	C-O	-5.64	1.16	1.24
1	E	325	ASN	CA-C	-5.64	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	145	VAL	CA-CB	-5.64	1.48	1.55
1	E	254	ASN	C-O	-5.64	1.17	1.23
1	D	221	GLU	C-O	-5.64	1.16	1.24
1	A	258	GLN	C-O	-5.63	1.16	1.24
1	F	201	THR	N-CA	-5.63	1.39	1.46
1	D	133	LEU	C-O	-5.63	1.16	1.24
1	E	159	CYS	N-CA	5.63	1.52	1.46
1	E	219	ASP	C-O	-5.63	1.17	1.24
1	D	196	HIS	CA-C	-5.63	1.45	1.52
1	C	244	LEU	N-CA	-5.62	1.39	1.46
1	E	80	MET	C-O	-5.62	1.12	1.23
1	D	80	MET	C-N	-5.62	1.28	1.33
1	D	150	PHE	CA-C	-5.61	1.45	1.52
1	E	195	CYS	C-O	-5.61	1.17	1.24
1	E	276	LEU	CA-C	5.61	1.59	1.52
1	F	356	THR	N-CA	5.61	1.53	1.46
1	B	197	THR	C-O	-5.61	1.17	1.24
1	A	312	ARG	C-O	-5.60	1.17	1.24
1	D	316	GLN	C-O	-5.60	1.17	1.24
1	D	319	VAL	CA-CB	5.60	1.62	1.54
1	E	180	ILE	C-N	-5.60	1.26	1.33
1	A	366	CYS	N-CA	5.60	1.53	1.46
1	B	235	ARG	CA-C	-5.60	1.44	1.52
1	A	225	ARG	CA-C	5.60	1.59	1.52
1	D	216	LEU	CA-C	-5.59	1.46	1.52
1	F	143	GLY	CA-C	-5.59	1.44	1.51
1	A	129	ALA	CA-CB	-5.59	1.44	1.53
1	E	288	THR	CA-C	5.59	1.60	1.52
1	B	285	LEU	CA-C	5.59	1.60	1.52
1	F	210	GLY	C-O	-5.59	1.16	1.23
1	E	322	VAL	CA-CB	-5.59	1.47	1.54
1	D	139	LEU	CA-C	5.58	1.60	1.52
1	D	285	LEU	C-O	-5.58	1.16	1.24
1	A	249	TYR	C-O	-5.58	1.17	1.24
1	E	298	ALA	CA-C	-5.58	1.45	1.52
1	B	325	ASN	CA-C	-5.57	1.46	1.52
1	D	182	GLU	C-O	-5.57	1.17	1.24
1	F	279	VAL	CA-C	-5.57	1.45	1.52
1	C	194	LEU	C-O	-5.56	1.17	1.24
1	D	385	PHE	CA-C	-5.56	1.45	1.53
1	A	369	LEU	C-O	-5.55	1.16	1.23
1	A	145	VAL	CA-C	-5.55	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	ILE	CA-C	-5.55	1.45	1.52
1	B	180	ILE	C-O	-5.54	1.16	1.24
1	A	326	GLN	C-O	-5.54	1.17	1.24
1	D	93	MET	C-O	-5.54	1.17	1.24
1	A	88	VAL	C-O	-5.53	1.15	1.23
1	A	93	MET	C-O	-5.53	1.17	1.24
1	A	277	ILE	C-N	-5.53	1.26	1.33
1	F	369	LEU	C-O	-5.53	1.16	1.23
1	F	200	VAL	CA-CB	-5.52	1.47	1.55
1	A	255	ALA	C-O	-5.52	1.17	1.24
1	C	257	HIS	CA-C	-5.51	1.45	1.52
1	A	151	HIS	C-O	-5.51	1.17	1.24
1	F	270	SER	CA-C	-5.51	1.45	1.53
1	A	200	VAL	CA-CB	-5.50	1.47	1.55
1	F	96	VAL	CA-C	-5.49	1.46	1.52
1	E	102	SER	C-O	-5.49	1.17	1.24
1	A	360	PHE	C-O	-5.49	1.17	1.24
1	F	87	GLN	C-O	-5.48	1.17	1.23
1	B	162	THR	C-O	-5.47	1.16	1.24
1	A	269	MET	SD-CE	-5.47	1.65	1.79
1	A	201	THR	C-O	-5.47	1.17	1.24
1	F	393	GLY	C-O	-5.46	1.17	1.24
1	A	358	LEU	C-N	-5.46	1.29	1.33
1	E	150	PHE	CA-C	-5.46	1.45	1.52
1	F	360	PHE	CD2-CE2	-5.46	1.22	1.38
1	E	196	HIS	CA-C	-5.45	1.45	1.52
1	C	215	CYS	CA-C	5.45	1.59	1.52
1	E	136	ALA	C-O	-5.45	1.17	1.24
1	C	248	ALA	CA-C	-5.44	1.46	1.52
1	B	321	VAL	N-CA	-5.44	1.39	1.46
1	C	306	PHE	CA-C	-5.44	1.47	1.53
1	A	372	VAL	CA-C	-5.44	1.45	1.52
1	F	118	LEU	C-O	-5.43	1.17	1.23
1	D	282	VAL	N-CA	-5.43	1.39	1.46
1	E	99	LEU	C-O	-5.43	1.17	1.23
1	A	303	LEU	CA-C	-5.43	1.45	1.52
1	C	279	VAL	N-CA	-5.43	1.40	1.46
1	D	305	LYS	CD-CE	5.42	1.68	1.52
1	E	92	THR	C-O	-5.42	1.17	1.23
1	E	277	ILE	C-O	-5.42	1.17	1.24
1	C	362	LYS	C-O	-5.41	1.17	1.24
1	D	348	ASN	CA-C	-5.41	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	PHE	CE1-CZ	-5.41	1.22	1.38
1	F	267	GLN	C-O	-5.40	1.17	1.24
1	A	149	ASP	CA-C	-5.40	1.45	1.52
1	D	384	VAL	CA-CB	-5.39	1.47	1.54
1	A	152	MET	CA-C	-5.39	1.45	1.52
1	B	322	VAL	CA-CB	-5.39	1.47	1.54
1	B	307	MET	SD-CE	-5.38	1.66	1.79
1	B	324	THR	CA-C	-5.38	1.46	1.52
1	B	307	MET	CG-SD	-5.37	1.67	1.80
1	A	221	GLU	C-O	-5.37	1.18	1.24
1	B	181	THR	C-O	-5.37	1.17	1.23
1	E	385	PHE	CA-C	-5.36	1.46	1.52
1	F	355	THR	CA-C	-5.35	1.45	1.52
1	E	142	MET	CA-C	-5.35	1.44	1.52
1	E	164	SER	N-CA	-5.35	1.40	1.46
1	F	279	VAL	N-CA	-5.34	1.39	1.46
1	B	153	ARG	N-CA	5.34	1.53	1.46
1	E	268	MET	C-O	-5.34	1.17	1.23
1	C	197	THR	CA-CB	-5.34	1.44	1.53
1	F	286	TYR	CZ-OH	5.34	1.49	1.38
1	A	306	PHE	CE1-CZ	-5.33	1.22	1.38
1	A	146	THR	CB-CG2	5.33	1.70	1.52
1	F	392	VAL	CA-CB	-5.33	1.48	1.54
1	A	265	ALA	CA-C	-5.33	1.45	1.52
1	C	173	GLY	CA-C	5.33	1.57	1.52
1	A	227	VAL	C-O	-5.32	1.17	1.24
1	D	100	ARG	CG-CD	5.32	1.68	1.52
1	A	278	VAL	CB-CG2	-5.32	1.35	1.52
1	F	354	SER	C-O	-5.32	1.17	1.23
1	B	146	THR	CA-C	-5.31	1.45	1.53
1	A	100	ARG	CA-C	-5.31	1.45	1.52
1	B	274	PHE	N-CA	5.31	1.52	1.45
1	C	141	PRO	C-O	-5.31	1.17	1.24
1	F	250	ALA	CA-C	-5.30	1.46	1.52
1	E	93	MET	C-O	-5.29	1.17	1.24
1	E	230	VAL	C-O	-5.29	1.17	1.24
1	B	142	MET	CA-C	-5.29	1.46	1.52
1	D	164	SER	N-CA	-5.29	1.40	1.46
1	F	217	TYR	C-O	-5.29	1.18	1.24
1	F	145	VAL	CA-C	-5.29	1.45	1.52
1	C	109	ALA	CA-CB	-5.29	1.45	1.53
1	A	324	THR	CA-CB	-5.28	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	296	LEU	N-CA	5.28	1.52	1.46
1	B	91	ILE	CA-CB	5.27	1.61	1.54
1	D	284	ALA	C-N	-5.26	1.26	1.33
1	D	359	GLY	C-O	-5.26	1.16	1.23
1	F	146	THR	CA-C	-5.25	1.46	1.53
1	D	387	ILE	C-O	-5.25	1.18	1.24
1	A	165	LYS	CA-C	-5.25	1.45	1.52
1	B	146	THR	C-O	-5.25	1.15	1.23
1	E	321	VAL	C-O	-5.25	1.18	1.24
1	A	302	HIS	CA-C	-5.25	1.46	1.52
1	F	100	ARG	CA-C	-5.25	1.45	1.52
1	D	355	THR	CA-C	-5.24	1.45	1.52
1	F	234	GLN	C-N	-5.24	1.26	1.33
1	A	107	ALA	CA-CB	-5.24	1.45	1.53
1	F	269	MET	C-O	-5.23	1.17	1.24
1	D	226	PRO	C-O	-5.23	1.17	1.24
1	F	368	ARG	C-O	-5.23	1.17	1.24
1	E	234	GLN	C-O	-5.23	1.17	1.24
1	E	358	LEU	CA-C	-5.23	1.46	1.52
1	C	385	PHE	CA-C	-5.23	1.46	1.52
1	E	247	VAL	C-O	-5.23	1.18	1.24
1	F	88	VAL	C-O	-5.22	1.17	1.24
1	A	83	ILE	CA-C	-5.21	1.45	1.52
1	E	145	VAL	CB-CG2	-5.20	1.35	1.52
1	E	200	VAL	CA-CB	-5.20	1.47	1.55
1	E	88	VAL	C-O	-5.20	1.17	1.23
1	A	306	PHE	CA-C	-5.20	1.48	1.53
1	B	180	ILE	CA-CB	-5.20	1.48	1.54
1	C	217	TYR	CG-CD1	-5.19	1.28	1.39
1	B	208	ILE	C-O	-5.19	1.17	1.24
1	E	133	LEU	C-O	-5.19	1.17	1.24
1	D	285	LEU	N-CA	-5.19	1.39	1.46
1	A	102	SER	C-O	-5.18	1.17	1.24
1	E	232	ILE	C-O	-5.18	1.18	1.24
1	C	296	LEU	N-CA	5.18	1.52	1.46
1	E	306	PHE	CE1-CZ	-5.18	1.23	1.38
1	E	81	VAL	C-O	-5.18	1.18	1.24
1	F	165	LYS	C-O	-5.17	1.18	1.24
1	C	265	ALA	CA-C	-5.17	1.45	1.52
1	C	146	THR	CA-CB	5.17	1.62	1.53
1	B	189	THR	CA-CB	-5.16	1.46	1.53
1	E	260	ARG	C-N	-5.16	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	SER	C-O	-5.16	1.18	1.24
1	A	387	ILE	C-O	-5.16	1.18	1.24
1	D	319	VAL	CA-C	5.16	1.59	1.52
1	B	214	LYS	C-O	-5.16	1.17	1.24
1	C	230	VAL	CA-C	-5.16	1.46	1.52
1	D	219	ASP	CA-C	-5.16	1.46	1.52
1	F	129	ALA	C-O	-5.15	1.18	1.24
1	C	221	GLU	C-O	-5.15	1.17	1.24
1	F	359	GLY	N-CA	-5.15	1.38	1.45
1	D	234	GLN	C-O	-5.14	1.18	1.24
1	D	307	MET	SD-CE	-5.14	1.66	1.79
1	F	304	ALA	N-CA	-5.13	1.40	1.46
1	A	359	GLY	N-CA	-5.13	1.38	1.45
1	C	326	GLN	CA-C	-5.13	1.46	1.52
1	F	289	ASP	CA-C	5.13	1.63	1.52
1	E	180	ILE	CA-CB	-5.13	1.48	1.54
1	A	306	PHE	C-N	-5.13	1.26	1.33
1	B	312	ARG	CA-C	-5.13	1.45	1.52
1	F	378	LEU	N-CA	5.13	1.53	1.46
1	D	144	PHE	CG-CD1	-5.12	1.28	1.38
1	D	181	THR	CA-CB	5.12	1.61	1.53
1	E	257	HIS	CA-C	5.12	1.59	1.52
1	F	248	ALA	CA-CB	-5.12	1.46	1.53
1	C	147	ALA	CA-C	-5.12	1.45	1.52
1	D	227	VAL	C-O	-5.12	1.18	1.24
1	B	391	GLY	CA-C	-5.11	1.46	1.52
1	D	215	CYS	C-O	-5.10	1.18	1.23
1	C	220	THR	CA-C	-5.10	1.46	1.53
1	D	119	LEU	C-O	5.10	1.30	1.24
1	E	283	MET	C-O	-5.10	1.17	1.24
1	C	93	MET	SD-CE	5.10	1.92	1.79
1	A	121	ILE	CA-C	-5.09	1.47	1.52
1	A	251	ARG	CA-CB	-5.09	1.46	1.53
1	F	326	GLN	CG-CD	5.09	1.64	1.52
1	F	218	ILE	C-O	-5.09	1.18	1.24
1	F	308	ARG	NE-CZ	5.09	1.38	1.33
1	D	224	PHE	CA-C	-5.08	1.46	1.52
1	C	231	SER	CA-C	-5.08	1.46	1.52
1	B	191	LYS	CA-C	-5.08	1.48	1.53
1	F	255	ALA	C-N	-5.07	1.26	1.33
1	C	247	VAL	C-O	-5.07	1.18	1.24
1	A	157	LEU	CA-CB	5.07	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	ARG	CA-C	5.07	1.59	1.52
1	C	130	ASP	CA-C	5.07	1.59	1.52
1	C	384	VAL	CA-CB	-5.07	1.48	1.54
1	B	238	LEU	C-O	-5.06	1.17	1.23
1	F	302	HIS	CA-C	-5.06	1.46	1.52
1	A	200	VAL	C-O	-5.06	1.17	1.24
1	A	356	THR	C-O	-5.06	1.18	1.24
1	E	254	ASN	CA-C	-5.06	1.46	1.52
1	E	391	GLY	C-O	-5.05	1.18	1.24
1	F	249	TYR	CA-CB	-5.05	1.46	1.53
1	A	85	LYS	C-O	-5.05	1.17	1.24
1	E	319	VAL	CA-C	5.05	1.59	1.52
1	D	317	PHE	CE2-CZ	-5.05	1.23	1.38
1	F	164	SER	C-O	-5.05	1.18	1.24
1	C	251	ARG	N-CA	-5.04	1.40	1.46
1	B	283	MET	CA-C	5.04	1.59	1.52
1	A	97	LYS	C-O	-5.04	1.18	1.24
1	D	268	MET	C-O	-5.04	1.17	1.23
1	F	208	ILE	C-O	-5.04	1.17	1.24
1	B	227	VAL	C-O	-5.04	1.18	1.24
1	F	253	TYR	C-O	-5.04	1.17	1.24
1	A	187	PHE	CD2-CE2	5.03	1.53	1.38
1	C	256	ASP	CB-CG	5.03	1.64	1.52
1	B	191	LYS	C-O	-5.03	1.19	1.23
1	A	388	TYR	C-O	-5.02	1.17	1.24
1	E	305	LYS	C-O	-5.02	1.17	1.24
1	A	228	ARG	NE-CZ	5.02	1.38	1.33
1	E	200	VAL	N-CA	-5.02	1.41	1.46
1	B	95	ASP	CA-C	5.02	1.59	1.52
1	A	253	TYR	CZ-OH	5.01	1.48	1.38
1	A	205	PRO	C-O	-5.01	1.16	1.23
1	D	225	ARG	CD-NE	-5.01	1.39	1.46
1	B	248	ALA	C-O	-5.01	1.17	1.24
1	F	276	LEU	C-O	-5.01	1.17	1.23
1	F	280	ASP	CA-CB	-5.00	1.45	1.53

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	ARG	N-CA-C	-12.68	97.45	111.14
1	E	115	ARG	N-CA-C	-11.83	98.36	111.14
1	A	95	ASP	N-CA-C	-11.80	98.40	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	359	GLY	O-C-N	-10.92	115.20	123.61
1	F	115	ARG	N-CA-C	-10.89	99.38	111.14
1	F	95	ASP	N-CA-C	-10.15	100.17	111.14
1	D	95	ASP	N-CA-C	-10.11	99.80	111.03
1	D	146	THR	N-CA-C	-10.05	97.26	110.43
1	E	95	ASP	N-CA-C	-9.70	100.66	111.14
1	F	285	LEU	N-CA-C	-9.04	101.35	112.38
1	A	221	GLU	N-CA-C	8.98	120.76	110.97
1	E	288	THR	N-CA-C	8.95	121.85	111.11
1	F	359	GLY	CA-C-O	8.83	128.59	120.91
1	C	279	VAL	N-CA-C	-8.79	95.81	108.11
1	C	200	VAL	CB-CA-C	-8.73	103.28	111.05
1	F	266	ALA	N-CA-C	-8.70	102.25	113.12
1	E	146	THR	N-CA-C	-8.67	99.07	110.43
1	E	284	ALA	N-CA-C	8.40	128.70	110.80
1	A	359	GLY	O-C-N	-8.38	117.15	123.61
1	F	151	HIS	N-CA-C	8.20	123.00	112.34
1	C	266	ALA	N-CA-C	-8.12	102.97	113.12
1	B	102	SER	N-CA-C	-8.11	103.91	113.88
1	A	115	ARG	N-CA-C	-8.11	102.39	111.14
1	A	146	THR	N-CA-C	-8.04	100.15	110.53
1	F	146	THR	N-CA-C	-7.89	100.70	110.41
1	F	267	GLN	N-CA-C	-7.70	101.89	111.75
1	B	267	GLN	N-CA-C	-7.70	101.90	111.75
1	E	96	VAL	CB-CA-C	-7.69	101.86	111.70
1	D	376	PRO	N-CD-CG	-7.61	91.79	103.20
1	B	367	GLN	N-CA-C	-7.60	101.06	110.41
1	F	375	SER	CA-C-N	7.56	129.29	119.84
1	F	375	SER	C-N-CA	7.56	129.29	119.84
1	D	279	VAL	N-CA-C	-7.54	97.61	108.17
1	A	308	ARG	N-CA-C	-7.52	102.68	111.03
1	B	279	VAL	CB-CA-C	-7.48	99.56	110.63
1	B	324	THR	CB-CA-C	-7.39	97.01	109.50
1	B	247	VAL	CB-CA-C	-7.38	99.19	111.29
1	F	384	VAL	CB-CA-C	-7.33	99.14	110.95
1	A	200	VAL	CB-CA-C	-7.32	104.54	111.05
1	A	266	ALA	N-CA-C	-7.28	104.02	113.12
1	F	353	SER	N-CA-C	7.27	121.98	113.18
1	F	221	GLU	N-CA-C	7.16	118.78	110.97
1	D	284	ALA	N-CA-C	7.15	126.02	110.80
1	E	384	VAL	CB-CA-C	-7.14	101.78	111.63
1	F	376	PRO	N-CD-CG	-7.09	92.56	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	LEU	N-CA-C	7.05	118.75	111.14
1	B	393	GLY	N-CA-C	7.00	122.04	110.55
1	F	378	LEU	N-CA-C	6.98	125.23	109.81
1	B	279	VAL	N-CA-C	-6.97	98.35	108.11
1	C	276	LEU	N-CA-C	6.90	119.66	108.76
1	A	191	LYS	N-CA-C	-6.86	101.06	111.56
1	E	205	PRO	N-CA-C	6.86	122.06	110.95
1	E	376	PRO	N-CD-CG	-6.85	92.93	103.20
1	D	185	GLY	CA-C-O	-6.82	114.79	121.75
1	C	152	MET	N-CA-C	-6.81	96.29	110.80
1	F	186	GLU	N-CA-CB	6.73	120.07	110.44
1	F	308	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	C	267	GLN	N-CA-C	-6.71	103.16	111.75
1	E	279	VAL	N-CA-C	-6.65	98.86	108.17
1	A	145	VAL	CB-CA-C	-6.62	105.51	111.74
1	A	384	VAL	CB-CA-C	-6.59	100.33	110.95
1	F	191	LYS	N-CA-C	-6.58	101.49	111.56
1	F	319	VAL	CB-CA-C	-6.56	100.53	111.29
1	C	223	THR	CB-CA-C	-6.56	100.90	111.06
1	A	208	ILE	CB-CA-C	-6.50	103.25	112.22
1	A	183	LEU	CB-CA-C	-6.49	100.29	110.74
1	E	276	LEU	N-CA-C	6.49	119.06	108.55
1	C	257	HIS	CB-CA-C	-6.48	97.52	110.42
1	F	276	LEU	N-CA-C	6.48	119.00	108.76
1	A	276	LEU	N-CA-C	6.47	119.02	108.55
1	C	363	GLY	N-CA-C	-6.46	102.72	112.60
1	C	205	PRO	N-CA-C	6.43	120.93	111.03
1	D	96	VAL	CB-CA-C	-6.42	103.49	111.70
1	F	183	LEU	CB-CA-C	-6.42	100.41	110.74
1	F	357	ARG	CA-C-O	6.42	127.51	120.71
1	C	102	SER	N-CA-C	-6.33	105.69	113.41
1	D	267	GLN	N-CA-C	-6.29	103.70	111.75
1	A	386	ALA	N-CA-C	6.27	117.75	108.60
1	B	266	ALA	N-CA-C	-6.27	103.74	112.45
1	D	316	GLN	N-CA-C	6.24	118.88	111.33
1	D	348	ASN	N-CA-C	-6.22	103.09	112.04
1	C	215	CYS	N-CA-C	6.20	119.64	108.48
1	E	102	SER	CB-CA-C	-6.17	98.46	110.11
1	F	260	ARG	N-CA-C	-6.15	104.58	111.28
1	C	208	ILE	CB-CA-C	-6.15	104.00	112.24
1	B	353	SER	N-CA-C	6.13	118.05	111.36
1	E	232	ILE	CB-CA-C	-6.13	104.00	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	324	THR	CB-CA-C	-6.12	99.17	109.50
1	B	223	THR	CB-CA-C	-6.05	101.68	111.06
1	B	276	LEU	N-CA-C	6.05	118.31	108.76
1	A	324	THR	CB-CA-C	-6.04	99.29	109.50
1	F	355	THR	N-CA-C	-6.03	106.05	113.41
1	D	113	ALA	CA-C-N	6.03	126.37	119.92
1	D	113	ALA	C-N-CA	6.03	126.37	119.92
1	C	384	VAL	N-CA-C	6.02	116.59	108.17
1	A	160	LEU	N-CA-C	-6.00	102.61	110.53
1	C	161	THR	OG1-CB-CG2	-5.99	97.32	109.30
1	C	155	SER	N-CA-C	5.97	117.78	111.28
1	D	215	CYS	N-CA-C	5.96	119.22	108.48
1	B	152	MET	N-CA-C	-5.96	98.10	110.80
1	C	177	THR	OG1-CB-CG2	-5.95	97.40	109.30
1	E	141	PRO	CA-C-O	-5.94	114.84	121.32
1	D	141	PRO	CA-C-O	-5.93	114.88	121.23
1	D	160	LEU	N-CA-C	-5.93	102.54	110.55
1	E	353	SER	CA-C-N	-5.89	114.69	123.00
1	E	353	SER	C-N-CA	-5.89	114.69	123.00
1	A	147	ALA	CA-C-O	-5.88	114.84	120.90
1	A	375	SER	CA-C-N	5.85	127.16	119.84
1	A	375	SER	C-N-CA	5.85	127.16	119.84
1	E	151	HIS	N-CA-C	5.84	123.23	110.80
1	A	359	GLY	CA-C-O	5.83	125.98	120.91
1	A	173	GLY	CA-C-O	5.82	124.78	119.83
1	B	279	VAL	O-C-N	5.80	129.52	123.26
1	F	173	GLY	CA-C-O	5.80	124.76	119.83
1	B	317	PHE	CA-C-O	5.79	125.35	118.69
1	D	266	ALA	N-CA-C	-5.79	105.89	113.12
1	D	151	HIS	N-CA-C	5.78	123.12	110.80
1	C	270	SER	N-CA-C	-5.77	102.74	111.56
1	B	210	GLY	N-CA-C	5.76	122.99	112.27
1	B	205	PRO	N-CA-C	5.74	119.86	111.03
1	F	352	HIS	N-CA-CB	5.72	118.26	109.91
1	A	378	LEU	N-CA-C	5.71	122.44	109.81
1	F	308	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	80	MET	CG-SD-CE	5.70	113.44	100.90
1	A	357	ARG	CG-CD-NE	-5.68	99.50	112.00
1	F	215	CYS	N-CA-C	5.68	118.71	108.48
1	A	100	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	D	322	VAL	CA-C-O	5.67	126.00	120.27
1	F	152	MET	N-CA-C	-5.67	98.71	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	208	ILE	CB-CA-C	-5.67	104.64	112.24
1	C	247	VAL	N-CA-C	5.65	116.20	107.78
1	C	279	VAL	O-C-N	5.64	129.35	123.26
1	D	225	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	F	200	VAL	CB-CA-C	-5.62	106.04	111.05
1	A	360	PHE	N-CA-C	5.61	118.55	109.40
1	C	107	ALA	CA-C-N	5.61	128.11	120.54
1	C	107	ALA	C-N-CA	5.61	128.11	120.54
1	E	110	VAL	CB-CA-C	-5.57	104.57	111.70
1	E	384	VAL	N-CA-C	5.55	117.21	109.55
1	A	357	ARG	CA-C-O	5.55	126.59	120.71
1	C	230	VAL	CB-CA-C	-5.55	104.60	111.70
1	A	142	MET	N-CA-C	-5.54	99.00	110.80
1	A	315	ASP	CA-C-N	5.53	127.96	120.38
1	A	315	ASP	C-N-CA	5.53	127.96	120.38
1	A	267	GLN	N-CA-C	-5.53	104.67	111.75
1	E	324	THR	CB-CA-C	-5.51	100.18	109.50
1	C	100	ARG	N-CA-C	5.51	117.75	111.02
1	B	220	THR	OG1-CB-CG2	-5.51	98.28	109.30
1	C	119	LEU	N-CA-C	5.51	117.36	111.36
1	D	386	ALA	N-CA-C	5.50	116.63	108.60
1	A	210	GLY	N-CA-C	5.50	126.22	113.18
1	A	151	HIS	N-CA-C	5.48	122.48	110.80
1	A	387	ILE	N-CA-C	5.48	115.84	108.17
1	F	169	THR	CA-C-O	5.48	126.34	120.20
1	C	367	GLN	N-CA-C	-5.47	103.48	110.53
1	E	185	GLY	CA-C-O	-5.46	116.18	121.75
1	C	247	VAL	CB-CA-C	-5.46	102.70	110.12
1	C	210	GLY	N-CA-C	5.46	126.11	113.18
1	D	115	ARG	N-CA-CB	5.45	117.97	110.07
1	A	389	GLU	N-CA-C	5.43	119.16	112.54
1	C	324	THR	CB-CA-C	-5.42	100.33	109.50
1	F	247	VAL	N-CA-C	5.42	115.85	107.78
1	E	128	LYS	N-CA-CB	5.42	118.19	110.06
1	B	384	VAL	N-CA-C	5.42	116.38	108.53
1	E	266	ALA	N-CA-C	-5.41	106.36	113.12
1	E	113	ALA	CA-C-N	5.40	125.38	120.03
1	E	113	ALA	C-N-CA	5.40	125.38	120.03
1	A	173	GLY	N-CA-C	5.39	119.35	113.58
1	A	356	THR	O-C-N	-5.39	116.97	123.27
1	C	244	LEU	O-C-N	-5.37	116.54	122.07
1	D	142	MET	N-CA-C	-5.37	99.69	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	247	VAL	CB-CA-C	-5.37	102.49	111.29
1	E	208	ILE	CB-CA-C	-5.36	105.06	112.24
1	F	82	PRO	CA-C-O	-5.36	115.34	121.56
1	B	225	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	C	317	PHE	CA-C-O	5.36	124.85	118.69
1	B	299	ARG	N-CA-C	-5.35	104.49	111.02
1	D	208	ILE	CB-CA-C	-5.35	105.07	112.24
1	F	159	CYS	CB-CA-C	-5.35	103.64	111.23
1	B	215	CYS	N-CA-C	5.32	118.05	108.48
1	C	301	MET	N-CA-C	-5.31	105.62	112.68
1	D	223	THR	CA-C-N	-5.31	115.94	122.84
1	D	223	THR	C-N-CA	-5.31	115.94	122.84
1	F	280	ASP	CB-CA-C	-5.31	102.87	110.62
1	D	99	LEU	CB-CA-C	-5.31	100.84	110.56
1	E	146	THR	N-CA-CB	5.31	117.85	110.26
1	F	308	ARG	N-CA-C	-5.28	105.17	111.03
1	F	359	GLY	N-CA-C	5.28	120.14	110.95
1	A	205	PRO	N-CA-C	5.27	119.85	111.26
1	C	393	GLY	N-CA-C	5.27	118.83	111.19
1	C	140	VAL	CA-C-O	5.26	123.25	119.25
1	B	285	LEU	N-CA-C	-5.26	106.70	113.01
1	D	296	LEU	N-CA-CB	5.24	119.34	110.49
1	F	315	ASP	CA-C-N	5.23	127.55	120.38
1	F	315	ASP	C-N-CA	5.23	127.55	120.38
1	A	162	THR	OG1-CB-CG2	-5.23	98.84	109.30
1	E	348	ASN	N-CA-C	-5.23	105.02	111.40
1	B	161	THR	OG1-CB-CG2	-5.22	98.85	109.30
1	F	249	TYR	N-CA-C	5.22	117.75	109.24
1	F	387	ILE	N-CA-C	5.21	115.47	108.17
1	B	100	ARG	N-CA-C	5.21	117.38	111.02
1	A	280	ASP	CB-CA-C	-5.21	103.02	110.62
1	D	159	CYS	N-CA-C	5.20	117.27	108.02
1	A	321	VAL	CA-C-O	5.19	126.25	120.59
1	A	138	ARG	N-CA-C	-5.19	105.69	112.23
1	D	146	THR	N-CA-CB	5.19	117.68	110.26
1	B	369	LEU	N-CA-C	5.18	117.26	109.23
1	B	230	VAL	CB-CA-C	-5.18	105.07	111.70
1	E	322	VAL	CB-CA-C	-5.17	103.44	110.42
1	F	376	PRO	N-CA-C	5.17	123.12	112.47
1	A	141	PRO	N-CA-C	-5.17	101.83	112.47
1	B	200	VAL	O-C-N	-5.17	118.00	121.98
1	C	279	VAL	CB-CA-C	-5.16	102.99	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	232	ILE	CB-CA-C	-5.16	105.16	111.92
1	A	353	SER	N-CA-C	5.16	119.43	113.18
1	B	208	ILE	CB-CA-C	-5.16	105.33	112.24
1	C	151	HIS	N-CA-C	5.16	118.67	112.38
1	E	359	GLY	O-C-N	-5.16	120.10	123.35
1	F	386	ALA	N-CA-C	5.15	116.12	108.60
1	F	239	ASP	N-CA-CB	5.15	119.54	110.37
1	A	201	THR	CA-CB-OG1	5.15	117.32	109.60
1	A	249	TYR	N-CA-C	5.15	117.63	109.24
1	B	177	THR	OG1-CB-CG2	-5.13	99.03	109.30
1	A	220	THR	N-CA-CB	5.12	118.25	110.42
1	D	384	VAL	CB-CA-C	-5.12	104.05	111.68
1	E	322	VAL	CA-C-O	5.11	125.44	120.27
1	B	273	ARG	CB-CA-C	-5.11	102.61	110.78
1	F	321	VAL	CA-C-O	5.09	126.02	120.57
1	C	260	ARG	N-CA-C	-5.09	105.23	111.75
1	E	112	TYR	N-CA-C	5.09	116.91	111.36
1	A	164	SER	N-CA-C	5.08	117.07	108.02
1	F	220	THR	N-CA-CB	5.08	117.82	110.26
1	D	261	LEU	N-CA-C	5.07	116.50	110.97
1	C	217	TYR	CB-CA-C	-5.06	102.97	110.62
1	B	107	ALA	N-CA-C	-5.06	105.04	111.11
1	B	151	HIS	N-CA-C	5.05	118.55	112.38
1	E	386	ALA	N-CA-C	5.05	116.48	108.96
1	E	261	LEU	N-CA-C	5.05	116.47	110.97
1	F	140	VAL	CB-CA-C	-5.04	102.18	111.36
1	B	107	ALA	O-C-N	5.04	127.33	122.09
1	B	370	CYS	CA-CB-SG	-5.03	102.82	114.40
1	E	285	LEU	N-CA-C	-5.03	106.65	112.89
1	B	384	VAL	CB-CA-C	-5.02	103.18	110.81
1	F	317	PHE	CA-C-O	5.02	124.70	119.03
1	C	282	VAL	O-C-N	5.02	126.81	121.89
1	C	220	THR	OG1-CB-CG2	-5.01	99.28	109.30
1	E	304	ALA	CA-C-O	5.01	126.88	121.02
1	F	138	ARG	N-CA-C	-5.00	106.35	112.90

There are no chirality outliers.

There are no planarity outliers.

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	2148	0	2095	162	0
1	B	1985	0	1931	177	0
1	C	1995	0	1944	171	0
1	D	2143	0	2094	158	0
1	E	2147	0	2095	150	1
1	F	2135	0	2075	180	1
2	A	5	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
2	E	5	0	0	2	0
2	F	5	0	0	0	0
All	All	12583	0	12234	970	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 39.

All (970) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:VAL:CB	1:B:227:VAL:CG2	1.75	1.62
1:F:308:ARG:CD	1:F:308:ARG:CG	1.84	1.55
1:A:308:ARG:CD	1:A:308:ARG:CG	1.76	1.52
1:A:93:MET:CE	1:A:93:MET:SD	2.02	1.45
1:F:93:MET:CE	1:F:93:MET:SD	2.05	1.44
1:E:80:MET:SD	1:E:80:MET:CE	2.06	1.42
1:C:283:MET:SD	1:C:283:MET:CE	2.09	1.40
1:D:283:MET:SD	1:D:283:MET:CE	2.16	1.33
1:E:283:MET:HE1	1:E:303:LEU:HD22	1.22	1.17
1:C:158:ILE:O	1:C:177:THR:HG23	1.49	1.12
1:A:230:VAL:HG23	1:A:231:SER:H	1.18	1.08
1:A:230:VAL:HG23	1:A:231:SER:N	1.68	1.07
1:B:158:ILE:O	1:B:177:THR:HG23	1.56	1.05
1:F:230:VAL:HG23	1:F:231:SER:H	1.14	1.02
1:C:355:THR:O	1:C:356:THR:OG1	1.77	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:PHE:CE2	1:B:370:CYS:SG	2.55	0.99
1:A:327:VAL:O	1:A:328:VAL:HB	1.62	0.99
1:E:283:MET:HE1	1:E:303:LEU:CD2	1.94	0.98
1:A:230:VAL:CG2	1:A:231:SER:H	1.76	0.96
1:B:367:GLN:O	1:B:368:ARG:HG2	1.66	0.96
1:B:281:SER:OG	1:B:324:THR:O	1.83	0.95
1:F:230:VAL:CG2	1:F:231:SER:H	1.80	0.95
1:F:230:VAL:HG23	1:F:231:SER:N	1.74	0.94
1:C:367:GLN:O	1:C:368:ARG:HG2	1.69	0.93
1:C:158:ILE:O	1:C:177:THR:CG2	2.15	0.93
1:F:296:LEU:O	1:F:297:SER:C	2.09	0.93
1:C:281:SER:OG	1:C:324:THR:O	1.86	0.93
1:C:191:LYS:HB2	2:C:503:SO4:O2	1.71	0.91
1:A:296:LEU:O	1:A:297:SER:C	2.11	0.91
1:F:286:TYR:OH	1:F:346:GLY:HA2	1.70	0.91
1:B:230:VAL:HG23	1:B:231:SER:N	1.84	0.91
1:A:146:THR:HG23	1:A:149:ASP:HB2	1.52	0.90
1:C:171:LEU:HD21	1:C:358:LEU:HD11	1.52	0.90
1:B:230:VAL:HG23	1:B:231:SER:H	1.37	0.89
1:B:191:LYS:HB2	2:B:502:SO4:O3	1.73	0.88
1:D:240:PRO:O	1:D:242:ASP:N	2.06	0.88
1:C:230:VAL:HG23	1:C:231:SER:N	1.89	0.87
1:A:286:TYR:OH	1:A:346:GLY:HA2	1.75	0.86
1:F:196:HIS:O	1:F:199:ALA:HB3	1.76	0.85
1:C:159:CYS:SG	1:C:176:GLU:HA	2.16	0.85
1:A:374:ASP:O	1:A:375:SER:OG	1.94	0.85
1:E:240:PRO:O	1:E:242:ASP:N	2.10	0.84
1:A:196:HIS:O	1:A:199:ALA:HB3	1.77	0.84
1:B:355:THR:OG1	1:B:356:THR:N	1.99	0.84
1:C:193:GLN:HG3	1:C:387:ILE:HD13	1.57	0.84
1:A:80:MET:HE3	1:A:270:SER:HA	1.60	0.83
1:A:288:THR:HG23	1:D:305:LYS:NZ	1.94	0.82
1:D:177:THR:HG22	1:D:320:ALA:HB2	1.61	0.82
1:A:160:LEU:HD22	1:A:202:CYS:HA	1.61	0.81
1:C:182:GLU:OE2	1:C:350:MET:HE2	1.81	0.81
1:C:244:LEU:C	1:C:246:ASN:H	1.85	0.81
1:A:288:THR:HG23	1:D:305:LYS:HZ1	1.45	0.80
1:B:193:GLN:HG3	1:B:387:ILE:HD13	1.64	0.80
1:C:244:LEU:O	1:C:246:ASN:N	2.15	0.80
1:F:146:THR:HG23	1:F:149:ASP:HB2	1.62	0.80
1:B:244:LEU:C	1:B:246:ASN:H	1.89	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:SER:OG	1:A:128:LYS:HB2	1.82	0.79
1:B:110:VAL:O	1:B:113:ALA:HB3	1.83	0.79
1:F:348:ASN:O	1:F:349:ILE:C	2.25	0.79
1:C:355:THR:C	1:C:356:THR:HG1	1.90	0.79
1:D:238:LEU:O	1:D:240:PRO:HD3	1.84	0.78
1:B:360:PHE:CD2	1:B:370:CYS:SG	2.77	0.78
1:C:110:VAL:O	1:C:113:ALA:HB3	1.84	0.78
1:F:125:SER:OG	1:F:128:LYS:HB2	1.84	0.78
1:B:158:ILE:O	1:B:177:THR:CG2	2.31	0.78
1:B:159:CYS:SG	1:B:176:GLU:HA	2.24	0.78
1:B:240:PRO:O	1:B:242:ASP:N	2.17	0.78
1:C:240:PRO:O	1:C:242:ASP:N	2.16	0.77
1:A:141:PRO:O	1:A:142:MET:HG3	1.84	0.77
1:B:230:VAL:CG2	1:B:231:SER:H	1.98	0.76
1:D:224:PHE:C	1:D:225:ARG:HD3	2.10	0.76
1:B:184:PHE:O	1:B:359:GLY:HA2	1.84	0.76
1:C:230:VAL:HG23	1:C:231:SER:H	1.50	0.76
1:E:296:LEU:O	1:E:297:SER:C	2.26	0.76
1:F:244:LEU:C	1:F:246:ASN:H	1.94	0.76
1:A:327:VAL:O	1:A:328:VAL:CB	2.34	0.76
1:E:238:LEU:O	1:E:240:PRO:HD3	1.85	0.76
1:C:194:LEU:O	1:C:195:CYS:C	2.27	0.75
1:E:140:VAL:O	1:E:142:MET:HG2	1.86	0.75
1:F:384:VAL:HG12	1:F:385:PHE:N	2.00	0.75
1:F:175:VAL:HG11	1:F:198:LEU:HD11	1.69	0.75
1:B:201:THR:HA	1:B:204:ILE:HG12	1.68	0.74
1:A:239:ASP:O	1:A:242:ASP:HB3	1.87	0.74
1:F:374:ASP:O	1:F:375:SER:OG	2.06	0.74
1:B:230:VAL:CG2	1:B:231:SER:N	2.51	0.73
1:D:201:THR:HA	1:D:204:ILE:HG12	1.71	0.73
1:C:191:LYS:O	1:C:192:SER:C	2.31	0.72
1:F:201:THR:HA	1:F:204:ILE:HG12	1.71	0.72
1:C:158:ILE:O	1:C:177:THR:OG1	2.07	0.72
1:C:189:THR:O	1:C:368:ARG:HD2	1.90	0.71
1:F:239:ASP:O	1:F:242:ASP:HB3	1.90	0.71
1:A:110:VAL:O	1:A:113:ALA:HB3	1.90	0.71
1:B:171:LEU:HD21	1:B:358:LEU:HD11	1.72	0.71
1:C:183:LEU:O	1:C:324:THR:HA	1.91	0.71
1:C:194:LEU:C	1:C:194:LEU:HD23	2.14	0.71
1:C:99:LEU:O	1:C:102:SER:HB3	1.90	0.71
1:F:99:LEU:O	1:F:102:SER:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:LYS:O	1:E:192:SER:C	2.33	0.71
1:E:230:VAL:HG23	1:E:231:SER:N	2.05	0.70
1:B:349:ILE:O	1:B:353:SER:OG	2.09	0.70
1:D:191:LYS:O	1:D:192:SER:C	2.32	0.70
1:E:170:LEU:HD21	1:E:381:ALA:O	1.91	0.70
1:A:235:ARG:NH1	1:A:392:VAL:O	2.25	0.70
1:E:201:THR:HA	1:E:204:ILE:HG12	1.74	0.70
1:C:164:SER:OG	1:C:167:LEU:HB2	1.92	0.69
1:E:283:MET:O	1:E:285:LEU:N	2.24	0.69
1:F:177:THR:HG22	1:F:320:ALA:HB2	1.73	0.69
1:A:258:GLN:NE2	1:A:306:PHE:CZ	2.58	0.69
1:B:191:LYS:O	1:B:192:SER:C	2.31	0.69
1:B:240:PRO:C	1:B:242:ASP:H	2.00	0.69
1:D:230:VAL:HG23	1:D:231:SER:N	2.06	0.69
1:C:230:VAL:CG2	1:C:231:SER:N	2.54	0.69
1:B:164:SER:OG	1:B:167:LEU:HB2	1.92	0.69
1:D:140:VAL:O	1:D:142:MET:HG2	1.93	0.69
1:D:239:ASP:HB2	1:D:242:ASP:HB3	1.74	0.69
1:E:240:PRO:C	1:E:242:ASP:H	1.99	0.69
1:A:295:GLU:O	1:A:296:LEU:C	2.36	0.69
1:B:191:LYS:HG2	1:B:360:PHE:HD1	1.58	0.69
1:C:240:PRO:C	1:C:242:ASP:H	2.00	0.69
1:D:296:LEU:O	1:D:297:SER:C	2.36	0.68
1:E:191:LYS:N	2:E:505:SO4:O3	2.24	0.68
1:E:96:VAL:HG12	1:E:97:LYS:N	2.09	0.68
1:E:175:VAL:HG11	1:E:198:LEU:HD11	1.76	0.68
1:A:175:VAL:HG11	1:A:198:LEU:HD11	1.75	0.67
1:C:230:VAL:CG2	1:C:231:SER:H	2.06	0.67
1:C:239:ASP:HB2	1:C:242:ASP:HB3	1.77	0.67
1:F:235:ARG:NH1	1:F:392:VAL:O	2.26	0.67
1:B:194:LEU:O	1:B:195:CYS:C	2.34	0.67
1:E:239:ASP:HB2	1:E:242:ASP:HB3	1.77	0.67
1:A:244:LEU:HB2	1:D:148:ALA:HB2	1.75	0.67
1:B:99:LEU:O	1:B:102:SER:HB3	1.95	0.67
1:D:240:PRO:C	1:D:242:ASP:H	2.03	0.67
1:A:254:ASN:HB3	1:D:112:TYR:O	1.96	0.66
1:C:360:PHE:CE2	1:C:370:CYS:SG	2.89	0.66
1:D:238:LEU:O	1:D:240:PRO:CD	2.43	0.66
1:A:244:LEU:C	1:A:246:ASN:H	2.04	0.66
1:E:224:PHE:CD2	1:E:249:TYR:CE1	2.84	0.66
1:A:239:ASP:HB2	1:A:242:ASP:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:THR:O	1:B:109:ALA:HB3	1.95	0.66
1:B:189:THR:O	1:B:368:ARG:HD2	1.96	0.66
1:C:196:HIS:O	1:C:199:ALA:HB3	1.95	0.66
1:A:80:MET:CE	1:A:270:SER:HA	2.24	0.66
1:C:106:THR:HG22	1:C:107:ALA:N	2.09	0.66
1:D:258:GLN:NE2	1:D:306:PHE:CZ	2.64	0.66
1:A:374:ASP:C	1:A:375:SER:HG	2.01	0.65
1:F:106:THR:O	1:F:107:ALA:C	2.32	0.65
1:F:171:LEU:HD21	1:F:358:LEU:HD11	1.78	0.65
1:B:194:LEU:HD23	1:B:194:LEU:C	2.21	0.65
1:E:230:VAL:HG23	1:E:231:SER:H	1.60	0.65
1:D:106:THR:O	1:D:109:ALA:N	2.30	0.65
1:F:303:LEU:HG	1:F:303:LEU:O	1.97	0.65
1:B:159:CYS:SG	1:B:176:GLU:HG3	2.37	0.65
1:C:255:ALA:HA	1:C:285:LEU:HD23	1.78	0.64
1:A:204:ILE:O	1:A:210:GLY:HA3	1.97	0.64
1:C:350:MET:O	1:C:354:SER:N	2.22	0.64
1:A:282:VAL:HG22	1:A:306:PHE:CE2	2.33	0.64
1:D:194:LEU:O	1:D:195:CYS:C	2.34	0.64
1:F:204:ILE:O	1:F:210:GLY:HA3	1.97	0.64
1:A:146:THR:HG23	1:A:149:ASP:CB	2.26	0.64
1:C:159:CYS:SG	1:C:176:GLU:HG3	2.37	0.64
1:D:350:MET:O	1:D:351:ALA:C	2.37	0.64
1:B:244:LEU:C	1:B:246:ASN:N	2.55	0.64
1:C:114:PRO:O	1:C:118:LEU:HG	1.98	0.63
1:E:253:TYR:CE2	1:F:112:TYR:CE1	2.86	0.63
1:E:297:SER:O	1:E:300:GLN:N	2.31	0.63
1:B:183:LEU:O	1:B:324:THR:HA	1.98	0.63
1:F:146:THR:HG23	1:F:149:ASP:CB	2.29	0.63
1:B:93:MET:O	1:B:97:LYS:HG3	1.98	0.63
1:F:296:LEU:O	1:F:297:SER:O	2.17	0.63
1:A:193:GLN:HG3	1:A:387:ILE:HG21	1.79	0.63
1:E:261:LEU:O	1:E:262:LEU:C	2.40	0.63
1:A:384:VAL:HG12	1:A:385:PHE:N	2.14	0.63
1:C:95:ASP:O	1:C:96:VAL:C	2.40	0.63
1:F:384:VAL:CG1	1:F:385:PHE:N	2.61	0.63
1:E:200:VAL:C	1:E:202:CYS:H	2.06	0.63
1:C:148:ALA:O	1:C:149:ASP:C	2.40	0.63
1:D:312:ARG:O	1:D:315:ASP:N	2.32	0.63
1:D:83:ILE:HG21	1:D:96:VAL:HG13	1.81	0.62
1:C:200:VAL:C	1:C:202:CYS:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:HIS:O	1:D:199:ALA:HB3	1.99	0.62
1:E:240:PRO:C	1:E:242:ASP:N	2.54	0.62
1:C:354:SER:C	1:C:356:THR:H	2.07	0.62
1:C:367:GLN:C	1:C:368:ARG:HG2	2.24	0.62
1:D:283:MET:O	1:D:285:LEU:N	2.32	0.62
1:E:164:SER:OG	1:E:167:LEU:HB2	2.00	0.62
1:F:370:CYS:O	1:F:370:CYS:SG	2.56	0.62
1:C:93:MET:O	1:C:97:LYS:HG3	2.00	0.62
1:C:226:PRO:O	1:C:227:VAL:C	2.39	0.62
1:C:296:LEU:O	1:C:297:SER:C	2.43	0.62
1:A:100:ARG:NH1	1:A:100:ARG:HG2	2.15	0.61
1:E:194:LEU:O	1:E:195:CYS:C	2.41	0.61
1:B:240:PRO:C	1:B:242:ASP:N	2.57	0.61
1:A:286:TYR:CZ	1:A:346:GLY:HA2	2.35	0.61
1:B:194:LEU:HA	1:B:392:VAL:CG2	2.30	0.61
1:F:194:LEU:C	1:F:194:LEU:HD23	2.25	0.61
1:F:197:THR:OG1	1:F:392:VAL:HG23	1.99	0.61
1:A:171:LEU:HD21	1:A:358:LEU:HD11	1.83	0.61
1:C:100:ARG:C	1:C:102:SER:H	2.09	0.61
1:B:106:THR:HG22	1:B:107:ALA:N	2.13	0.61
1:C:350:MET:O	1:C:353:SER:N	2.34	0.61
1:D:170:LEU:HD21	1:D:381:ALA:O	1.98	0.61
1:E:238:LEU:O	1:E:240:PRO:CD	2.48	0.61
1:E:350:MET:O	1:E:351:ALA:C	2.44	0.61
1:C:226:PRO:O	1:C:228:ARG:N	2.33	0.60
1:C:306:PHE:O	1:C:308:ARG:N	2.34	0.60
1:E:106:THR:O	1:E:109:ALA:N	2.34	0.60
1:B:100:ARG:C	1:B:102:SER:H	2.10	0.60
1:C:140:VAL:O	1:C:142:MET:HG2	2.02	0.60
1:C:201:THR:HA	1:C:204:ILE:HG12	1.83	0.60
1:C:318:GLY:O	1:C:319:VAL:O	2.19	0.60
1:D:230:VAL:HG23	1:D:231:SER:H	1.64	0.60
1:B:350:MET:O	1:B:351:ALA:C	2.43	0.60
1:D:204:ILE:HB	1:D:210:GLY:HA3	1.84	0.60
1:D:287:ARG:O	1:D:288:THR:C	2.40	0.60
1:F:244:LEU:C	1:F:246:ASN:N	2.58	0.60
1:A:240:PRO:O	1:A:242:ASP:N	2.35	0.60
1:C:191:LYS:HG2	1:C:360:PHE:CD1	2.37	0.60
1:C:347:GLY:CA	1:C:357:ARG:HH22	2.14	0.60
1:B:350:MET:O	1:B:352:HIS:N	2.33	0.60
1:A:201:THR:HA	1:A:204:ILE:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:HG2	1:B:360:PHE:CD1	2.36	0.60
1:E:272:SER:OG	1:E:273:ARG:N	2.33	0.60
1:D:348:ASN:O	1:D:349:ILE:C	2.43	0.59
1:B:244:LEU:O	1:B:246:ASN:N	2.35	0.59
1:C:347:GLY:CA	1:C:357:ARG:NH2	2.65	0.59
1:F:135:GLU:O	1:F:136:ALA:C	2.43	0.59
1:E:253:TYR:CD2	1:F:112:TYR:CD1	2.90	0.59
1:D:146:THR:HG23	1:D:149:ASP:HB2	1.84	0.59
1:A:177:THR:HG22	1:A:320:ALA:HB2	1.84	0.59
1:A:348:ASN:O	1:A:349:ILE:C	2.42	0.59
1:F:265:ALA:O	1:F:269:MET:HG3	2.03	0.59
1:A:300:GLN:O	1:A:349:ILE:HD13	2.02	0.59
1:D:360:PHE:N	1:D:360:PHE:CD1	2.68	0.59
1:A:106:THR:O	1:A:107:ALA:C	2.41	0.59
1:B:194:LEU:HG	1:B:392:VAL:HG21	1.85	0.59
1:D:175:VAL:HG11	1:D:198:LEU:HD11	1.84	0.59
1:F:348:ASN:O	1:F:350:MET:N	2.35	0.59
1:C:240:PRO:C	1:C:242:ASP:N	2.57	0.59
1:F:110:VAL:O	1:F:113:ALA:HB3	2.01	0.59
1:F:240:PRO:O	1:F:242:ASP:N	2.35	0.59
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.68	0.59
1:E:125:SER:OG	1:E:128:LYS:HB2	2.02	0.59
1:D:104:LEU:CD2	1:D:109:ALA:HB1	2.33	0.58
1:E:224:PHE:CD2	1:E:249:TYR:CD1	2.91	0.58
1:C:347:GLY:HA3	1:C:357:ARG:HH22	1.67	0.58
1:D:261:LEU:O	1:D:262:LEU:C	2.44	0.58
1:F:244:LEU:O	1:F:246:ASN:N	2.36	0.58
1:D:289:ASP:OD1	1:D:289:ASP:C	2.46	0.58
1:F:261:LEU:O	1:F:262:LEU:C	2.45	0.58
1:D:88:VAL:O	1:D:89:ASN:C	2.45	0.58
1:D:224:PHE:CD2	1:D:249:TYR:CE1	2.92	0.58
1:B:99:LEU:HD23	1:B:121:ILE:HD13	1.85	0.58
1:D:106:THR:O	1:D:107:ALA:C	2.47	0.58
1:A:272:SER:OG	1:A:273:ARG:N	2.34	0.58
1:A:287:ARG:C	1:A:289:ASP:H	2.12	0.58
1:B:144:PHE:CE2	1:C:250:ALA:HB2	2.39	0.58
1:B:197:THR:O	1:B:198:LEU:C	2.43	0.58
1:C:99:LEU:HD23	1:C:121:ILE:HD13	1.84	0.58
1:D:265:ALA:O	1:D:269:MET:HG3	2.03	0.58
1:E:276:LEU:C	1:E:276:LEU:HD23	2.28	0.58
1:B:227:VAL:CG2	1:B:227:VAL:CG1	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LEU:C	1:D:246:ASN:H	2.12	0.57
1:E:250:ALA:HB2	1:F:144:PHE:CE2	2.38	0.57
1:F:240:PRO:C	1:F:242:ASP:H	2.12	0.57
1:F:272:SER:OG	1:F:273:ARG:N	2.37	0.57
1:B:114:PRO:O	1:B:118:LEU:HG	2.04	0.57
1:C:182:GLU:OE2	1:C:350:MET:CE	2.51	0.57
1:D:240:PRO:C	1:D:242:ASP:N	2.57	0.57
1:A:106:THR:HG22	1:A:108:GLU:H	1.69	0.57
1:C:360:PHE:CD2	1:C:370:CYS:SG	2.97	0.57
1:E:83:ILE:HG21	1:E:96:VAL:HG13	1.86	0.57
1:A:179:SER:HB2	1:A:355:THR:HG21	1.86	0.57
1:E:106:THR:O	1:E:107:ALA:C	2.48	0.57
1:F:106:THR:HG22	1:F:108:GLU:H	1.69	0.57
1:E:244:LEU:C	1:E:246:ASN:H	2.12	0.57
1:B:281:SER:HB2	1:B:324:THR:OG1	2.04	0.57
1:D:186:GLU:O	1:D:189:THR:HG23	2.04	0.57
1:D:311:GLN:NE2	1:D:311:GLN:O	2.37	0.57
1:E:250:ALA:HB2	1:F:144:PHE:CD2	2.39	0.57
1:A:151:HIS:CG	1:A:151:HIS:O	2.57	0.57
1:A:152:MET:O	1:A:154:ARG:N	2.37	0.57
1:C:297:SER:O	1:C:300:GLN:N	2.38	0.57
1:D:200:VAL:C	1:D:202:CYS:H	2.12	0.57
1:D:238:LEU:O	1:D:240:PRO:N	2.37	0.57
1:D:254:ASN:OD1	1:D:254:ASN:C	2.48	0.57
1:E:146:THR:HG23	1:E:149:ASP:HB2	1.87	0.57
1:A:288:THR:CG2	1:D:305:LYS:NZ	2.67	0.57
1:A:132:LEU:O	1:A:133:LEU:C	2.48	0.56
1:A:306:PHE:O	1:A:307:MET:C	2.44	0.56
1:D:297:SER:O	1:D:300:GLN:N	2.39	0.56
1:E:276:LEU:HD23	1:E:276:LEU:O	2.05	0.56
1:C:350:MET:C	1:C:354:SER:OG	2.49	0.56
1:B:258:GLN:NE2	1:B:306:PHE:CE1	2.65	0.56
1:B:306:PHE:O	1:B:308:ARG:N	2.38	0.56
1:F:297:SER:O	1:F:298:ALA:C	2.49	0.56
1:C:350:MET:HA	1:C:353:SER:OG	2.05	0.56
1:A:240:PRO:C	1:A:242:ASP:H	2.14	0.56
1:B:124:ILE:HG22	1:B:129:ALA:HB2	1.87	0.56
1:B:312:ARG:O	1:B:315:ASP:N	2.38	0.56
1:E:186:GLU:O	1:E:189:THR:HG23	2.06	0.56
1:F:284:ALA:C	1:F:286:TYR:N	2.60	0.56
1:B:126:GLU:O	1:B:130:ASP:OD2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:C	1:B:202:CYS:H	2.13	0.56
1:A:197:THR:OG1	1:A:392:VAL:HG23	2.06	0.56
1:A:240:PRO:C	1:A:242:ASP:N	2.63	0.56
1:B:180:ILE:HB	1:B:355:THR:HG23	1.88	0.56
1:B:296:LEU:O	1:B:297:SER:C	2.49	0.56
1:D:191:LYS:NZ	1:D:326:GLN:HG2	2.21	0.56
1:E:244:LEU:HB2	1:F:148:ALA:HB2	1.87	0.56
1:A:373:VAL:O	1:A:374:ASP:O	2.23	0.55
1:C:124:ILE:HG22	1:C:129:ALA:HB2	1.88	0.55
1:A:200:VAL:C	1:A:202:CYS:H	2.14	0.55
1:C:200:VAL:C	1:C:202:CYS:N	2.63	0.55
1:E:230:VAL:CG2	1:E:231:SER:H	2.18	0.55
1:E:239:ASP:O	1:E:242:ASP:HB3	2.06	0.55
1:B:96:VAL:HG12	1:B:100:ARG:HE	1.71	0.55
1:B:168:ASP:O	1:B:171:LEU:N	2.39	0.55
1:B:258:GLN:HB2	1:B:285:LEU:CD2	2.36	0.55
1:C:200:VAL:O	1:C:202:CYS:N	2.40	0.55
1:C:306:PHE:O	1:C:307:MET:C	2.46	0.55
1:D:225:ARG:HD3	1:D:225:ARG:N	2.22	0.55
1:A:175:VAL:HG23	1:A:175:VAL:O	2.06	0.55
1:A:245:ASN:HA	1:D:146:THR:OG1	2.05	0.55
1:B:360:PHE:CE2	1:B:370:CYS:HB2	2.40	0.55
1:D:104:LEU:HD23	1:D:109:ALA:HB1	1.89	0.55
1:D:272:SER:OG	1:D:273:ARG:N	2.39	0.55
1:D:276:LEU:HD23	1:D:276:LEU:C	2.32	0.55
1:D:296:LEU:O	1:D:299:ARG:N	2.39	0.55
1:F:295:GLU:O	1:F:296:LEU:C	2.49	0.55
1:A:196:HIS:O	1:A:199:ALA:CB	2.53	0.55
1:B:164:SER:O	1:B:165:LYS:C	2.50	0.55
1:E:230:VAL:CG2	1:E:231:SER:N	2.69	0.55
1:F:240:PRO:C	1:F:242:ASP:N	2.63	0.55
1:A:305:LYS:O	1:A:308:ARG:HG2	2.06	0.55
1:B:360:PHE:CE2	1:B:370:CYS:CB	2.89	0.55
1:B:148:ALA:O	1:B:149:ASP:C	2.48	0.55
1:F:304:ALA:C	1:F:306:PHE:N	2.63	0.55
1:A:227:VAL:HG11	1:D:377:CYS:HB3	1.89	0.55
1:F:170:LEU:HG	1:F:372:VAL:HG21	1.89	0.55
1:B:227:VAL:CG2	1:B:227:VAL:CA	2.77	0.55
1:C:194:LEU:HG	1:C:392:VAL:HG21	1.89	0.55
1:D:88:VAL:O	1:D:90:GLY:N	2.40	0.55
1:D:303:LEU:O	1:D:304:ALA:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:TYR:CD2	1:F:112:TYR:CE1	2.95	0.55
1:A:164:SER:O	1:A:165:LYS:C	2.48	0.55
1:B:300:GLN:O	1:B:349:ILE:HG21	2.06	0.55
1:C:264:ALA:O	1:C:268:MET:HG3	2.07	0.55
1:C:265:ALA:O	1:C:269:MET:HE2	2.07	0.55
1:D:239:ASP:O	1:D:242:ASP:HB3	2.07	0.55
1:F:194:LEU:O	1:F:195:CYS:C	2.46	0.55
1:E:162:THR:HG21	1:E:167:LEU:HD23	1.89	0.54
1:C:145:VAL:HG23	1:C:145:VAL:O	2.07	0.54
1:C:350:MET:O	1:C:354:SER:OG	2.25	0.54
1:C:164:SER:O	1:C:165:LYS:C	2.46	0.54
1:D:295:GLU:O	1:D:296:LEU:C	2.50	0.54
1:F:155:SER:C	1:F:157:LEU:H	2.16	0.54
1:C:118:LEU:HB3	1:C:129:ALA:HB1	1.89	0.54
1:C:347:GLY:O	1:C:348:ASN:C	2.50	0.54
1:F:392:VAL:HG12	1:F:393:GLY:N	2.22	0.54
1:C:238:LEU:O	1:C:239:ASP:C	2.49	0.54
1:F:300:GLN:O	1:F:349:ILE:HD13	2.07	0.54
1:B:258:GLN:HB2	1:B:285:LEU:HD23	1.90	0.54
1:C:268:MET:C	1:C:270:SER:H	2.16	0.54
1:D:105:HIS:O	1:D:106:THR:OG1	2.23	0.54
1:D:132:LEU:O	1:D:135:GLU:N	2.41	0.54
1:E:132:LEU:O	1:E:135:GLU:N	2.41	0.54
1:E:196:HIS:O	1:E:199:ALA:HB3	2.08	0.54
1:B:192:SER:N	2:B:502:SO4:O3	2.26	0.54
1:D:171:LEU:HD21	1:D:358:LEU:HD21	1.89	0.54
1:F:193:GLN:HG3	1:F:387:ILE:HD13	1.89	0.54
1:F:348:ASN:C	1:F:350:MET:N	2.64	0.54
1:D:203:GLN:OE1	1:D:246:ASN:HB3	2.08	0.53
1:F:140:VAL:HG12	1:F:141:PRO:HD2	1.91	0.53
1:A:282:VAL:HG22	1:A:306:PHE:HE2	1.73	0.53
1:A:304:ALA:C	1:A:306:PHE:N	2.60	0.53
1:E:200:VAL:C	1:E:202:CYS:N	2.64	0.53
1:B:239:ASP:HB2	1:B:242:ASP:HB3	1.90	0.53
1:C:191:LYS:N	2:C:503:SO4:O4	2.41	0.53
1:D:358:LEU:HB3	1:D:360:PHE:HE1	1.72	0.53
1:D:385:PHE:CD1	1:D:386:ALA:N	2.76	0.53
1:E:359:GLY:O	1:E:370:CYS:HA	2.09	0.53
1:F:266:ALA:C	1:F:268:MET:N	2.64	0.53
1:F:306:PHE:O	1:F:307:MET:C	2.46	0.53
1:B:227:VAL:CG2	1:B:227:VAL:HB	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:THR:HG23	1:F:161:THR:O	2.08	0.53
1:F:394:ASP:HB3	1:F:395:PRO:HD2	1.90	0.53
1:A:125:SER:OG	1:A:128:LYS:CB	2.54	0.53
1:B:265:ALA:O	1:B:269:MET:HE2	2.08	0.53
1:B:267:GLN:O	1:B:271:GLU:HG2	2.08	0.53
1:C:196:HIS:O	1:C:197:THR:C	2.48	0.53
1:F:151:HIS:O	1:F:151:HIS:CG	2.62	0.53
1:A:237:GLY:O	1:A:238:LEU:HG	2.09	0.53
1:A:282:VAL:HB	1:A:323:VAL:CG1	2.39	0.53
1:F:179:SER:HB2	1:F:355:THR:HG21	1.89	0.53
1:C:359:GLY:O	1:C:370:CYS:HA	2.09	0.53
1:F:385:PHE:CD1	1:F:385:PHE:C	2.86	0.53
1:A:194:LEU:O	1:A:195:CYS:C	2.51	0.53
1:B:112:TYR:CD1	1:C:253:TYR:CG	2.97	0.53
1:E:348:ASN:O	1:E:351:ALA:N	2.42	0.53
1:B:140:VAL:O	1:B:142:MET:HG2	2.08	0.53
1:B:226:PRO:O	1:B:227:VAL:C	2.48	0.53
1:C:194:LEU:HA	1:C:392:VAL:CG2	2.39	0.53
1:C:238:LEU:O	1:C:240:PRO:HD3	2.09	0.53
1:A:200:VAL:O	1:A:202:CYS:N	2.42	0.52
1:C:168:ASP:O	1:C:171:LEU:N	2.42	0.52
1:F:286:TYR:CZ	1:F:346:GLY:HA2	2.45	0.52
1:A:193:GLN:HG3	1:A:387:ILE:CG2	2.39	0.52
1:B:155:SER:O	1:B:156:GLU:C	2.47	0.52
1:B:158:ILE:O	1:B:177:THR:OG1	2.20	0.52
1:F:299:ARG:HG3	1:F:299:ARG:HH11	1.74	0.52
1:D:276:LEU:HD23	1:D:276:LEU:O	2.09	0.52
1:E:200:VAL:O	1:E:202:CYS:N	2.42	0.52
1:F:237:GLY:O	1:F:238:LEU:HG	2.10	0.52
1:A:196:HIS:O	1:A:197:THR:C	2.50	0.52
1:B:200:VAL:C	1:B:202:CYS:N	2.64	0.52
1:B:367:GLN:C	1:B:368:ARG:HG2	2.35	0.52
1:A:167:LEU:O	1:A:168:ASP:C	2.52	0.52
1:A:288:THR:CG2	1:D:305:LYS:HZ3	2.23	0.52
1:B:118:LEU:HB3	1:B:129:ALA:HB1	1.89	0.52
1:D:238:LEU:O	1:D:239:ASP:C	2.53	0.52
1:B:230:VAL:O	1:B:231:SER:C	2.50	0.52
1:E:238:LEU:O	1:E:240:PRO:N	2.42	0.52
1:E:295:GLU:O	1:E:296:LEU:C	2.52	0.52
1:B:359:GLY:O	1:B:370:CYS:HA	2.10	0.52
1:D:385:PHE:HD1	1:D:386:ALA:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:VAL:HB	1:F:323:VAL:CG1	2.39	0.52
1:C:238:LEU:O	1:C:240:PRO:N	2.43	0.51
1:D:254:ASN:OD1	1:D:254:ASN:O	2.28	0.51
1:B:196:HIS:O	1:B:199:ALA:HB3	2.10	0.51
1:C:266:ALA:C	1:C:268:MET:N	2.64	0.51
1:D:230:VAL:CG2	1:D:231:SER:H	2.22	0.51
1:B:201:THR:HA	1:B:204:ILE:CG1	2.38	0.51
1:D:201:THR:O	1:D:210:GLY:HA2	2.10	0.51
1:F:160:LEU:HD22	1:F:202:CYS:HA	1.92	0.51
1:F:299:ARG:HG3	1:F:299:ARG:NH1	2.25	0.51
1:A:237:GLY:C	1:A:238:LEU:HG	2.35	0.51
1:B:196:HIS:O	1:B:197:THR:C	2.51	0.51
1:D:303:LEU:C	1:D:303:LEU:HD12	2.36	0.51
1:F:141:PRO:HG2	1:F:142:MET:H	1.75	0.51
1:B:204:ILE:HB	1:B:210:GLY:HA3	1.93	0.51
1:C:99:LEU:O	1:C:102:SER:CB	2.59	0.51
1:F:152:MET:O	1:F:154:ARG:N	2.42	0.51
1:F:230:VAL:O	1:F:231:SER:C	2.52	0.51
1:A:235:ARG:HD2	1:A:390:ASP:OD1	2.10	0.51
1:B:266:ALA:C	1:B:268:MET:N	2.66	0.51
1:B:277:ILE:HG22	1:B:278:VAL:N	2.24	0.51
1:C:106:THR:CG2	1:C:107:ALA:N	2.74	0.51
1:D:180:ILE:HG22	1:D:181:THR:N	2.26	0.51
1:C:220:THR:HG21	1:C:281:SER:O	2.10	0.51
1:D:310:LEU:O	1:D:311:GLN:C	2.47	0.51
1:D:367:GLN:O	1:D:368:ARG:HG2	2.10	0.51
1:E:104:LEU:CD2	1:E:109:ALA:HB1	2.41	0.51
1:E:312:ARG:O	1:E:315:ASP:N	2.43	0.51
1:F:106:THR:O	1:F:109:ALA:HB3	2.10	0.51
1:F:175:VAL:HG23	1:F:175:VAL:O	2.10	0.51
1:F:200:VAL:O	1:F:202:CYS:N	2.43	0.51
1:C:389:GLU:HG2	1:C:389:GLU:O	2.11	0.51
1:E:253:TYR:CG	1:F:112:TYR:CD1	2.98	0.51
1:D:240:PRO:O	1:D:241:ASP:C	2.52	0.51
1:E:384:VAL:HG12	1:E:385:PHE:N	2.26	0.51
1:C:230:VAL:O	1:C:231:SER:C	2.53	0.51
1:E:274:PHE:CD1	1:E:274:PHE:N	2.78	0.51
1:E:303:LEU:O	1:E:304:ALA:C	2.52	0.51
1:F:164:SER:O	1:F:165:LYS:C	2.49	0.51
1:A:200:VAL:C	1:A:202:CYS:N	2.67	0.50
1:B:360:PHE:CD2	1:B:370:CYS:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:TYR:CD2	1:B:303:LEU:HD13	2.46	0.50
1:C:234:GLN:O	1:C:235:ARG:C	2.52	0.50
1:C:254:ASN:OD1	1:C:254:ASN:O	2.29	0.50
1:D:258:GLN:NE2	1:D:306:PHE:CE1	2.75	0.50
1:E:160:LEU:HD22	1:E:202:CYS:HA	1.92	0.50
1:A:277:ILE:HB	1:A:321:VAL:HG22	1.94	0.50
1:B:306:PHE:C	1:B:308:ARG:N	2.67	0.50
1:B:352:HIS:NE2	1:C:326:GLN:OE1	2.44	0.50
1:C:195:CYS:O	1:C:196:HIS:C	2.54	0.50
1:C:238:LEU:O	1:C:240:PRO:CD	2.60	0.50
1:D:230:VAL:CG2	1:D:231:SER:N	2.71	0.50
1:E:162:THR:CB	1:E:167:LEU:HD23	2.41	0.50
1:E:281:SER:C	1:E:283:MET:N	2.67	0.50
1:F:100:ARG:NH1	1:F:100:ARG:HG2	2.27	0.50
1:C:306:PHE:C	1:C:308:ARG:N	2.67	0.50
1:D:240:PRO:O	1:D:243:ALA:N	2.45	0.50
1:E:296:LEU:O	1:E:299:ARG:N	2.44	0.50
1:F:200:VAL:C	1:F:202:CYS:H	2.20	0.50
1:E:177:THR:HG22	1:E:320:ALA:HB2	1.94	0.50
1:E:247:VAL:O	1:F:147:ALA:N	2.44	0.50
1:A:244:LEU:C	1:A:246:ASN:N	2.65	0.50
1:B:147:ALA:HB2	1:C:247:VAL:HB	1.93	0.50
1:C:282:VAL:HB	1:C:323:VAL:CG1	2.42	0.50
1:E:204:ILE:HB	1:E:210:GLY:HA3	1.94	0.50
1:A:370:CYS:O	1:A:370:CYS:SG	2.68	0.50
1:B:286:TYR:HE2	1:B:303:LEU:N	2.10	0.50
1:C:106:THR:HG22	1:C:108:GLU:H	1.77	0.50
1:F:282:VAL:CG2	1:F:323:VAL:HG13	2.41	0.50
1:F:385:PHE:HD1	1:F:386:ALA:N	2.10	0.50
1:D:191:LYS:HZ2	1:D:326:GLN:HG2	1.76	0.50
1:A:239:ASP:HB2	1:A:242:ASP:CB	2.42	0.50
1:A:348:ASN:C	1:A:350:MET:N	2.66	0.50
1:D:96:VAL:HG12	1:D:97:LYS:N	2.22	0.50
1:D:184:PHE:CD1	1:D:184:PHE:C	2.90	0.50
1:E:99:LEU:HD23	1:E:121:ILE:HD13	1.93	0.49
1:F:144:PHE:O	1:F:145:VAL:HG13	2.12	0.49
1:A:244:LEU:CB	1:D:148:ALA:HB2	2.40	0.49
1:F:125:SER:OG	1:F:128:LYS:CB	2.57	0.49
1:F:237:GLY:C	1:F:238:LEU:HG	2.37	0.49
1:B:283:MET:O	1:B:286:TYR:HB2	2.12	0.49
1:D:348:ASN:O	1:D:350:MET:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:PRO:O	1:E:243:ALA:N	2.46	0.49
1:F:239:ASP:HB2	1:F:242:ASP:HB3	1.95	0.49
1:A:180:ILE:HG12	1:A:321:VAL:CG1	2.42	0.49
1:B:318:GLY:O	1:B:319:VAL:O	2.30	0.49
1:E:88:VAL:O	1:E:89:ASN:C	2.53	0.49
1:E:201:THR:O	1:E:210:GLY:HA2	2.12	0.49
1:F:194:LEU:HD21	1:F:198:LEU:HD12	1.94	0.49
1:F:232:ILE:O	1:F:235:ARG:HB3	2.12	0.49
1:A:140:VAL:C	1:A:141:PRO:O	2.51	0.49
1:A:384:VAL:CG1	1:A:385:PHE:N	2.75	0.49
1:B:200:VAL:O	1:B:202:CYS:N	2.46	0.49
1:F:226:PRO:O	1:F:227:VAL:C	2.54	0.49
1:D:175:VAL:CG1	1:D:198:LEU:HD11	2.43	0.49
1:F:284:ALA:C	1:F:286:TYR:H	2.18	0.49
1:F:366:CYS:HA	1:F:368:ARG:HH12	1.78	0.49
1:B:306:PHE:O	1:B:307:MET:C	2.48	0.49
1:C:106:THR:O	1:C:109:ALA:HB3	2.12	0.49
1:E:265:ALA:O	1:E:269:MET:HG3	2.13	0.49
1:F:167:LEU:O	1:F:168:ASP:C	2.54	0.49
1:A:368:ARG:HG3	1:A:387:ILE:HD11	1.95	0.49
1:B:311:GLN:O	1:B:312:ARG:C	2.53	0.49
1:D:108:GLU:OE1	1:D:108:GLU:N	2.45	0.49
1:E:375:SER:O	1:E:376:PRO:C	2.54	0.49
1:F:371:LYS:HG2	1:F:372:VAL:N	2.28	0.49
1:F:374:ASP:C	1:F:375:SER:HG	2.12	0.49
1:A:152:MET:O	1:A:153:ARG:C	2.56	0.49
1:B:360:PHE:CD2	1:B:370:CYS:CB	2.95	0.49
1:D:83:ILE:HG21	1:D:96:VAL:CG1	2.42	0.49
1:D:200:VAL:C	1:D:202:CYS:N	2.69	0.49
1:B:238:LEU:O	1:B:239:ASP:C	2.49	0.49
1:E:164:SER:O	1:E:165:LYS:C	2.56	0.49
1:F:196:HIS:O	1:F:199:ALA:CB	2.55	0.49
1:F:250:ALA:HB1	1:F:261:LEU:HD13	1.94	0.49
1:A:175:VAL:O	1:A:175:VAL:CG2	2.61	0.48
1:B:151:HIS:O	1:B:151:HIS:CG	2.66	0.48
1:B:226:PRO:O	1:B:228:ARG:N	2.46	0.48
1:D:162:THR:O	1:D:197:THR:HG21	2.13	0.48
1:D:360:PHE:N	1:D:360:PHE:HD1	2.07	0.48
1:E:106:THR:O	1:E:109:ALA:HB3	2.13	0.48
1:B:161:THR:OG1	1:B:162:THR:N	2.44	0.48
1:C:161:THR:OG1	1:C:162:THR:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:LYS:HG2	1:D:372:VAL:N	2.28	0.48
1:F:144:PHE:C	1:F:145:VAL:HG13	2.39	0.48
1:F:194:LEU:C	1:F:194:LEU:CD2	2.86	0.48
1:A:258:GLN:NE2	1:A:306:PHE:CE1	2.71	0.48
1:B:198:LEU:C	1:B:200:VAL:N	2.71	0.48
1:E:311:GLN:O	1:E:311:GLN:NE2	2.45	0.48
1:F:148:ALA:O	1:F:149:ASP:C	2.55	0.48
1:C:354:SER:C	1:C:356:THR:N	2.72	0.48
1:D:160:LEU:HD22	1:D:202:CYS:HA	1.95	0.48
1:F:254:ASN:OD1	1:F:254:ASN:C	2.56	0.48
1:A:100:ARG:NH1	1:A:100:ARG:CG	2.68	0.48
1:E:132:LEU:O	1:E:133:LEU:C	2.57	0.48
1:E:203:GLN:OE1	1:E:246:ASN:HB3	2.12	0.48
1:F:191:LYS:O	1:F:192:SER:C	2.54	0.48
1:F:196:HIS:O	1:F:197:THR:C	2.54	0.48
1:A:304:ALA:C	1:A:306:PHE:H	2.21	0.48
1:B:140:VAL:O	1:B:141:PRO:C	2.56	0.48
1:C:197:THR:O	1:C:198:LEU:C	2.53	0.48
1:C:106:THR:O	1:C:107:ALA:C	2.55	0.48
1:C:194:LEU:C	1:C:194:LEU:CD2	2.86	0.48
1:D:247:VAL:O	1:D:247:VAL:HG12	2.09	0.48
1:B:198:LEU:C	1:B:200:VAL:H	2.20	0.48
1:C:355:THR:O	1:C:356:THR:CB	2.62	0.48
1:F:200:VAL:C	1:F:202:CYS:N	2.72	0.48
1:A:205:PRO:O	1:A:206:LEU:C	2.56	0.47
1:B:194:LEU:CD2	1:B:198:LEU:HD12	2.44	0.47
1:D:164:SER:O	1:D:164:SER:OG	2.30	0.47
1:B:268:MET:C	1:B:270:SER:H	2.21	0.47
1:C:196:HIS:O	1:C:199:ALA:N	2.47	0.47
1:D:200:VAL:O	1:D:202:CYS:N	2.47	0.47
1:F:372:VAL:O	1:F:372:VAL:HG12	2.14	0.47
1:A:226:PRO:O	1:A:227:VAL:C	2.56	0.47
1:B:164:SER:OG	1:B:167:LEU:CB	2.60	0.47
1:C:255:ALA:HB1	1:C:286:TYR:CE2	2.49	0.47
1:D:224:PHE:CD2	1:D:249:TYR:CD1	3.02	0.47
1:E:162:THR:CG2	1:E:167:LEU:HD23	2.44	0.47
1:B:145:VAL:HG23	1:B:145:VAL:O	2.14	0.47
1:B:259:LEU:O	1:B:260:ARG:C	2.56	0.47
1:D:92:THR:C	1:D:94:ALA:N	2.70	0.47
1:A:144:PHE:O	1:A:145:VAL:HG13	2.14	0.47
1:D:267:GLN:O	1:D:270:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:CG1	1:A:198:LEU:HD11	2.42	0.47
1:A:304:ALA:O	1:A:306:PHE:N	2.47	0.47
1:C:298:ALA:O	1:C:299:ARG:C	2.55	0.47
1:A:244:LEU:O	1:A:246:ASN:N	2.47	0.47
1:B:255:ALA:HA	1:B:285:LEU:CD2	2.44	0.47
1:B:355:THR:HG1	1:B:356:THR:H	1.58	0.47
1:D:280:ASP:HA	1:D:281:SER:HA	1.68	0.47
1:F:88:VAL:O	1:F:89:ASN:C	2.57	0.47
1:F:132:LEU:O	1:F:133:LEU:C	2.56	0.47
1:A:348:ASN:O	1:A:350:MET:N	2.48	0.47
1:B:106:THR:HG22	1:B:108:GLU:H	1.79	0.47
1:D:191:LYS:HB2	2:D:504:SO4:O3	2.14	0.47
1:C:100:ARG:C	1:C:102:SER:N	2.71	0.47
1:D:244:LEU:C	1:D:246:ASN:N	2.72	0.47
1:D:367:GLN:C	1:D:368:ARG:HG2	2.40	0.47
1:F:115:ARG:O	1:F:116:LYS:C	2.58	0.47
1:F:266:ALA:O	1:F:267:GLN:C	2.58	0.47
1:F:296:LEU:O	1:F:299:ARG:N	2.47	0.47
1:B:117:ASP:O	1:B:121:ILE:HD11	2.15	0.47
1:C:280:ASP:HA	1:C:281:SER:HA	1.77	0.47
1:C:302:HIS:O	1:C:303:LEU:C	2.57	0.47
1:C:312:ARG:O	1:C:315:ASP:N	2.47	0.47
1:A:374:ASP:C	1:A:375:SER:OG	2.54	0.46
1:B:110:VAL:O	1:B:111:ALA:C	2.58	0.46
1:B:182:GLU:OE1	1:B:357:ARG:HG2	2.14	0.46
1:E:253:TYR:CZ	1:F:112:TYR:CE1	3.03	0.46
1:B:350:MET:O	1:B:353:SER:N	2.49	0.46
1:E:238:LEU:O	1:E:239:ASP:C	2.58	0.46
1:F:104:LEU:H	1:F:104:LEU:HG	1.40	0.46
1:A:191:LYS:O	1:A:192:SER:C	2.57	0.46
1:A:280:ASP:HA	1:A:281:SER:HA	1.69	0.46
1:A:266:ALA:C	1:A:268:MET:N	2.72	0.46
1:C:255:ALA:HA	1:C:285:LEU:CD2	2.45	0.46
1:C:254:ASN:OD1	1:C:254:ASN:C	2.57	0.46
1:E:371:LYS:HG2	1:E:372:VAL:N	2.31	0.46
1:A:350:MET:O	1:A:351:ALA:C	2.59	0.46
1:C:117:ASP:O	1:C:121:ILE:HD11	2.16	0.46
1:D:145:VAL:O	1:D:146:THR:C	2.57	0.46
1:E:244:LEU:C	1:E:246:ASN:N	2.72	0.46
1:E:281:SER:O	1:E:282:VAL:C	2.58	0.46
1:E:296:LEU:O	1:E:298:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:TYR:CE1	1:F:303:LEU:HD22	2.50	0.46
1:A:227:VAL:HG22	1:D:151:HIS:CE1	2.51	0.46
1:B:144:PHE:O	1:B:145:VAL:HG13	2.16	0.46
1:D:132:LEU:O	1:D:133:LEU:C	2.58	0.46
1:E:197:THR:OG1	1:E:392:VAL:HG23	2.15	0.46
1:F:203:GLN:OE1	1:F:246:ASN:HB3	2.16	0.46
1:A:180:ILE:HD11	1:A:310:LEU:HB3	1.98	0.46
1:A:304:ALA:O	1:A:305:LYS:C	2.59	0.46
1:D:92:THR:C	1:D:94:ALA:H	2.24	0.46
1:B:115:ARG:O	1:B:116:LYS:C	2.58	0.46
1:D:237:GLY:O	1:D:238:LEU:HG	2.16	0.46
1:A:247:VAL:O	1:D:147:ALA:N	2.49	0.46
1:A:261:LEU:O	1:A:262:LEU:C	2.58	0.46
1:B:112:TYR:O	1:C:254:ASN:HB3	2.16	0.46
1:C:276:LEU:HG	1:C:277:ILE:N	2.31	0.46
1:E:254:ASN:C	1:E:254:ASN:OD1	2.59	0.46
1:A:230:VAL:O	1:A:231:SER:C	2.60	0.45
1:A:392:VAL:HG12	1:A:393:GLY:N	2.31	0.45
1:B:256:ASP:O	1:B:257:HIS:C	2.58	0.45
1:D:281:SER:O	1:D:282:VAL:C	2.59	0.45
1:E:125:SER:O	1:E:127:ALA:N	2.48	0.45
1:E:160:LEU:HB2	1:E:175:VAL:HG22	1.97	0.45
1:C:204:ILE:HG23	1:C:205:PRO:HD2	1.97	0.45
1:D:96:VAL:O	1:D:97:LYS:C	2.59	0.45
1:D:206:LEU:HG	1:D:212:GLU:OE2	2.17	0.45
1:E:224:PHE:C	1:E:225:ARG:HD3	2.42	0.45
1:F:285:LEU:HA	1:F:285:LEU:HD23	1.60	0.45
1:A:111:ALA:HB1	1:A:142:MET:SD	2.57	0.45
1:B:204:ILE:HA	1:B:205:PRO:HD3	1.79	0.45
1:C:194:LEU:O	1:C:194:LEU:HD23	2.17	0.45
1:C:244:LEU:O	1:C:245:ASN:C	2.56	0.45
1:D:107:ALA:O	1:D:108:GLU:C	2.58	0.45
1:F:268:MET:C	1:F:270:SER:H	2.24	0.45
1:D:274:PHE:CD1	1:D:274:PHE:N	2.84	0.45
1:F:384:VAL:CG1	1:F:385:PHE:H	2.30	0.45
1:B:350:MET:C	1:B:352:HIS:N	2.72	0.45
1:D:308:ARG:O	1:D:309:ALA:C	2.58	0.45
1:F:88:VAL:O	1:F:90:GLY:N	2.49	0.45
1:F:230:VAL:CG2	1:F:231:SER:N	2.43	0.45
1:F:238:LEU:O	1:F:240:PRO:HD3	2.16	0.45
1:A:232:ILE:O	1:A:235:ARG:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:VAL:HG12	1:D:393:GLY:N	2.32	0.45
1:A:170:LEU:HD11	1:A:381:ALA:O	2.17	0.45
1:A:286:TYR:CE1	1:A:346:GLY:HA2	2.51	0.45
1:B:136:ALA:O	1:B:137:ALA:C	2.59	0.45
1:B:183:LEU:HD22	1:B:360:PHE:CE1	2.52	0.45
1:B:255:ALA:HB1	1:B:286:TYR:CE1	2.52	0.45
1:A:282:VAL:CG2	1:A:306:PHE:HE2	2.29	0.45
1:B:145:VAL:C	1:B:146:THR:O	2.55	0.45
1:F:140:VAL:CG1	1:F:141:PRO:HD2	2.47	0.45
1:E:108:GLU:O	1:E:111:ALA:HB3	2.17	0.45
1:A:93:MET:O	1:A:93:MET:HG2	2.16	0.44
1:B:100:ARG:C	1:B:102:SER:N	2.71	0.44
1:B:261:LEU:O	1:B:262:LEU:C	2.60	0.44
1:C:148:ALA:C	1:C:150:PHE:N	2.72	0.44
1:C:164:SER:OG	1:C:167:LEU:CB	2.63	0.44
1:E:162:THR:O	1:E:197:THR:HG21	2.17	0.44
1:E:371:LYS:CG	1:E:372:VAL:N	2.80	0.44
1:F:262:LEU:HD11	1:F:306:PHE:CE1	2.52	0.44
1:F:373:VAL:O	1:F:373:VAL:HG13	2.17	0.44
1:A:183:LEU:HD23	1:A:358:LEU:HB2	1.99	0.44
1:C:255:ALA:HB1	1:C:286:TYR:HE2	1.82	0.44
1:D:125:SER:OG	1:D:128:LYS:HB2	2.18	0.44
1:F:238:LEU:O	1:F:239:ASP:C	2.60	0.44
1:F:389:GLU:O	1:F:389:GLU:HG2	2.16	0.44
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.88	0.44
1:B:303:LEU:O	1:B:303:LEU:HG	2.17	0.44
1:C:258:GLN:HB2	1:C:285:LEU:CD2	2.47	0.44
1:C:283:MET:CE	1:C:283:MET:CG	2.94	0.44
1:C:311:GLN:O	1:C:312:ARG:C	2.60	0.44
1:E:92:THR:OG1	1:E:95:ASP:OD2	2.31	0.44
1:E:306:PHE:C	1:E:308:ARG:N	2.75	0.44
1:E:371:LYS:HG2	1:E:372:VAL:C	2.43	0.44
1:F:99:LEU:HD23	1:F:121:ILE:HD13	2.00	0.44
1:F:299:ARG:O	1:F:300:GLN:C	2.60	0.44
1:B:106:THR:CG2	1:B:107:ALA:N	2.79	0.44
1:B:216:LEU:HD23	1:B:277:ILE:HG23	1.99	0.44
1:C:191:LYS:HG2	1:C:360:PHE:HD1	1.80	0.44
1:D:99:LEU:HD23	1:D:121:ILE:HD13	1.99	0.44
1:F:318:GLY:O	1:F:319:VAL:O	2.36	0.44
1:A:255:ALA:HB2	1:A:289:ASP:O	2.17	0.44
1:A:296:LEU:O	1:A:297:SER:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASP:O	1:B:242:ASP:HB3	2.18	0.44
1:B:255:ALA:HA	1:B:285:LEU:HD23	2.00	0.44
1:D:239:ASP:HB2	1:D:242:ASP:CB	2.47	0.44
1:E:204:ILE:HG22	1:E:205:PRO:N	2.31	0.44
1:E:240:PRO:O	1:E:241:ASP:C	2.57	0.44
1:B:282:VAL:HB	1:B:323:VAL:CG1	2.48	0.44
1:D:170:LEU:HD11	1:D:381:ALA:HB3	1.99	0.44
1:E:281:SER:O	1:E:283:MET:N	2.51	0.44
1:E:285:LEU:HD13	1:E:285:LEU:HA	1.78	0.44
1:A:371:LYS:HG2	1:A:372:VAL:N	2.33	0.44
1:B:194:LEU:O	1:B:194:LEU:HD23	2.18	0.44
1:D:205:PRO:O	1:D:206:LEU:C	2.61	0.44
1:A:203:GLN:OE1	1:A:246:ASN:HB3	2.18	0.44
1:B:155:SER:C	1:B:157:LEU:N	2.76	0.44
1:D:155:SER:C	1:D:157:LEU:H	2.26	0.44
1:D:162:THR:HB	1:D:167:LEU:HD23	1.98	0.44
1:D:297:SER:OG	1:D:298:ALA:N	2.47	0.44
1:E:162:THR:HB	1:E:167:LEU:HD23	2.00	0.44
1:E:244:LEU:CB	1:F:148:ALA:HB2	2.48	0.44
1:E:256:ASP:O	1:E:257:HIS:C	2.61	0.44
1:E:281:SER:C	1:E:283:MET:H	2.26	0.44
1:F:375:SER:HA	1:F:376:PRO:HD2	1.62	0.44
1:A:385:PHE:CD1	1:A:385:PHE:C	2.96	0.43
1:D:205:PRO:O	1:D:207:ASP:N	2.51	0.43
1:E:88:VAL:O	1:E:90:GLY:N	2.51	0.43
1:E:162:THR:HG21	1:E:167:LEU:CD2	2.48	0.43
1:F:158:ILE:HG21	1:F:158:ILE:HD13	1.70	0.43
1:A:257:HIS:O	1:A:258:GLN:C	2.61	0.43
1:B:124:ILE:CG2	1:B:129:ALA:HB2	2.47	0.43
1:C:151:HIS:O	1:C:151:HIS:CG	2.70	0.43
1:C:272:SER:OG	1:C:273:ARG:N	2.51	0.43
1:D:256:ASP:O	1:D:257:HIS:C	2.61	0.43
1:E:350:MET:O	1:E:353:SER:N	2.50	0.43
1:E:367:GLN:C	1:E:368:ARG:HG2	2.43	0.43
1:E:385:PHE:CD1	1:E:386:ALA:N	2.86	0.43
1:F:109:ALA:O	1:F:110:VAL:C	2.60	0.43
1:F:194:LEU:CD2	1:F:198:LEU:HD12	2.48	0.43
1:A:106:THR:O	1:A:109:ALA:HB3	2.18	0.43
1:B:145:VAL:O	1:B:146:THR:C	2.56	0.43
1:D:81:VAL:O	1:D:106:THR:HG23	2.19	0.43
1:D:125:SER:O	1:D:127:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:ILE:HD13	1:F:180:ILE:HG21	1.77	0.43
1:C:124:ILE:CG2	1:C:129:ALA:HB2	2.47	0.43
1:E:277:ILE:HG21	1:E:277:ILE:HD13	1.75	0.43
1:E:306:PHE:O	1:E:307:MET:C	2.59	0.43
1:E:392:VAL:HG12	1:E:393:GLY:N	2.34	0.43
1:F:100:ARG:HG2	1:F:100:ARG:HH11	1.83	0.43
1:B:254:ASN:OD1	1:B:254:ASN:C	2.60	0.43
1:C:145:VAL:O	1:C:146:THR:C	2.61	0.43
1:D:104:LEU:HD22	1:D:109:ALA:HB1	2.00	0.43
1:D:183:LEU:O	1:D:324:THR:HA	2.19	0.43
1:E:125:SER:OG	1:E:128:LYS:CB	2.65	0.43
1:E:167:LEU:HD12	1:E:167:LEU:HA	1.84	0.43
1:F:92:THR:C	1:F:94:ALA:N	2.75	0.43
1:A:250:ALA:HB2	1:D:144:PHE:CE2	2.53	0.43
1:A:284:ALA:C	1:A:286:TYR:N	2.74	0.43
1:C:110:VAL:O	1:C:113:ALA:CB	2.61	0.43
1:C:211:GLY:C	1:C:213:GLY:H	2.27	0.43
1:E:164:SER:OG	1:E:167:LEU:CB	2.66	0.43
1:F:269:MET:HE1	1:F:313:LEU:HD13	2.00	0.43
1:B:110:VAL:O	1:B:113:ALA:CB	2.62	0.43
1:E:125:SER:O	1:E:126:GLU:C	2.61	0.43
1:B:254:ASN:OD1	1:B:254:ASN:O	2.36	0.43
1:C:204:ILE:HA	1:C:205:PRO:HD3	1.72	0.43
1:B:226:PRO:O	1:B:229:LEU:N	2.50	0.43
1:C:308:ARG:O	1:C:309:ALA:C	2.61	0.43
1:E:183:LEU:O	1:E:324:THR:HA	2.19	0.43
1:F:164:SER:OG	1:F:167:LEU:HB2	2.19	0.43
1:F:170:LEU:HG	1:F:372:VAL:CG2	2.48	0.43
1:F:205:PRO:HA	1:F:212:GLU:HG3	2.00	0.43
1:A:115:ARG:O	1:A:116:LYS:C	2.62	0.43
1:A:390:ASP:OD1	1:A:390:ASP:C	2.61	0.43
1:B:197:THR:O	1:B:199:ALA:N	2.51	0.43
1:E:170:LEU:HD12	1:E:170:LEU:HA	1.80	0.43
1:E:274:PHE:N	1:E:274:PHE:HD1	2.17	0.43
1:E:310:LEU:O	1:E:311:GLN:C	2.58	0.43
1:F:194:LEU:HD23	1:F:194:LEU:O	2.19	0.43
1:F:385:PHE:CD1	1:F:386:ALA:N	2.86	0.43
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.70	0.42
1:A:226:PRO:O	1:A:228:ARG:N	2.51	0.42
1:B:112:TYR:HB3	1:C:253:TYR:HB3	2.00	0.42
1:C:347:GLY:HA2	1:C:357:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.83	0.42
1:F:125:SER:C	1:F:127:ALA:N	2.76	0.42
1:A:155:SER:C	1:A:157:LEU:H	2.26	0.42
1:A:296:LEU:HG	1:A:297:SER:N	2.34	0.42
1:B:309:ALA:O	1:B:310:LEU:C	2.60	0.42
1:C:180:ILE:HG22	1:C:181:THR:N	2.33	0.42
1:A:88:VAL:O	1:A:91:ILE:HD12	2.19	0.42
1:B:304:ALA:C	1:B:306:PHE:N	2.75	0.42
1:C:186:GLU:O	1:C:189:THR:HG23	2.18	0.42
1:D:253:TYR:N	1:D:253:TYR:CD1	2.87	0.42
1:D:306:PHE:C	1:D:308:ARG:N	2.76	0.42
1:E:145:VAL:C	1:E:146:THR:O	2.57	0.42
1:E:198:LEU:C	1:E:200:VAL:H	2.28	0.42
1:E:198:LEU:HD23	1:E:198:LEU:HA	1.65	0.42
1:F:125:SER:O	1:F:127:ALA:N	2.51	0.42
1:F:312:ARG:O	1:F:313:LEU:C	2.60	0.42
1:D:204:ILE:HG22	1:D:205:PRO:N	2.35	0.42
1:E:92:THR:C	1:E:94:ALA:H	2.27	0.42
1:E:92:THR:C	1:E:94:ALA:N	2.76	0.42
1:A:175:VAL:HG11	1:A:198:LEU:CD1	2.46	0.42
1:A:186:GLU:O	1:A:189:THR:HG23	2.19	0.42
1:A:312:ARG:O	1:A:315:ASP:N	2.52	0.42
1:B:301:MET:O	1:B:304:ALA:HB3	2.20	0.42
1:C:226:PRO:O	1:C:229:LEU:N	2.53	0.42
1:A:312:ARG:O	1:A:315:ASP:HB2	2.20	0.42
1:B:303:LEU:O	1:B:307:MET:HG2	2.19	0.42
1:E:108:GLU:OE1	1:E:108:GLU:N	2.48	0.42
1:C:257:HIS:HA	1:C:260:ARG:HE	1.85	0.42
1:E:254:ASN:OD1	1:E:254:ASN:O	2.38	0.42
1:A:268:MET:C	1:A:270:SER:H	2.28	0.42
1:B:369:LEU:HD23	1:B:370:CYS:N	2.35	0.42
1:C:205:PRO:HA	1:C:212:GLU:HG3	2.02	0.42
1:D:106:THR:O	1:D:109:ALA:HB3	2.20	0.42
1:D:280:ASP:OD1	1:D:280:ASP:C	2.63	0.42
1:F:125:SER:O	1:F:126:GLU:C	2.63	0.42
1:F:392:VAL:HG12	1:F:393:GLY:H	1.83	0.42
1:A:125:SER:C	1:A:127:ALA:N	2.76	0.42
1:A:161:THR:O	1:A:161:THR:HG23	2.19	0.42
1:B:198:LEU:HA	1:B:198:LEU:HD23	1.82	0.42
1:C:96:VAL:O	1:C:97:LYS:C	2.63	0.42
1:C:232:ILE:HG12	1:C:390:ASP:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ILE:HB	1:C:321:VAL:HG22	2.01	0.42
1:C:281:SER:HB2	1:C:324:THR:OG1	2.20	0.42
1:E:80:MET:CE	1:E:80:MET:CG	2.94	0.42
1:E:351:ALA:O	1:E:352:HIS:C	2.63	0.42
1:F:280:ASP:HA	1:F:281:SER:HA	1.77	0.42
1:F:303:LEU:O	1:F:303:LEU:CG	2.64	0.42
1:F:374:ASP:C	1:F:375:SER:OG	2.61	0.42
1:F:268:MET:C	1:F:270:SER:N	2.77	0.42
1:A:389:GLU:O	1:A:389:GLU:HG2	2.19	0.41
1:A:394:ASP:HB3	1:A:395:PRO:HD2	2.01	0.41
1:B:220:THR:HG21	1:B:281:SER:O	2.20	0.41
1:B:360:PHE:HA	1:B:369:LEU:O	2.20	0.41
1:B:384:VAL:CG1	1:B:385:PHE:N	2.78	0.41
1:D:239:ASP:O	1:D:240:PRO:C	2.62	0.41
1:E:104:LEU:H	1:E:104:LEU:HG	1.58	0.41
1:F:288:THR:HA	1:F:299:ARG:NH2	2.35	0.41
1:A:257:HIS:C	1:A:259:LEU:N	2.77	0.41
1:B:146:THR:HG23	1:B:149:ASP:HB2	2.01	0.41
1:B:194:LEU:C	1:B:194:LEU:CD2	2.90	0.41
1:B:196:HIS:O	1:B:199:ALA:N	2.52	0.41
1:B:230:VAL:O	1:B:232:ILE:N	2.54	0.41
1:C:240:PRO:O	1:C:243:ALA:N	2.53	0.41
1:D:105:HIS:C	1:D:106:THR:OG1	2.63	0.41
1:D:162:THR:CB	1:D:167:LEU:HD23	2.50	0.41
1:E:96:VAL:O	1:E:97:LYS:C	2.59	0.41
1:E:280:ASP:HA	1:E:281:SER:HA	1.74	0.41
1:F:105:HIS:C	1:F:106:THR:HG1	2.28	0.41
1:F:268:MET:O	1:F:270:SER:N	2.53	0.41
1:F:376:PRO:HB2	1:F:377:CYS:H	1.64	0.41
1:B:256:ASP:O	1:B:258:GLN:N	2.53	0.41
1:D:145:VAL:C	1:D:146:THR:O	2.52	0.41
1:E:152:MET:O	1:E:153:ARG:C	2.63	0.41
1:E:233:ALA:O	1:E:234:GLN:C	2.62	0.41
1:F:306:PHE:C	1:F:308:ARG:N	2.78	0.41
1:A:96:VAL:O	1:A:97:LYS:C	2.63	0.41
1:B:347:GLY:O	1:B:350:MET:HB2	2.20	0.41
1:B:389:GLU:O	1:B:389:GLU:HG2	2.21	0.41
1:C:232:ILE:O	1:C:233:ALA:C	2.63	0.41
1:E:113:ALA:HA	1:E:114:PRO:HD3	1.66	0.41
1:F:92:THR:O	1:F:95:ASP:N	2.51	0.41
1:B:104:LEU:O	1:B:105:HIS:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLU:OE1	1:B:357:ARG:CG	2.69	0.41
1:C:240:PRO:O	1:C:241:ASP:C	2.61	0.41
1:D:234:GLN:C	1:D:236:PHE:N	2.77	0.41
1:F:100:ARG:NH1	1:F:100:ARG:CG	2.77	0.41
1:F:226:PRO:O	1:F:228:ARG:N	2.53	0.41
1:A:265:ALA:O	1:A:269:MET:HG3	2.20	0.41
1:A:369:LEU:O	1:A:370:CYS:CB	2.68	0.41
1:C:167:LEU:O	1:C:168:ASP:C	2.63	0.41
1:C:369:LEU:HD21	1:C:382:GLU:HB2	2.03	0.41
1:D:230:VAL:O	1:D:232:ILE:N	2.54	0.41
1:D:266:ALA:C	1:D:268:MET:N	2.74	0.41
1:D:296:LEU:O	1:D:298:ALA:N	2.53	0.41
1:D:301:MET:O	1:D:302:HIS:C	2.64	0.41
1:F:164:SER:O	1:F:164:SER:OG	2.34	0.41
1:F:211:GLY:C	1:F:213:GLY:H	2.28	0.41
1:A:360:PHE:CD1	1:A:360:PHE:N	2.88	0.41
1:B:211:GLY:C	1:B:213:GLY:H	2.28	0.41
1:C:115:ARG:O	1:C:116:LYS:C	2.63	0.41
1:C:194:LEU:HA	1:C:392:VAL:HG21	2.02	0.41
1:C:384:VAL:O	1:C:384:VAL:HG12	2.13	0.41
1:C:387:ILE:C	1:C:388:TYR:HD1	2.28	0.41
1:D:144:PHE:O	1:D:145:VAL:HG13	2.20	0.41
1:E:301:MET:O	1:E:302:HIS:C	2.62	0.41
1:F:83:ILE:O	1:F:84:GLU:C	2.63	0.41
1:F:175:VAL:O	1:F:175:VAL:CG2	2.68	0.41
1:F:204:ILE:HB	1:F:210:GLY:HA3	2.02	0.41
1:F:257:HIS:C	1:F:259:LEU:N	2.77	0.41
1:A:158:ILE:HG21	1:A:158:ILE:HD13	1.77	0.41
1:A:254:ASN:OD1	1:A:254:ASN:C	2.63	0.41
1:B:175:VAL:O	1:B:175:VAL:HG23	2.19	0.41
1:C:136:ALA:O	1:C:137:ALA:C	2.60	0.41
1:C:166:ASN:HB3	1:C:383:CYS:SG	2.61	0.41
1:C:257:HIS:O	1:C:258:GLN:C	2.58	0.41
1:D:188:ARG:HA	2:D:504:SO4:O4	2.20	0.41
1:E:125:SER:O	1:E:128:LYS:N	2.54	0.41
1:E:170:LEU:HG	1:E:372:VAL:HG21	2.02	0.41
1:E:192:SER:O	1:E:193:GLN:C	2.60	0.41
1:E:368:ARG:HG3	1:E:387:ILE:HD11	2.03	0.41
1:A:81:VAL:HB	1:A:107:ALA:HB3	2.02	0.41
1:A:83:ILE:O	1:A:84:GLU:C	2.64	0.41
1:A:141:PRO:O	1:A:142:MET:CG	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:O	1:A:150:PHE:HB3	2.21	0.41
1:B:96:VAL:CG1	1:B:100:ARG:HE	2.34	0.41
1:B:106:THR:O	1:B:107:ALA:C	2.63	0.41
1:B:234:GLN:O	1:B:235:ARG:C	2.60	0.41
1:B:311:GLN:O	1:B:314:ALA:HB3	2.21	0.41
1:C:196:HIS:O	1:C:199:ALA:CB	2.66	0.41
1:C:261:LEU:O	1:C:262:LEU:C	2.62	0.41
1:C:304:ALA:C	1:C:306:PHE:N	2.79	0.41
1:D:170:LEU:O	1:D:378:LEU:HD22	2.20	0.41
1:D:319:VAL:HB	1:D:320:ALA:H	1.76	0.41
1:F:147:ALA:O	1:F:150:PHE:HB3	2.21	0.41
1:F:211:GLY:C	1:F:213:GLY:N	2.78	0.41
1:F:306:PHE:O	1:F:308:ARG:N	2.53	0.41
1:B:183:LEU:HD23	1:B:358:LEU:HB2	2.03	0.41
1:C:325:ASN:HD22	1:C:326:GLN:N	2.19	0.41
1:D:224:PHE:O	1:D:225:ARG:HD3	2.21	0.41
1:E:180:ILE:HG21	1:E:180:ILE:HD13	1.81	0.41
1:E:259:LEU:O	1:E:260:ARG:C	2.63	0.41
1:F:92:THR:HG1	1:F:95:ASP:CG	2.29	0.41
1:F:155:SER:C	1:F:157:LEU:N	2.76	0.41
1:A:300:GLN:CB	1:A:349:ILE:HD11	2.51	0.40
1:A:306:PHE:O	1:A:308:ARG:N	2.55	0.40
1:B:144:PHE:C	1:B:145:VAL:HG13	2.46	0.40
1:D:163:GLY:O	1:D:393:GLY:HA2	2.21	0.40
1:D:368:ARG:HG3	1:D:387:ILE:HD11	2.02	0.40
1:E:267:GLN:O	1:E:270:SER:HB3	2.21	0.40
1:F:282:VAL:HG22	1:F:306:PHE:CE2	2.56	0.40
1:C:216:LEU:HB3	1:C:277:ILE:HG12	2.03	0.40
1:D:125:SER:O	1:D:126:GLU:C	2.64	0.40
1:D:180:ILE:CG2	1:D:181:THR:N	2.80	0.40
1:D:198:LEU:C	1:D:200:VAL:H	2.28	0.40
1:E:188:ARG:HA	2:E:505:SO4:O2	2.21	0.40
1:E:360:PHE:N	1:E:360:PHE:CD1	2.88	0.40
1:F:282:VAL:HG23	1:F:323:VAL:HG13	2.01	0.40
1:B:184:PHE:CD2	1:B:358:LEU:O	2.74	0.40
1:C:193:GLN:CG	1:C:387:ILE:HD13	2.41	0.40
1:C:211:GLY:C	1:C:213:GLY:N	2.77	0.40
1:C:239:ASP:O	1:C:240:PRO:C	2.62	0.40
1:E:229:LEU:O	1:E:230:VAL:C	2.65	0.40
1:E:234:GLN:C	1:E:236:PHE:N	2.78	0.40
1:F:170:LEU:HD21	1:F:372:VAL:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HA	1:A:119:LEU:HD23	1.84	0.40
1:B:184:PHE:HZ	1:B:373:VAL:CG1	2.34	0.40
1:B:186:GLU:O	1:B:189:THR:OG1	2.30	0.40
1:C:257:HIS:C	1:C:259:LEU:N	2.77	0.40
1:C:268:MET:O	1:C:270:SER:N	2.54	0.40
1:E:348:ASN:O	1:E:349:ILE:C	2.62	0.40
1:F:304:ALA:C	1:F:306:PHE:H	2.29	0.40
1:F:373:VAL:O	1:F:374:ASP:O	2.39	0.40
1:F:388:TYR:CD1	1:F:388:TYR:N	2.88	0.40
1:A:148:ALA:O	1:A:149:ASP:C	2.61	0.40
1:A:192:SER:HB2	2:A:501:SO4:S	2.60	0.40
1:F:170:LEU:HD11	1:F:381:ALA:O	2.21	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:E:305:LYS:NZ	1:F:288:THR:OG1[2_545]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/321 (90%)	206 (71%)	55 (19%)	28 (10%)	0	3
1	B	266/321 (83%)	187 (70%)	58 (22%)	21 (8%)	1	4
1	C	266/321 (83%)	189 (71%)	57 (21%)	20 (8%)	1	5
1	D	287/321 (89%)	195 (68%)	73 (25%)	19 (7%)	1	7
1	E	288/321 (90%)	200 (69%)	66 (23%)	22 (8%)	1	5
1	F	288/321 (90%)	206 (72%)	57 (20%)	25 (9%)	0	4
All	All	1684/1926 (87%)	1183 (70%)	366 (22%)	135 (8%)	1	4

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	MET
1	A	153	ARG
1	A	257	HIS
1	A	296	LEU
1	A	297	SER
1	A	319	VAL
1	A	351	ALA
1	A	376	PRO
1	B	227	VAL
1	B	297	SER
1	B	319	VAL
1	C	227	VAL
1	C	297	SER
1	C	319	VAL
1	D	151	HIS
1	D	241	ASP
1	D	284	ALA
1	D	288	THR
1	D	296	LEU
1	D	297	SER
1	D	319	VAL
1	D	374	ASP
1	D	376	PRO
1	E	151	HIS
1	E	241	ASP
1	E	284	ALA
1	E	296	LEU
1	E	297	SER
1	E	319	VAL
1	E	376	PRO
1	F	227	VAL
1	F	257	HIS
1	F	296	LEU
1	F	319	VAL
1	F	351	ALA
1	F	374	ASP
1	F	376	PRO
1	A	151	HIS
1	A	227	VAL
1	A	241	ASP
1	A	255	ALA
1	A	350	MET

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Mol	Chain	Res	Type
1	A	374	ASP
1	B	241	ASP
1	B	257	HIS
1	C	153	ARG
1	C	241	ASP
1	C	296	LEU
1	C	307	MET
1	C	356	THR
1	D	201	THR
1	D	227	VAL
1	D	240	PRO
1	D	257	HIS
1	D	313	LEU
1	E	201	THR
1	E	227	VAL
1	E	240	PRO
1	E	257	HIS
1	E	289	ASP
1	E	313	LEU
1	E	370	CYS
1	E	374	ASP
1	F	153	ARG
1	F	201	THR
1	F	241	ASP
1	F	297	SER
1	A	198	LEU
1	A	201	THR
1	A	269	MET
1	A	307	MET
1	B	127	ALA
1	B	264	ALA
1	B	307	MET
1	C	127	ALA
1	C	201	THR
1	C	245	ASN
1	C	257	HIS
1	C	258	GLN
1	C	264	ALA
1	C	269	MET
1	C	372	VAL
1	D	197	THR
1	D	198	LEU

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Mol	Chain	Res	Type
1	E	237	GLY
1	E	255	ALA
1	F	117	ASP
1	F	141	PRO
1	F	198	LEU
1	F	264	ALA
1	F	269	MET
1	F	350	MET
1	A	197	THR
1	A	381	ALA
1	B	101	GLU
1	B	111	ALA
1	B	153	ARG
1	B	256	ASP
1	B	258	GLN
1	B	296	LEU
1	C	101	GLU
1	C	111	ALA
1	C	240	PRO
1	D	237	GLY
1	E	197	THR
1	E	379	PRO
1	F	197	THR
1	F	256	ASP
1	F	283	MET
1	F	349	ILE
1	A	84	GLU
1	A	117	ASP
1	A	240	PRO
1	A	256	ASP
1	A	370	CYS
1	B	201	THR
1	B	214	LYS
1	B	240	PRO
1	C	355	THR
1	D	307	MET
1	D	379	PRO
1	E	198	LEU
1	F	240	PRO
1	F	245	ASN
1	F	258	GLN
1	F	378	LEU

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Mol	Chain	Res	Type
1	A	346	GLY
1	A	378	LEU
1	B	313	LEU
1	B	350	MET
1	B	372	VAL
1	E	305	LYS
1	A	237	GLY
1	B	237	GLY
1	E	378	LEU

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	217/260 (84%)	203 (94%)	14 (6%)	15	42
1	B	197/260 (76%)	184 (93%)	13 (7%)	15	42
1	C	199/260 (76%)	183 (92%)	16 (8%)	11	35
1	D	217/260 (84%)	195 (90%)	22 (10%)	7	26
1	E	217/260 (84%)	194 (89%)	23 (11%)	6	24
1	F	215/260 (83%)	197 (92%)	18 (8%)	10	33
All	All	1262/1560 (81%)	1156 (92%)	106 (8%)	10	33

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	A	140	VAL
1	A	146	THR
1	A	194	LEU
1	A	207	ASP
1	A	216	LEU
1	A	231	SER
1	A	254	ASN
1	A	276	LEU

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Mol	Chain	Res	Type
1	A	282	VAL
1	A	285	LEU
1	A	370	CYS
1	A	377	CYS
1	A	383	CYS
1	B	146	THR
1	B	161	THR
1	B	216	LEU
1	B	225	ARG
1	B	227	VAL
1	B	242	ASP
1	B	271	GLU
1	B	276	LEU
1	B	280	ASP
1	B	282	VAL
1	B	296	LEU
1	B	353	SER
1	B	355	THR
1	C	139	LEU
1	C	141	PRO
1	C	146	THR
1	C	161	THR
1	C	216	LEU
1	C	218	ILE
1	C	227	VAL
1	C	242	ASP
1	C	276	LEU
1	C	280	ASP
1	C	282	VAL
1	C	283	MET
1	C	302	HIS
1	C	354	SER
1	C	355	THR
1	C	384	VAL
1	D	83	ILE
1	D	87	GLN
1	D	89	ASN
1	D	102	SER
1	D	140	VAL
1	D	146	THR
1	D	164	SER
1	D	207	ASP

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Mol	Chain	Res	Type
1	D	216	LEU
1	D	225	ARG
1	D	227	VAL
1	D	228	ARG
1	D	231	SER
1	D	245	ASN
1	D	276	LEU
1	D	280	ASP
1	D	282	VAL
1	D	288	THR
1	D	289	ASP
1	D	370	CYS
1	D	377	CYS
1	D	383	CYS
1	E	80	MET
1	E	83	ILE
1	E	89	ASN
1	E	102	SER
1	E	140	VAL
1	E	146	THR
1	E	164	SER
1	E	207	ASP
1	E	216	LEU
1	E	218	ILE
1	E	225	ARG
1	E	227	VAL
1	E	231	SER
1	E	276	LEU
1	E	280	ASP
1	E	282	VAL
1	E	285	LEU
1	E	326	GLN
1	E	370	CYS
1	E	376	PRO
1	E	377	CYS
1	E	383	CYS
1	E	384	VAL
1	F	80	MET
1	F	89	ASN
1	F	108	GLU
1	F	146	THR
1	F	155	SER

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Mol	Chain	Res	Type
1	F	164	SER
1	F	194	LEU
1	F	207	ASP
1	F	216	LEU
1	F	231	SER
1	F	254	ASN
1	F	276	LEU
1	F	281	SER
1	F	282	VAL
1	F	326	GLN
1	F	370	CYS
1	F	377	CYS
1	F	383	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	193	GLN
1	A	267	GLN
1	B	89	ASN
1	B	105	HIS
1	B	245	ASN
1	B	325	ASN
1	C	89	ASN
1	C	105	HIS
1	C	267	GLN
1	C	311	GLN
1	C	325	ASN
1	D	89	ASN
1	D	151	HIS
1	D	193	GLN
1	D	311	GLN
1	E	89	ASN
1	E	193	GLN
1	E	245	ASN
1	E	257	HIS
1	E	311	GLN
1	E	325	ASN
1	F	89	ASN
1	F	166	ASN
1	F	193	GLN

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Mol	Chain	Res	Type
1	F	245	ASN
1	F	311	GLN
1	F	325	ASN
1	F	352	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	501	-	4,4,4	1.00	0	6,6,6	1.29	1 (16%)
2	SO4	D	504	-	4,4,4	0.79	0	6,6,6	2.13	3 (50%)
2	SO4	E	505	-	4,4,4	1.22	1 (25%)	6,6,6	1.51	1 (16%)
2	SO4	F	506	-	4,4,4	0.42	0	6,6,6	0.94	0
2	SO4	B	502	-	4,4,4	0.56	0	6,6,6	1.83	2 (33%)
2	SO4	C	503	-	4,4,4	0.58	0	6,6,6	1.62	2 (33%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	505	SO4	O1-S	-2.06	1.32	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	SO4	O3-S-O2	3.25	126.57	109.56
2	D	504	SO4	O2-S-O1	-3.02	87.78	109.06
2	B	502	SO4	O4-S-O1	2.95	124.97	109.56
2	C	503	SO4	O4-S-O1	-2.73	95.29	109.56
2	C	503	SO4	O4-S-O3	2.68	123.31	108.54
2	B	502	SO4	O2-S-O1	-2.51	91.34	109.06
2	E	505	SO4	O4-S-O3	2.32	121.30	108.54
2	A	501	SO4	O3-S-O1	-2.13	98.45	109.56
2	D	504	SO4	O4-S-O2	-2.07	98.76	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	0
2	D	504	SO4	2	0
2	E	505	SO4	2	0
2	B	502	SO4	2	0
2	C	503	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/321 (91%)	-1.46	0 100 100	6, 36, 69, 98	0
1	B	274/321 (85%)	-1.29	0 100 100	23, 64, 98, 128	0
1	C	274/321 (85%)	-1.29	0 100 100	22, 63, 99, 121	0
1	D	293/321 (91%)	-1.40	0 100 100	12, 51, 81, 112	0
1	E	294/321 (91%)	-1.37	0 100 100	15, 53, 82, 112	0
1	F	294/321 (91%)	-1.48	0 100 100	5, 35, 72, 93	0
All	All	1724/1926 (89%)	-1.38	0 100 100	5, 49, 93, 128	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	502	5/5	0.99	0.03	55,58,62,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	503	5/5	0.99	0.03	49,52,62,65	0
2	SO4	D	504	5/5	0.99	0.03	33,36,42,43	0
2	SO4	E	505	5/5	0.99	0.03	32,35,35,39	0
2	SO4	A	501	5/5	1.00	0.04	37,40,47,48	0
2	SO4	F	506	5/5	1.00	0.02	36,41,44,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.