



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:58 PM UTC

PDB ID : 7KQY / pdb_00007kqy
Title : Crystal Structure and Characterization of Human Heavy-Chain only Antibodies reveals a novel, stable dimeric structure similar to Monoclonal Antibodies
Authors : Bahmanjah, S.; Mieczkowski, C.; Yu, Y.; Baker, J.; Raghunathan, G.; Tomazela, D.; Hsieh, M.; McCoy, M.; Strickland, C.; Fayadat-Dilman, L.
Deposited on : 2020-11-18
Resolution : 2.91 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
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

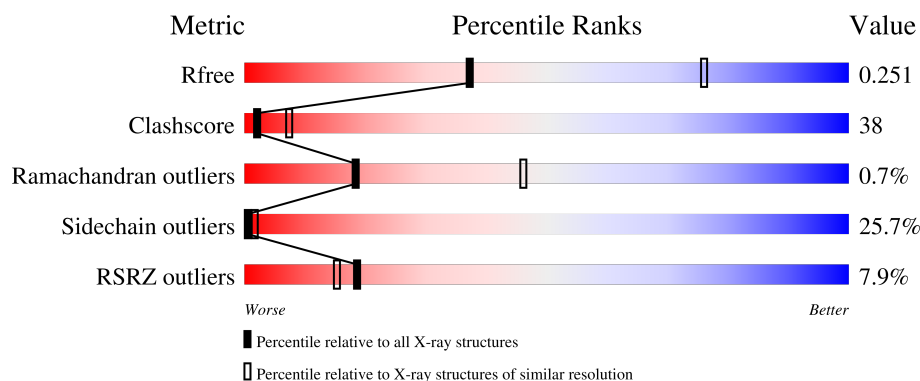
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	

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Mol	Chain	Length	Quality of chain
1	F	448	4%14%19%11%54%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9265 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.

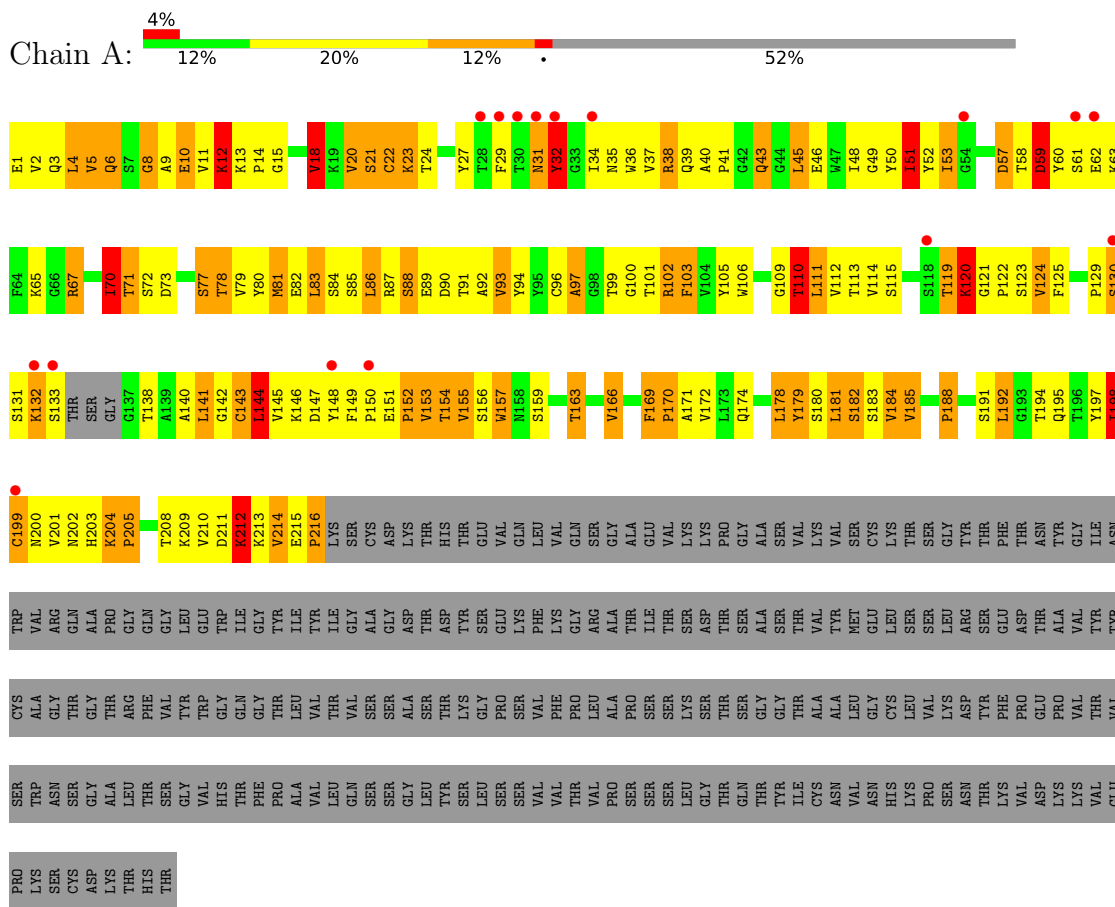
- Molecule 1 is a protein called Heavy-Chain only Human Antibodies.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1588	1006	259	318	5			
1	B	203	Total	C	N	O	S	0	0	0
			1504	953	244	302	5			
1	C	202	Total	C	N	O	S	0	0	0
			1508	959	246	298	5			
1	D	207	Total	C	N	O	S	0	0	0
			1542	981	249	307	5			
1	E	216	Total	C	N	O	S	0	0	0
			1605	1015	262	323	5			
1	F	204	Total	C	N	O	S	0	0	0
			1518	962	248	303	5			

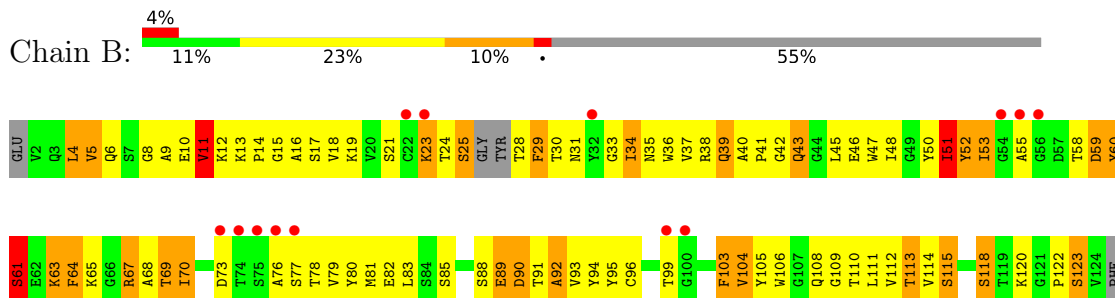
3 Residue-property plots [i](#)

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.

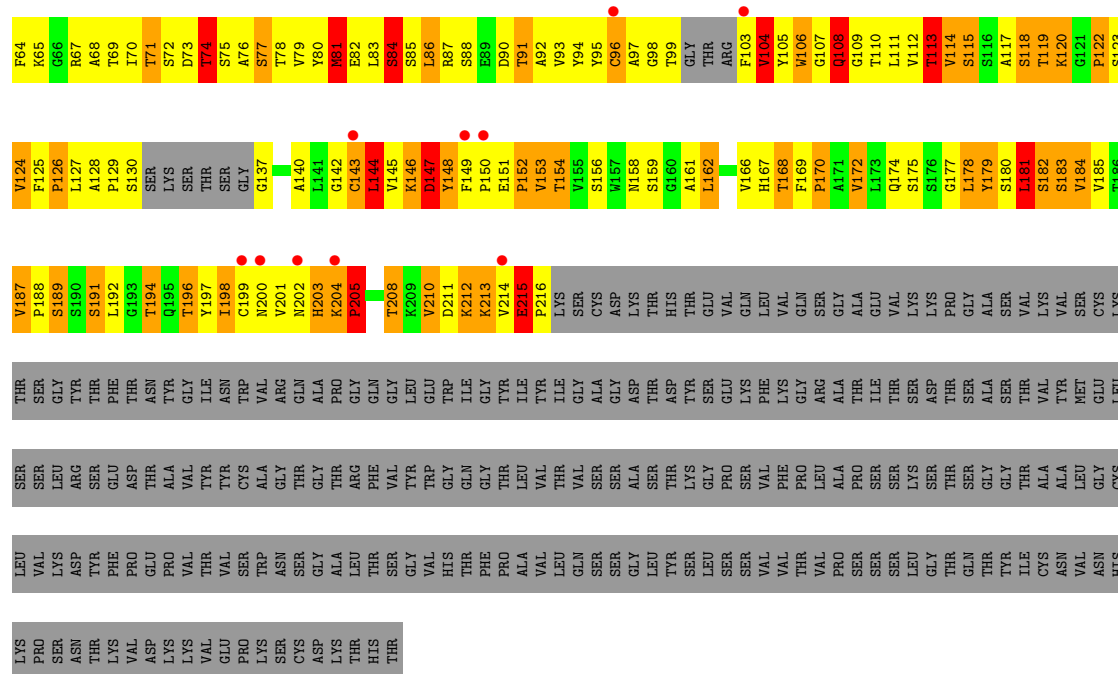
• Molecule 1: Heavy-Chain only Human Antibodies



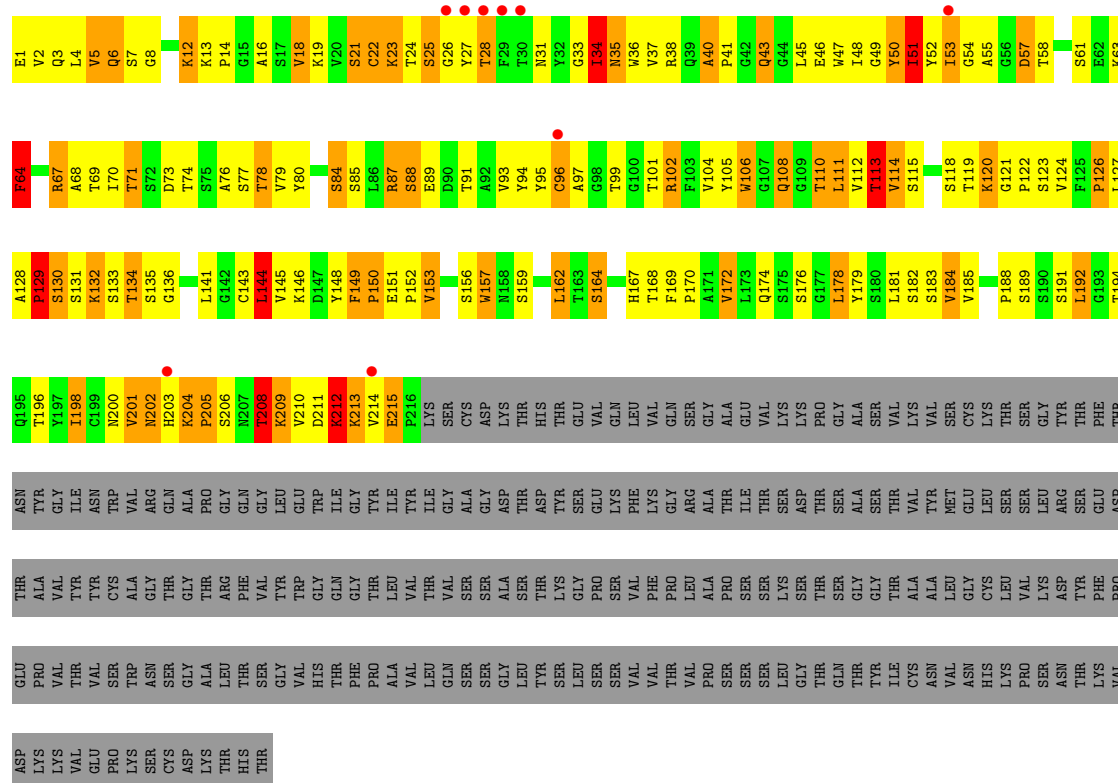
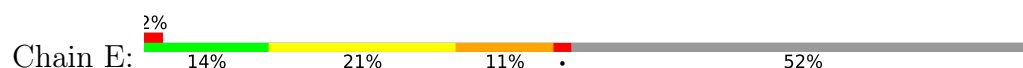
• Molecule 1: Heavy-Chain only Human Antibodies



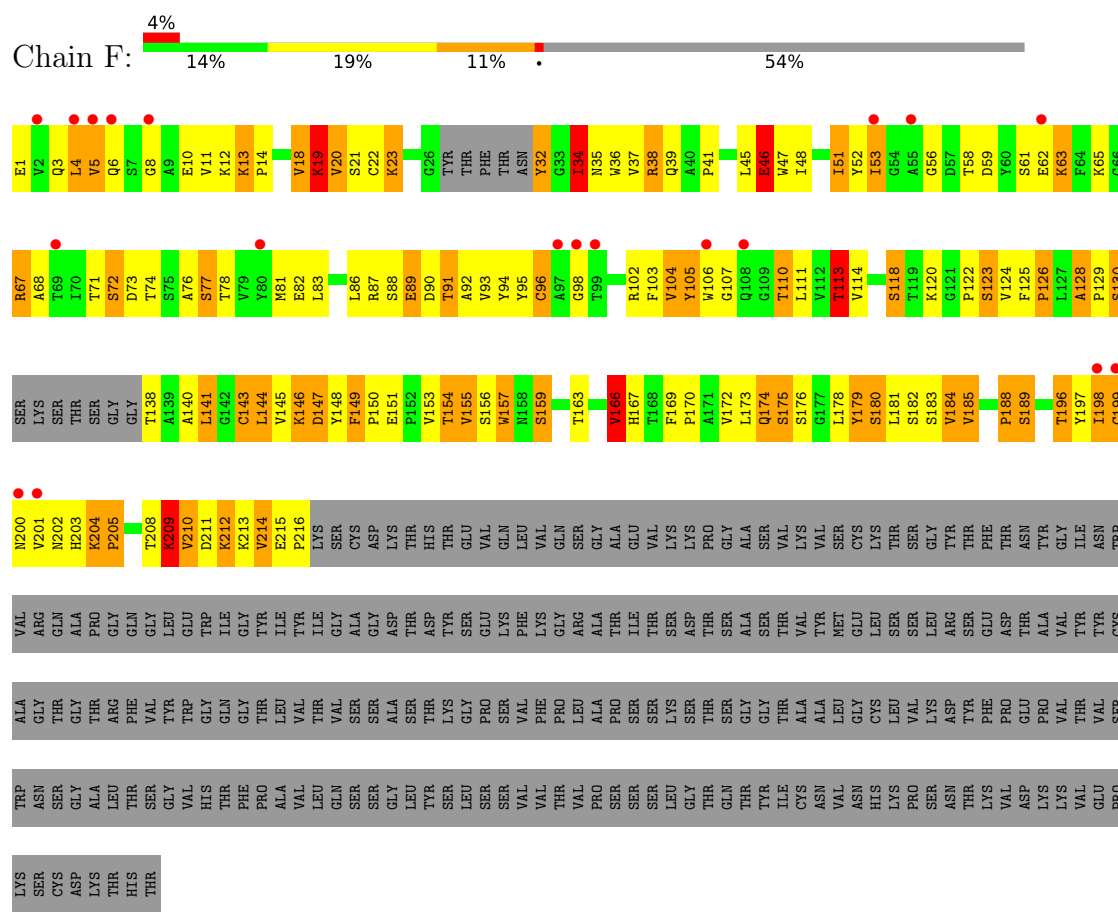




• Molecule 1: Heavy-Chain only Human Antibodies



• Molecule 1: Heavy-Chain only Human Antibodies



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.62Å 73.42Å 140.41Å 90.00° 125.71° 90.00°	Depositor
Resolution (Å)	114.01 – 2.91 114.01 – 2.91	Depositor EDS
% Data completeness (in resolution range)	73.4 (114.01-2.91) 73.5 (114.01-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.207 , 0.260 (Not available) , 0.251	Depositor DCC
R_{free} test set	1082 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9265	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.71% 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 ⓘ

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	2.19	103/1625 (6.3%)	1.63	19/2215 (0.9%)
1	B	2.27	109/1536 (7.1%)	1.70	21/2094 (1.0%)
1	C	2.09	81/1542 (5.3%)	1.66	12/2102 (0.6%)
1	D	2.36	111/1578 (7.0%)	1.83	24/2152 (1.1%)
1	E	2.10	83/1643 (5.1%)	1.71	24/2241 (1.1%)
1	F	1.95	63/1552 (4.1%)	1.59	12/2115 (0.6%)
All	All	2.16	550/9476 (5.8%)	1.69	112/12919 (0.9%)

All (550) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	126	PRO	C-O	-10.80	1.13	1.23
1	E	210	VAL	C-O	-10.08	1.12	1.24
1	D	113	THR	C-O	-10.08	1.12	1.24
1	C	18	VAL	C-O	-10.02	1.14	1.24
1	B	41	PRO	C-O	-9.99	1.16	1.24
1	A	94	TYR	C-O	-9.80	1.12	1.24
1	C	37	VAL	C-O	-9.69	1.14	1.24
1	D	34	ILE	C-O	-9.47	1.14	1.24
1	E	209	LYS	C-O	-9.40	1.13	1.24
1	C	35	ASN	C-O	-9.30	1.12	1.23
1	B	37	VAL	C-O	-9.29	1.14	1.24
1	D	36	TRP	C-O	-9.27	1.12	1.24
1	D	114	VAL	C-O	-9.21	1.14	1.24
1	B	208	THR	C-O	-9.21	1.12	1.24
1	D	51	ILE	C-O	-9.17	1.14	1.24
1	D	203	HIS	C-O	-9.17	1.12	1.23
1	A	112	VAL	C-O	-9.16	1.14	1.24
1	D	14	PRO	C-O	-9.12	1.13	1.23
1	A	155	VAL	C-O	-8.99	1.14	1.24
1	E	200	ASN	C-O	-8.95	1.13	1.24
1	E	205	PRO	C-O	-8.95	1.12	1.24
1	A	78	THR	C-O	-8.94	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	79	VAL	C-O	-8.90	1.15	1.24
1	A	14	PRO	C-O	-8.88	1.13	1.23
1	A	4	LEU	C-O	-8.87	1.14	1.24
1	B	113	THR	C-O	-8.85	1.13	1.24
1	D	143	CYS	C-O	-8.78	1.14	1.24
1	D	82	GLU	C-O	-8.78	1.13	1.24
1	D	208	THR	C-O	-8.76	1.13	1.23
1	C	79	VAL	C-O	-8.72	1.15	1.24
1	A	144	LEU	C-O	-8.71	1.13	1.24
1	A	93	VAL	C-O	-8.67	1.14	1.24
1	B	36	TRP	C-O	-8.62	1.13	1.24
1	B	81	MET	C-O	-8.62	1.14	1.24
1	C	14	PRO	C-O	-8.58	1.13	1.23
1	B	93	VAL	C-O	-8.50	1.14	1.24
1	A	18	VAL	C-O	-8.48	1.15	1.24
1	B	46	GLU	C-O	-8.44	1.14	1.23
1	D	11	VAL	C-O	-8.42	1.15	1.24
1	F	182	SER	C-O	-8.40	1.14	1.24
1	D	37	VAL	C-O	-8.40	1.15	1.24
1	A	92	ALA	C-O	-8.38	1.14	1.23
1	E	188	PRO	C-O	-8.38	1.14	1.23
1	A	37	VAL	C-O	-8.33	1.15	1.24
1	D	5	VAL	C-O	-8.26	1.15	1.24
1	A	181	LEU	C-O	-8.26	1.13	1.23
1	D	123	SER	C-O	-8.23	1.14	1.24
1	D	20	VAL	C-O	-8.22	1.15	1.24
1	D	115	SER	C-O	-8.21	1.13	1.23
1	D	38	ARG	C-O	-8.20	1.13	1.23
1	C	92	ALA	C-O	-8.17	1.15	1.24
1	E	114	VAL	C-O	-8.17	1.15	1.24
1	B	200	ASN	C-O	-8.14	1.14	1.24
1	B	14	PRO	C-O	-8.13	1.13	1.23
1	E	170	PRO	C-O	-8.10	1.14	1.23
1	D	68	ALA	C-O	-8.09	1.14	1.23
1	C	182	SER	C-O	-8.07	1.15	1.23
1	D	48	ILE	C-O	-8.06	1.13	1.24
1	C	34	ILE	C-O	-8.02	1.15	1.24
1	E	172	VAL	C-O	-8.02	1.15	1.24
1	A	51	ILE	C-O	-7.98	1.16	1.24
1	D	153	VAL	C-O	-7.98	1.16	1.24
1	B	203	HIS	C-O	-7.97	1.14	1.23
1	D	182	SER	C-O	-7.96	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	LEU	C-O	-7.95	1.13	1.23
1	B	35	ASN	C-O	-7.95	1.14	1.23
1	C	51	ILE	C-O	-7.94	1.16	1.24
1	C	47	TRP	C-O	-7.94	1.14	1.23
1	A	208	THR	C-O	-7.92	1.14	1.24
1	A	96	CYS	C-O	-7.90	1.14	1.24
1	F	122	PRO	C-O	-7.88	1.15	1.23
1	F	148	TYR	C-O	-7.88	1.14	1.23
1	A	154	THR	C-O	-7.86	1.14	1.24
1	E	153	VAL	C-O	-7.86	1.15	1.24
1	F	170	PRO	C-O	-7.86	1.14	1.23
1	A	200	ASN	C-O	-7.85	1.13	1.23
1	B	178	LEU	C-O	-7.84	1.14	1.23
1	E	157	TRP	C-O	-7.84	1.14	1.24
1	E	212	LYS	C-O	-7.82	1.14	1.24
1	A	203	HIS	C-O	-7.80	1.14	1.23
1	E	184	VAL	C-O	-7.79	1.16	1.24
1	B	209	LYS	C-O	-7.78	1.15	1.24
1	D	154	THR	C-O	-7.78	1.15	1.24
1	B	18	VAL	C-O	-7.76	1.16	1.24
1	D	168	THR	C-O	-7.76	1.14	1.24
1	D	125	PHE	C-O	-7.75	1.14	1.24
1	A	113	THR	C-O	-7.71	1.14	1.24
1	B	110	THR	C-O	-7.71	1.14	1.24
1	D	111	LEU	C-O	-7.71	1.14	1.24
1	B	70	ILE	C-O	-7.70	1.15	1.24
1	C	94	TYR	C-O	-7.67	1.14	1.23
1	C	49	GLY	C-O	-7.67	1.16	1.23
1	A	39	GLN	C-O	-7.66	1.15	1.24
1	D	72	SER	C-O	-7.65	1.14	1.23
1	A	12	LYS	C-O	-7.65	1.14	1.23
1	D	18	VAL	C-O	-7.64	1.16	1.24
1	A	80	TYR	C-O	-7.63	1.14	1.23
1	D	178	LEU	C-O	-7.62	1.14	1.23
1	C	3	GLN	C-O	-7.62	1.15	1.23
1	D	179	TYR	C-O	-7.61	1.15	1.23
1	B	39	GLN	C-O	-7.61	1.15	1.24
1	A	172	VAL	C-O	-7.60	1.16	1.24
1	A	106	TRP	C-O	-7.60	1.14	1.23
1	B	172	VAL	C-O	-7.59	1.16	1.24
1	B	38	ARG	C-O	-7.59	1.14	1.23
1	D	94	TYR	C-O	-7.58	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	152	PRO	C-O	-7.57	1.13	1.23
1	A	2	VAL	C-O	-7.55	1.15	1.24
1	D	119	THR	C-O	-7.54	1.15	1.23
1	D	120	LYS	C-O	-7.51	1.14	1.23
1	C	17	SER	C-O	-7.51	1.14	1.23
1	E	95	TYR	C-O	-7.48	1.15	1.24
1	B	205	PRO	C-O	-7.48	1.14	1.24
1	A	9	ALA	C-O	-7.46	1.15	1.23
1	E	211	ASP	C-O	-7.45	1.15	1.24
1	C	111	LEU	C-O	-7.44	1.14	1.24
1	D	124	VAL	C-O	-7.44	1.16	1.24
1	F	124	VAL	C-O	-7.43	1.15	1.24
1	D	21	SER	C-O	-7.42	1.14	1.23
1	E	49	GLY	C-O	-7.42	1.15	1.24
1	B	90	ASP	C-O	-7.39	1.14	1.24
1	B	157	TRP	C-O	-7.38	1.15	1.24
1	B	182	SER	C-O	-7.38	1.15	1.24
1	C	113	THR	C-O	-7.37	1.15	1.23
1	D	10	GLU	C-O	-7.37	1.15	1.23
1	D	60	TYR	C-O	-7.37	1.14	1.23
1	C	5	VAL	C-O	-7.34	1.16	1.24
1	F	181	LEU	C-O	-7.34	1.14	1.23
1	B	95	TYR	C-O	-7.33	1.15	1.24
1	E	21	SER	C-O	-7.32	1.15	1.23
1	A	105	TYR	C-O	-7.32	1.15	1.24
1	B	184	VAL	C-O	-7.32	1.16	1.24
1	F	172	VAL	C-O	-7.31	1.16	1.24
1	C	52	TYR	C-O	-7.29	1.15	1.24
1	D	81	MET	C-O	-7.29	1.15	1.24
1	E	70	ILE	C-O	-7.28	1.16	1.24
1	C	70	ILE	C-O	-7.28	1.16	1.24
1	F	211	ASP	C-O	-7.28	1.15	1.24
1	D	144	LEU	C-O	-7.28	1.15	1.24
1	C	50	TYR	C-O	-7.27	1.15	1.23
1	A	45	LEU	C-O	-7.26	1.14	1.23
1	D	41	PRO	C-O	-7.26	1.14	1.24
1	D	129	PRO	C-O	-7.25	1.15	1.23
1	B	170	PRO	C-O	-7.24	1.15	1.23
1	A	123	SER	C-O	-7.24	1.15	1.24
1	B	122	PRO	C-O	-7.24	1.15	1.23
1	F	125	PHE	C-O	-7.23	1.16	1.25
1	A	38	ARG	C-O	-7.20	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	CYS	C-O	-7.18	1.15	1.24
1	B	10	GLU	C-O	-7.18	1.14	1.23
1	D	203	HIS	CE1-NE2	-7.17	1.25	1.32
1	B	19	LYS	C-O	-7.16	1.15	1.24
1	B	94	TYR	C-O	-7.15	1.15	1.24
1	C	23	LYS	C-O	-7.12	1.15	1.23
1	A	170	PRO	C-O	-7.11	1.15	1.23
1	D	126	PRO	C-O	-7.09	1.14	1.24
1	B	83	LEU	C-O	-7.09	1.16	1.24
1	F	143	CYS	C-O	-7.07	1.16	1.23
1	E	149	PHE	C-O	-7.07	1.15	1.24
1	D	93	VAL	C-O	-7.07	1.16	1.24
1	D	39	GLN	C-O	-7.06	1.16	1.24
1	E	36	TRP	C-O	-7.04	1.16	1.24
1	B	48	ILE	C-O	-7.03	1.16	1.23
1	B	204	LYS	C-O	-7.03	1.18	1.24
1	D	122	PRO	C-O	-7.03	1.16	1.23
1	F	157	TRP	C-O	-7.03	1.16	1.24
1	A	201	VAL	C-O	-7.02	1.16	1.24
1	C	48	ILE	C-O	-7.00	1.15	1.23
1	F	14	PRO	C-O	-6.99	1.15	1.23
1	A	73	ASP	C-O	-6.99	1.16	1.24
1	A	23	LYS	C-O	-6.98	1.15	1.23
1	D	50	TYR	C-O	-6.98	1.15	1.23
1	C	10	GLU	C-O	-6.98	1.15	1.24
1	B	17	SER	C-O	-6.95	1.15	1.23
1	E	118	SER	C-O	-6.92	1.15	1.23
1	D	83	LEU	C-O	-6.92	1.15	1.24
1	D	77	SER	C-O	-6.92	1.14	1.23
1	E	41	PRO	C-O	-6.92	1.15	1.23
1	C	67	ARG	C-O	-6.91	1.15	1.24
1	F	205	PRO	C-O	-6.91	1.15	1.24
1	E	106	TRP	C-O	-6.91	1.15	1.23
1	A	182	SER	C-O	-6.90	1.15	1.23
1	A	109	GLY	C-O	-6.89	1.14	1.23
1	A	185	VAL	C-O	-6.89	1.17	1.24
1	D	71	THR	C-O	-6.89	1.15	1.23
1	C	46	GLU	C-O	-6.88	1.15	1.23
1	E	201	VAL	C-O	-6.87	1.14	1.24
1	A	209	LYS	C-O	-6.85	1.16	1.24
1	B	152	PRO	N-CD	-6.85	1.38	1.47
1	F	155	VAL	C-O	-6.84	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	14	PRO	C-O	-6.83	1.15	1.23
1	D	52	TYR	C-O	-6.83	1.15	1.24
1	A	203	HIS	CE1-NE2	-6.82	1.25	1.32
1	D	49	GLY	C-O	-6.82	1.16	1.23
1	B	202	ASN	C-O	-6.82	1.16	1.24
1	E	129	PRO	C-O	-6.81	1.15	1.24
1	D	4	LEU	C-O	-6.80	1.16	1.24
1	B	211	ASP	C-O	-6.79	1.16	1.24
1	D	109	GLY	C-O	-6.77	1.14	1.23
1	D	142	GLY	C-O	-6.77	1.15	1.24
1	E	50	TYR	C-O	-6.76	1.16	1.24
1	F	146	LYS	C-O	-6.75	1.15	1.23
1	A	211	ASP	C-O	-6.75	1.16	1.24
1	D	110	THR	C-O	-6.75	1.16	1.24
1	B	106	TRP	C-O	-6.74	1.15	1.24
1	A	205	PRO	C-O	-6.73	1.15	1.24
1	C	82	GLU	C-O	-6.73	1.16	1.24
1	C	21	SER	C-O	-6.72	1.15	1.23
1	F	179	TYR	C-O	-6.70	1.15	1.23
1	F	123	SER	C-O	-6.69	1.15	1.23
1	E	181	LEU	C-O	-6.69	1.15	1.23
1	E	198	ILE	C-O	-6.69	1.17	1.24
1	F	149	PHE	C-O	-6.69	1.14	1.25
1	D	181	LEU	C-O	-6.68	1.15	1.23
1	C	36	TRP	C-O	-6.68	1.16	1.24
1	A	210	VAL	C-O	-6.67	1.15	1.24
1	F	38	ARG	C-O	-6.67	1.15	1.23
1	F	126	PRO	C-O	-6.66	1.16	1.23
1	D	172	VAL	C-O	-6.66	1.16	1.24
1	B	34	ILE	C-O	-6.65	1.16	1.24
1	C	39	GLN	C-O	-6.63	1.16	1.24
1	C	19	LYS	C-O	-6.62	1.16	1.24
1	E	18	VAL	C-O	-6.62	1.17	1.24
1	B	5	VAL	C-O	-6.61	1.17	1.24
1	D	73	ASP	C-O	-6.61	1.16	1.24
1	B	109	GLY	C-O	-6.61	1.16	1.24
1	D	69	THR	C-O	-6.60	1.16	1.24
1	B	111	LEU	C-O	-6.60	1.15	1.24
1	B	212	LYS	C-O	-6.59	1.16	1.24
1	E	96	CYS	C-O	-6.58	1.16	1.24
1	A	82	GLU	C-O	-6.58	1.16	1.24
1	C	38	ARG	C-O	-6.57	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	TYR	C-O	-6.56	1.15	1.23
1	F	36	TRP	C-O	-6.56	1.16	1.24
1	E	110	THR	C-O	-6.55	1.16	1.24
1	A	179	TYR	C-O	-6.53	1.15	1.23
1	B	188	PRO	C-O	-6.53	1.15	1.23
1	C	4	LEU	C-O	-6.53	1.16	1.24
1	E	208	THR	C-O	-6.52	1.16	1.24
1	F	141	LEU	C-O	-6.51	1.16	1.24
1	A	204	LYS	C-O	-6.51	1.18	1.24
1	F	144	LEU	C-O	-6.50	1.16	1.24
1	A	3	GLN	C-O	-6.50	1.15	1.23
1	B	47	TRP	C-O	-6.50	1.16	1.24
1	C	81	MET	C-O	-6.50	1.16	1.24
1	E	145	VAL	C-O	-6.49	1.16	1.24
1	B	104	VAL	C-O	-6.47	1.17	1.24
1	A	111	LEU	C-O	-6.45	1.16	1.24
1	E	182	SER	C-O	-6.45	1.16	1.24
1	E	120	LYS	C-O	-6.44	1.16	1.23
1	D	198	ILE	C-O	-6.44	1.17	1.24
1	D	210	VAL	C-O	-6.43	1.17	1.23
1	F	188	PRO	C-O	-6.43	1.14	1.23
1	A	59	ASP	C-O	-6.43	1.16	1.23
1	E	94	TYR	C-O	-6.42	1.16	1.24
1	C	77	SER	CA-CB	-6.41	1.44	1.53
1	F	95	TYR	C-O	-6.41	1.15	1.23
1	D	95	TYR	C-O	-6.40	1.15	1.23
1	E	12	LYS	C-O	-6.39	1.15	1.23
1	C	96	CYS	C-O	-6.39	1.16	1.24
1	A	72	SER	C-O	-6.39	1.16	1.23
1	E	206	SER	CA-CB	-6.37	1.45	1.54
1	D	86	LEU	C-O	-6.37	1.15	1.23
1	D	35	ASN	C-O	-6.36	1.16	1.23
1	A	198	ILE	C-O	-6.36	1.17	1.24
1	E	113	THR	C-O	-6.35	1.16	1.24
1	C	22	CYS	C-O	-6.34	1.16	1.24
1	D	22	CYS	C-O	-6.34	1.16	1.23
1	F	167	HIS	C-O	-6.34	1.16	1.24
1	B	61	SER	CA-CB	-6.34	1.43	1.53
1	E	51	ILE	C-O	-6.34	1.17	1.24
1	D	205	PRO	C-O	-6.33	1.15	1.24
1	C	93	VAL	C-O	-6.33	1.17	1.24
1	A	49	GLY	C-O	-6.32	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	209	LYS	C-O	-6.32	1.16	1.24
1	D	9	ALA	C-O	-6.32	1.16	1.23
1	B	203	HIS	CE1-NE2	-6.31	1.26	1.32
1	A	48	ILE	C-O	-6.30	1.16	1.23
1	E	191	SER	CA-CB	-6.30	1.44	1.53
1	B	16	ALA	C-O	-6.29	1.15	1.23
1	B	29	PHE	C-O	-6.29	1.16	1.24
1	E	183	SER	C-O	-6.29	1.16	1.24
1	B	123	SER	C-O	-6.29	1.16	1.24
1	B	120	LYS	C-O	-6.27	1.16	1.23
1	F	111	LEU	C-O	-6.27	1.16	1.24
1	D	96	CYS	C-O	-6.25	1.16	1.23
1	F	202	ASN	C-O	-6.23	1.16	1.23
1	D	3	GLN	C-O	-6.22	1.17	1.24
1	B	52	TYR	C-O	-6.22	1.16	1.24
1	A	120	LYS	C-O	-6.22	1.16	1.23
1	C	183	SER	C-O	-6.21	1.16	1.24
1	F	46	GLU	C-O	-6.21	1.17	1.23
1	E	71	THR	C-O	-6.21	1.16	1.23
1	F	185	VAL	C-O	-6.21	1.17	1.24
1	C	64	PHE	C-O	-6.21	1.15	1.24
1	A	199	CYS	C-O	-6.19	1.16	1.24
1	A	70	ILE	C-O	-6.17	1.17	1.24
1	B	12	LYS	C-O	-6.17	1.16	1.23
1	E	156	SER	C-O	-6.17	1.16	1.23
1	B	33	GLY	C-O	-6.17	1.15	1.23
1	C	166	VAL	C-O	-6.16	1.16	1.23
1	B	80	TYR	C-O	-6.16	1.16	1.23
1	C	106	TRP	C-O	-6.16	1.16	1.23
1	B	167	HIS	C-O	-6.16	1.17	1.24
1	C	105	TYR	C-O	-6.14	1.16	1.23
1	B	179	TYR	C-O	-6.14	1.16	1.23
1	F	184	VAL	C-O	-6.14	1.17	1.24
1	D	85	SER	C-O	-6.13	1.15	1.23
1	F	93	VAL	C-O	-6.12	1.17	1.24
1	B	79	VAL	C-O	-6.11	1.17	1.24
1	A	184	VAL	C-O	-6.11	1.17	1.24
1	D	90	ASP	CG-OD1	-6.11	1.13	1.25
1	E	6	GLN	C-O	-6.10	1.15	1.23
1	A	81	MET	C-O	-6.09	1.17	1.24
1	E	167	HIS	C-O	-6.09	1.16	1.24
1	B	43	GLN	C-O	-6.08	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	VAL	C-O	-6.08	1.17	1.24
1	E	115	SER	C-O	-6.08	1.16	1.23
1	B	206	SER	C-O	-6.08	1.16	1.23
1	F	180	SER	C-O	-6.07	1.16	1.23
1	D	175	SER	C-O	-6.07	1.16	1.24
1	D	183	SER	C-O	-6.06	1.17	1.24
1	A	166	VAL	C-O	-6.06	1.17	1.24
1	B	60	TYR	C-O	-6.06	1.16	1.23
1	E	112	VAL	C-O	-6.04	1.17	1.24
1	D	90	ASP	C-O	-6.03	1.16	1.24
1	E	3	GLN	C-O	-6.03	1.16	1.23
1	A	5	VAL	C-O	-6.03	1.17	1.24
1	E	179	TYR	C-O	-6.03	1.16	1.23
1	E	38	ARG	C-O	-6.02	1.16	1.23
1	D	112	VAL	C-O	-6.01	1.17	1.24
1	C	112	VAL	C-O	-6.01	1.17	1.24
1	A	11	VAL	C-O	-6.01	1.17	1.24
1	D	19	LYS	C-O	-6.01	1.17	1.24
1	B	114	VAL	C-O	-6.00	1.17	1.24
1	B	9	ALA	C-O	-5.99	1.16	1.23
1	A	171	ALA	C-O	-5.99	1.16	1.23
1	C	87	ARG	C-O	-5.97	1.16	1.23
1	C	71	THR	C-O	-5.97	1.16	1.23
1	E	144	LEU	C-O	-5.97	1.16	1.24
1	A	114	VAL	C-O	-5.96	1.17	1.24
1	C	201	VAL	C-O	-5.95	1.17	1.24
1	C	95	TYR	C-O	-5.95	1.16	1.23
1	C	104	VAL	C-O	-5.94	1.18	1.24
1	C	141	LEU	C-O	-5.94	1.16	1.24
1	A	123	SER	CA-CB	-5.93	1.45	1.53
1	B	112	VAL	C-O	-5.92	1.17	1.24
1	D	46	GLU	C-O	-5.92	1.16	1.23
1	B	199	CYS	C-O	-5.92	1.16	1.24
1	F	118	SER	C-O	-5.91	1.16	1.23
1	B	166	VAL	C-O	-5.91	1.17	1.24
1	E	196	THR	C-O	-5.88	1.16	1.24
1	F	113	THR	C-O	-5.87	1.17	1.24
1	E	97	ALA	C-O	-5.87	1.17	1.24
1	A	197	TYR	C-O	-5.86	1.17	1.24
1	D	87	ARG	C-O	-5.86	1.16	1.23
1	B	155	VAL	C-O	-5.85	1.17	1.24
1	B	96	CYS	C-O	-5.85	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	GLY	C-O	-5.85	1.16	1.24
1	B	51	ILE	C-O	-5.84	1.18	1.24
1	B	92	ALA	C-O	-5.84	1.17	1.23
1	A	143	CYS	C-O	-5.83	1.17	1.23
1	F	153	VAL	C-O	-5.83	1.18	1.24
1	C	41	PRO	C-O	-5.83	1.17	1.23
1	F	189	SER	C-O	-5.83	1.16	1.24
1	B	210	VAL	C-O	-5.83	1.16	1.24
1	F	173	LEU	C-O	-5.83	1.17	1.24
1	A	91	THR	C-O	-5.82	1.16	1.24
1	C	69	THR	C-O	-5.82	1.17	1.24
1	A	6	GLN	C-O	-5.82	1.16	1.23
1	A	13	LYS	C-O	-5.82	1.17	1.23
1	C	16	ALA	C-O	-5.82	1.17	1.23
1	A	110	THR	C-O	-5.81	1.17	1.24
1	B	169	PHE	C-O	-5.81	1.16	1.23
1	D	47	TRP	C-O	-5.80	1.16	1.23
1	A	90	ASP	CG-OD2	-5.79	1.14	1.25
1	A	124	VAL	C-O	-5.79	1.16	1.24
1	C	83	LEU	C-O	-5.79	1.17	1.24
1	C	118	SER	C-O	-5.79	1.17	1.23
1	F	154	THR	C-O	-5.77	1.17	1.24
1	C	88	SER	C-O	-5.77	1.16	1.24
1	B	68	ALA	C-O	-5.76	1.17	1.23
1	B	151	GLU	CD-OE1	-5.76	1.14	1.25
1	B	82	GLU	C-O	-5.76	1.17	1.24
1	B	187	VAL	C-O	-5.74	1.18	1.24
1	A	159	SER	CA-CB	-5.72	1.44	1.53
1	F	214	VAL	C-O	-5.72	1.18	1.24
1	B	69	THR	C-O	-5.71	1.17	1.23
1	C	8	GLY	C-O	-5.71	1.16	1.23
1	D	170	PRO	C-O	-5.69	1.17	1.23
1	A	50	TYR	C-O	-5.69	1.16	1.23
1	D	76	ALA	C-O	-5.68	1.16	1.24
1	D	105	TYR	C-O	-5.68	1.17	1.23
1	D	146	LYS	C-O	-5.67	1.17	1.23
1	F	147	ASP	CG-OD1	-5.67	1.14	1.25
1	B	8	GLY	C-O	-5.65	1.15	1.23
1	B	183	SER	C-O	-5.64	1.17	1.24
1	E	185	VAL	C-O	-5.64	1.18	1.24
1	B	67	ARG	C-O	-5.64	1.17	1.24
1	C	20	VAL	C-O	-5.64	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	188	PRO	C-O	-5.64	1.17	1.23
1	D	147	ASP	C-O	-5.64	1.16	1.24
1	F	110	THR	C-O	-5.63	1.17	1.24
1	E	105	TYR	C-O	-5.62	1.16	1.23
1	E	35	ASN	C-O	-5.62	1.17	1.23
1	F	159	SER	CA-CB	-5.62	1.45	1.53
1	D	184	VAL	C-O	-5.62	1.18	1.24
1	C	185	VAL	C-O	-5.61	1.18	1.24
1	F	166	VAL	C-O	-5.61	1.17	1.24
1	A	141	LEU	C-O	-5.60	1.16	1.24
1	D	6	GLN	C-O	-5.59	1.16	1.23
1	D	12	LYS	C-O	-5.59	1.16	1.23
1	E	169	PHE	C-O	-5.58	1.16	1.23
1	D	45	LEU	C-O	-5.58	1.17	1.23
1	C	212	LYS	C-O	-5.58	1.17	1.24
1	F	208	THR	C-O	-5.57	1.16	1.24
1	B	6	GLN	C-O	-5.56	1.16	1.23
1	B	156	SER	C-O	-5.55	1.17	1.23
1	C	114	VAL	C-O	-5.55	1.17	1.24
1	A	153	VAL	C-O	-5.54	1.18	1.24
1	C	205	PRO	C-O	-5.54	1.17	1.24
1	E	80	TYR	C-O	-5.54	1.16	1.23
1	E	164	SER	C-O	-5.53	1.17	1.24
1	C	182	SER	CA-CB	-5.53	1.44	1.53
1	D	78	THR	C-O	-5.53	1.16	1.23
1	D	75	SER	CA-CB	-5.53	1.44	1.53
1	A	212	LYS	C-O	-5.52	1.17	1.23
1	D	70	ILE	C-O	-5.52	1.18	1.24
1	A	24	THR	C-O	-5.51	1.17	1.24
1	A	202	ASN	C-O	-5.51	1.17	1.24
1	A	86	LEU	C-O	-5.51	1.17	1.23
1	F	196	THR	C-O	-5.51	1.17	1.24
1	A	46	GLU	C-O	-5.50	1.17	1.23
1	F	34	ILE	C-O	-5.50	1.18	1.24
1	E	22	CYS	C-O	-5.50	1.17	1.24
1	F	41	PRO	C-O	-5.50	1.17	1.23
1	F	147	ASP	CG-OD2	-5.50	1.15	1.25
1	C	203	HIS	CE1-NE2	-5.49	1.27	1.32
1	B	61	SER	C-O	-5.49	1.17	1.23
1	A	156	SER	C-O	-5.48	1.17	1.23
1	B	40	ALA	C-O	-5.47	1.16	1.23
1	C	197	TYR	C-O	-5.47	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	93	VAL	C-O	-5.47	1.18	1.24
1	B	45	LEU	C-O	-5.47	1.17	1.23
1	D	98	GLY	C-O	-5.47	1.16	1.23
1	C	91	THR	C-O	-5.46	1.17	1.24
1	C	61	SER	CA-CB	-5.46	1.44	1.53
1	C	80	TYR	C-O	-5.46	1.17	1.23
1	D	88	SER	C-O	-5.46	1.17	1.24
1	E	34	ILE	C-O	-5.45	1.18	1.24
1	C	78	THR	C-O	-5.45	1.17	1.23
1	F	210	VAL	C-O	-5.44	1.17	1.24
1	A	169	PHE	C-O	-5.44	1.17	1.23
1	E	73	ASP	C-O	-5.43	1.17	1.23
1	B	108	GLN	C-O	-5.43	1.17	1.24
1	B	115	SER	C-O	-5.42	1.17	1.23
1	C	140	ALA	C-O	-5.42	1.17	1.24
1	E	84	SER	CA-CB	-5.41	1.45	1.53
1	A	71	THR	C-O	-5.40	1.17	1.23
1	A	89	GLU	C-O	-5.38	1.17	1.24
1	C	11	VAL	C-O	-5.38	1.18	1.24
1	C	12	LYS	C-O	-5.37	1.17	1.23
1	E	151	GLU	C-O	-5.37	1.15	1.24
1	C	168	THR	C-O	-5.36	1.17	1.24
1	A	8	GLY	C-O	-5.36	1.15	1.23
1	D	97	ALA	C-O	-5.36	1.17	1.23
1	B	201	VAL	C-O	-5.35	1.18	1.24
1	A	100	GLY	C-O	-5.35	1.16	1.23
1	A	83	LEU	C-O	-5.34	1.17	1.24
1	F	204	LYS	C-O	-5.34	1.19	1.24
1	E	61	SER	CA-CB	-5.34	1.45	1.53
1	F	183	SER	C-O	-5.33	1.18	1.24
1	C	86	LEU	C-O	-5.33	1.17	1.23
1	E	143	CYS	C-O	-5.32	1.17	1.24
1	E	8	GLY	C-O	-5.32	1.15	1.23
1	F	81	MET	C-O	-5.32	1.18	1.24
1	F	120	LYS	C-O	-5.32	1.17	1.23
1	A	90	ASP	CG-OD1	-5.31	1.15	1.25
1	B	118	SER	C-O	-5.31	1.17	1.24
1	B	182	SER	CA-CB	-5.30	1.43	1.53
1	A	90	ASP	C-O	-5.30	1.16	1.24
1	E	159	SER	CA-CB	-5.29	1.45	1.53
1	C	7	SER	CA-CB	-5.29	1.45	1.53
1	D	92	ALA	C-O	-5.29	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	48	ILE	C-O	-5.29	1.17	1.24
1	B	188	PRO	N-CA	-5.29	1.41	1.47
1	D	212	LYS	C-O	-5.28	1.17	1.24
1	D	90	ASP	CG-OD2	-5.28	1.15	1.25
1	D	91	THR	C-O	-5.27	1.17	1.24
1	D	203	HIS	CG-ND1	-5.26	1.32	1.38
1	E	178	LEU	C-O	-5.25	1.17	1.24
1	A	157	TRP	C-O	-5.25	1.17	1.24
1	B	50	TYR	C-O	-5.25	1.17	1.23
1	E	89	GLU	C-O	-5.25	1.17	1.24
1	C	193	GLY	C-O	-5.23	1.16	1.23
1	C	164	SER	C-O	-5.23	1.17	1.24
1	D	62	GLU	C-O	-5.23	1.17	1.24
1	B	85	SER	C-O	-5.22	1.17	1.23
1	A	188	PRO	C-O	-5.22	1.16	1.23
1	E	182	SER	CA-CB	-5.20	1.43	1.53
1	B	59	ASP	C-O	-5.20	1.17	1.23
1	A	102	ARG	C-O	-5.20	1.17	1.23
1	B	63	LYS	C-O	-5.19	1.18	1.24
1	C	15	GLY	C-O	-5.18	1.16	1.24
1	A	103	PHE	C-O	-5.18	1.15	1.23
1	E	25	SER	C-O	-5.18	1.17	1.23
1	F	19	LYS	C-O	-5.17	1.18	1.24
1	F	145	VAL	C-O	-5.17	1.18	1.24
1	A	21	SER	C-O	-5.17	1.17	1.24
1	B	14	PRO	N-CA	-5.17	1.41	1.47
1	C	195	GLN	C-O	-5.17	1.17	1.23
1	D	61	SER	CA-CB	-5.16	1.44	1.53
1	F	91	THR	C-O	-5.16	1.17	1.23
1	B	64	PHE	C-O	-5.16	1.17	1.24
1	D	77	SER	CA-CB	-5.16	1.45	1.53
1	F	123	SER	CA-CB	-5.16	1.46	1.53
1	D	169	PHE	C-O	-5.16	1.16	1.23
1	A	183	SER	C-O	-5.15	1.18	1.24
1	B	30	THR	C-O	-5.15	1.17	1.23
1	A	88	SER	C-O	-5.13	1.17	1.24
1	A	41	PRO	C-O	-5.13	1.17	1.24
1	B	42	GLY	C-O	-5.13	1.16	1.24
1	B	21	SER	C-O	-5.12	1.17	1.23
1	A	79	VAL	C-O	-5.12	1.18	1.24
1	E	111	LEU	C-O	-5.12	1.17	1.24
1	A	122	PRO	C-O	-5.11	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	84	SER	C-O	-5.11	1.17	1.23
1	C	200	ASN	C-O	-5.11	1.17	1.23
1	D	117	ALA	C-O	-5.10	1.17	1.23
1	D	203	HIS	CD2-NE2	-5.10	1.32	1.37
1	F	128	ALA	CA-CB	-5.09	1.47	1.54
1	B	4	LEU	C-O	-5.08	1.18	1.24
1	B	149	PHE	C-O	-5.08	1.17	1.24
1	E	57	ASP	C-O	-5.08	1.17	1.23
1	F	96	CYS	C-O	-5.08	1.17	1.23
1	D	17	SER	C-O	-5.08	1.17	1.23
1	B	173	LEU	C-O	-5.07	1.17	1.23
1	E	16	ALA	C-O	-5.07	1.18	1.23
1	E	45	LEU	C-O	-5.07	1.17	1.23
1	F	203	HIS	C-O	-5.07	1.17	1.23
1	E	123	SER	C-O	-5.05	1.17	1.24
1	B	180	SER	C-O	-5.05	1.17	1.23
1	D	32	TYR	C-O	-5.03	1.17	1.24
1	E	5	VAL	C-O	-5.02	1.18	1.24
1	A	15	GLY	C-O	-5.01	1.17	1.24
1	A	20	VAL	C-O	-5.01	1.18	1.24
1	E	176	SER	CA-CB	-5.01	1.44	1.53
1	B	103	PHE	C-O	-5.01	1.17	1.23
1	A	52	TYR	C-O	-5.00	1.18	1.24
1	F	176	SER	CA-CB	-5.00	1.44	1.53

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	PRO	N-CD-CG	-11.01	90.59	103.80
1	D	148	TYR	CA-C-O	-10.61	110.12	121.36
1	D	104	VAL	CA-C-N	10.09	139.44	121.89
1	D	104	VAL	C-N-CA	10.09	139.44	121.89
1	A	110	THR	CB-CA-C	10.07	127.15	109.72
1	B	203	HIS	CA-C-N	9.56	131.44	120.06
1	B	203	HIS	C-N-CA	9.56	131.44	120.06
1	E	96	CYS	N-CA-C	9.00	123.59	108.20
1	F	105	TYR	CA-C-N	-8.87	106.66	121.39
1	F	105	TYR	C-N-CA	-8.87	106.66	121.39
1	D	194	THR	CB-CA-C	-8.86	95.20	110.88
1	F	35	ASN	CB-CA-C	-8.62	94.20	109.71
1	C	195	GLN	CB-CG-CD	8.52	127.08	112.60
1	E	188	PRO	CB-CA-C	-8.20	100.88	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	CYS	N-CA-C	8.08	122.28	107.99
1	B	52	TYR	CB-CA-C	-8.06	95.78	109.72
1	A	57	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	3	GLN	CB-CA-C	-7.43	93.86	109.38
1	C	10	GLU	CB-CG-CD	7.33	125.07	112.60
1	B	144	LEU	N-CA-CB	-7.31	98.51	110.42
1	B	58	THR	CB-CA-C	-7.27	97.76	109.75
1	A	97	ALA	CA-C-N	-7.19	115.40	121.58
1	A	97	ALA	C-N-CA	-7.19	115.40	121.58
1	A	194	THR	CA-CB-OG1	-7.18	98.82	109.60
1	D	44	GLY	CA-C-O	-7.07	117.62	122.22
1	D	104	VAL	N-CA-C	7.03	119.33	108.44
1	B	152	PRO	CA-N-CD	7.00	121.80	112.00
1	A	32	TYR	CB-CA-C	6.94	122.25	111.70
1	A	142	GLY	CA-C-N	6.81	132.47	122.39
1	A	142	GLY	C-N-CA	6.81	132.47	122.39
1	F	188	PRO	CB-CA-C	-6.70	103.13	111.64
1	D	106	TRP	CA-C-N	6.61	128.96	120.64
1	D	106	TRP	C-N-CA	6.61	128.96	120.64
1	B	215	GLU	CB-CG-CD	6.56	123.75	112.60
1	E	198	ILE	CA-C-O	-6.53	113.31	120.43
1	B	188	PRO	CB-CA-C	-6.47	103.48	111.64
1	E	88	SER	CA-C-N	6.42	130.87	120.60
1	E	88	SER	C-N-CA	6.42	130.87	120.60
1	D	105	TYR	CB-CA-C	-6.35	99.00	109.80
1	B	89	GLU	CB-CG-CD	6.27	123.26	112.60
1	E	67	ARG	CB-CA-C	-6.26	98.73	110.01
1	B	175	SER	CA-C-N	6.25	128.66	120.28
1	B	175	SER	C-N-CA	6.25	128.66	120.28
1	D	205	PRO	CB-CA-C	-6.23	103.00	111.85
1	D	146	LYS	CA-C-N	6.19	133.36	121.54
1	D	146	LYS	C-N-CA	6.19	133.36	121.54
1	C	119	THR	CA-C-O	-6.18	113.62	120.60
1	C	157	TRP	CA-C-N	-6.08	112.95	122.08
1	C	157	TRP	C-N-CA	-6.08	112.95	122.08
1	B	94	TYR	CB-CA-C	6.07	119.75	109.80
1	D	74	THR	CB-CA-C	6.04	122.27	110.67
1	A	59	ASP	CB-CA-C	-6.01	99.58	109.80
1	F	145	VAL	N-CA-CB	-5.98	103.94	111.41
1	A	48	ILE	N-CA-C	-5.92	106.47	111.56
1	E	134	THR	O-C-N	5.84	128.09	122.07
1	E	23	LYS	CB-CA-C	-5.82	100.50	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	LYS	CB-CA-C	-5.80	100.61	109.89
1	D	151	GLU	N-CA-C	5.78	121.37	113.16
1	D	46	GLU	CB-CA-C	-5.77	97.67	109.38
1	E	64	PHE	CB-CA-C	-5.71	101.07	110.72
1	E	149	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	143	CYS	CB-CA-C	-5.63	101.47	110.14
1	B	24	THR	CA-CB-OG1	-5.61	101.19	109.60
1	D	108	GLN	CB-CA-C	-5.59	102.07	110.90
1	A	203	HIS	CA-C-N	5.57	127.05	120.09
1	A	203	HIS	C-N-CA	5.57	127.05	120.09
1	C	119	THR	CA-C-N	-5.54	113.89	122.59
1	C	119	THR	C-N-CA	-5.54	113.89	122.59
1	E	55	ALA	N-CA-C	-5.47	106.65	113.55
1	E	46	GLU	CA-C-N	5.46	129.50	120.94
1	E	46	GLU	C-N-CA	5.46	129.50	120.94
1	D	118	SER	N-CA-CB	5.42	119.02	110.56
1	D	64	PHE	CB-CA-C	-5.40	102.28	111.02
1	E	95	TYR	N-CA-C	5.39	117.75	109.07
1	F	196	THR	CA-CB-OG1	-5.37	101.54	109.60
1	F	74	THR	CB-CA-C	-5.37	101.87	110.79
1	D	69	THR	CB-CA-C	-5.35	100.02	109.70
1	C	46	GLU	CB-CA-C	5.34	121.32	109.94
1	F	71	THR	CA-CB-OG1	-5.33	101.61	109.60
1	B	41	PRO	N-CA-C	5.33	119.58	110.74
1	B	41	PRO	N-CD-CG	-5.32	95.22	103.20
1	D	215	GLU	CB-CG-CD	5.32	121.65	112.60
1	E	3	GLN	N-CA-CB	-5.31	101.62	111.13
1	C	35	ASN	CB-CA-C	-5.31	100.53	109.50
1	D	123	SER	CA-C-N	-5.31	116.61	123.19
1	D	123	SER	C-N-CA	-5.31	116.61	123.19
1	E	46	GLU	CB-CA-C	5.29	118.90	109.65
1	F	20	VAL	CA-C-O	-5.28	115.59	121.98
1	E	119	THR	CB-CA-C	-5.27	101.94	109.84
1	B	46	GLU	CA-C-N	5.26	129.02	121.50
1	B	46	GLU	C-N-CA	5.26	129.02	121.50
1	E	96	CYS	CB-CA-C	-5.26	102.37	110.78
1	B	142	GLY	N-CA-C	-5.25	100.75	113.18
1	F	175	SER	CA-C-N	5.21	129.43	120.72
1	F	175	SER	C-N-CA	5.21	129.43	120.72
1	A	91	THR	CB-CA-C	5.21	119.47	110.77
1	E	192	LEU	CA-C-N	-5.19	114.28	119.94
1	E	192	LEU	C-N-CA	-5.19	114.28	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	GLY	CA-C-O	-5.18	117.06	121.57
1	F	154	THR	CB-CA-C	-5.18	100.77	109.72
1	D	146	LYS	CB-CA-C	-5.17	100.80	109.48
1	C	194	THR	CA-CB-OG1	-5.16	101.87	109.60
1	A	216	PRO	N-CD-CG	-5.15	95.47	103.20
1	B	64	PHE	CB-CA-C	-5.14	101.79	110.64
1	B	35	ASN	CB-CA-C	-5.13	100.83	109.50
1	B	14	PRO	N-CA-CB	-5.11	98.67	103.27
1	A	72	SER	CA-C-O	-5.07	115.32	120.99
1	E	40	ALA	CA-C-O	-5.04	114.80	120.25
1	A	170	PRO	N-CA-CB	-5.04	98.82	103.31
1	E	89	GLU	CB-CA-C	-5.04	99.69	110.32
1	E	168	THR	CB-CA-C	5.03	118.83	110.78
1	A	188	PRO	CB-CA-C	-5.02	105.26	111.64

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	1588	0	1558	93	0
1	B	1504	0	1468	83	22
1	C	1508	0	1478	188	22
1	D	1542	0	1511	127	0
1	E	1605	0	1570	123	0
1	F	1518	0	1494	141	0
All	All	9265	0	9079	683	22

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 38.

All (683) 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:F:4:LEU:CD1	1:F:107:GLY:HA3	1.19	1.57
1:F:4:LEU:HD12	1:F:107:GLY:CA	1.10	1.56
1:F:5:VAL:CG1	1:F:23:LYS:CB	1.89	1.50
1:D:200:ASN:ND2	1:D:211:ASP:CB	1.72	1.50
1:F:5:VAL:CG1	1:F:23:LYS:HB2	1.43	1.47
1:C:22:CYS:SG	1:C:96:CYS:CB	2.08	1.40
1:C:22:CYS:SG	1:C:96:CYS:SG	1.45	1.40
1:D:188:PRO:HG2	1:D:191:SER:OG	1.20	1.38
1:F:5:VAL:HG11	1:F:23:LYS:CB	1.48	1.35
1:F:67:ARG:NH2	1:F:90:ASP:OD2	1.62	1.32
1:F:4:LEU:CD1	1:F:107:GLY:CA	1.79	1.31
1:C:151:GLU:OE2	1:C:179:TYR:CD2	1.83	1.30
1:C:150:PRO:C	1:C:152:PRO:HD2	1.57	1.29
1:C:146:LYS:HG3	1:C:180:SER:OG	1.35	1.26
1:E:122:PRO:HD3	1:E:203:HIS:ND1	1.49	1.25
1:A:151:GLU:CG	1:A:152:PRO:HA	1.66	1.23
1:E:6:GLN:H	1:E:108:GLN:NE2	1.36	1.23
1:D:150:PRO:HD2	1:D:205:PRO:CB	1.67	1.22
1:F:4:LEU:CG	1:F:107:GLY:HA2	1.70	1.22
1:F:5:VAL:HG12	1:F:23:LYS:O	1.37	1.22
1:A:61:SER:OG	1:B:103:PHE:CE2	1.91	1.17
1:D:150:PRO:HD2	1:D:205:PRO:CG	1.75	1.17
1:F:18:VAL:HG12	1:F:86:LEU:HD11	1.27	1.14
1:C:73:ASP:OD2	1:C:76:ALA:CB	1.94	1.13
1:E:6:GLN:N	1:E:108:GLN:HE21	1.46	1.13
1:C:152:PRO:HG2	1:C:205:PRO:HG2	1.19	1.13
1:C:76:ALA:O	1:C:77:SER:OG	1.65	1.12
1:E:6:GLN:N	1:E:108:GLN:NE2	1.96	1.12
1:E:51:ILE:HG13	1:E:58:THR:CG2	1.81	1.10
1:F:19:LYS:HD2	1:F:82:GLU:OE1	1.51	1.10
1:C:151:GLU:OE2	1:C:179:TYR:HD2	1.23	1.09
1:F:46:GLU:OE1	1:F:63:LYS:NZ	1.84	1.09
1:C:22:CYS:SG	1:C:96:CYS:HB3	1.90	1.09
1:F:68:ALA:HB2	1:F:83:LEU:HD12	1.32	1.08
1:A:151:GLU:HG2	1:A:152:PRO:HA	1.32	1.08
1:A:184:VAL:CG1	1:B:144:LEU:HD22	1.83	1.07
1:C:159:SER:HA	1:C:200:ASN:ND2	1.67	1.07
1:B:142:GLY:HA2	1:B:157:TRP:CZ2	1.89	1.07
1:F:174:GLN:HG3	1:F:178:LEU:O	1.55	1.06
1:C:28:THR:HG23	1:E:101:THR:O	1.54	1.06
1:D:150:PRO:CD	1:D:205:PRO:CB	2.33	1.05
1:D:150:PRO:CD	1:D:205:PRO:HB3	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ASP:OD2	1:C:76:ALA:HB3	1.55	1.04
1:C:22:CYS:CB	1:C:96:CYS:SG	2.46	1.04
1:C:159:SER:HA	1:C:200:ASN:HD21	1.23	1.03
1:D:126:PRO:HB3	1:D:214:VAL:HG22	1.41	1.03
1:D:119:THR:HG23	1:D:149:PHE:O	1.59	1.02
1:F:4:LEU:HG	1:F:107:GLY:HA2	1.40	1.02
1:D:150:PRO:HD2	1:D:205:PRO:HG2	1.40	1.01
1:E:47:TRP:CE3	1:F:104:VAL:HG13	1.94	1.01
1:E:189:SER:HA	1:E:192:LEU:HD11	1.41	1.01
1:F:5:VAL:HG11	1:F:23:LYS:HB3	1.02	1.01
1:F:5:VAL:HG13	1:F:23:LYS:CB	1.69	1.01
1:C:212:LYS:HZ3	1:C:213:LYS:NZ	1.59	1.01
1:C:20:VAL:CG1	1:C:110:THR:HG21	1.88	1.01
1:F:51:ILE:HG13	1:F:58:THR:HG22	1.40	1.01
1:A:184:VAL:HG11	1:B:144:LEU:HD22	1.04	1.00
1:C:157:TRP:HB2	1:C:162:LEU:HD11	1.44	1.00
1:C:159:SER:CA	1:C:200:ASN:HD21	1.73	1.00
1:C:42:GLY:C	1:C:43:GLN:OE1	2.04	0.99
1:C:102:ARG:HD2	1:E:28:THR:HG22	1.44	0.99
1:E:192:LEU:H	1:E:192:LEU:HD12	1.26	0.99
1:C:102:ARG:HA	1:E:28:THR:HG23	1.43	0.99
1:F:157:TRP:CE3	1:F:198:ILE:O	2.15	0.99
1:C:28:THR:CG2	1:E:101:THR:O	2.11	0.98
1:C:157:TRP:CB	1:C:162:LEU:HD11	1.92	0.98
1:C:47:TRP:CD1	1:D:104:VAL:HG22	1.98	0.98
1:A:36:TRP:CD1	1:A:70:ILE:HD13	1.99	0.98
1:C:150:PRO:C	1:C:152:PRO:CD	2.36	0.97
1:D:150:PRO:HD3	1:D:205:PRO:HB3	1.43	0.97
1:D:156:SER:O	1:D:199:CYS:O	1.82	0.97
1:E:189:SER:O	1:E:192:LEU:CD1	2.12	0.97
1:A:36:TRP:HD1	1:A:70:ILE:HD13	1.24	0.97
1:F:156:SER:O	1:F:199:CYS:O	1.81	0.97
1:D:188:PRO:CG	1:D:191:SER:OG	2.13	0.96
1:C:152:PRO:CG	1:C:205:PRO:HG2	1.96	0.95
1:F:51:ILE:CG1	1:F:58:THR:HG22	1.96	0.95
1:E:67:ARG:HD2	1:E:84:SER:O	1.67	0.95
1:F:5:VAL:HG13	1:F:23:LYS:HB2	0.96	0.94
1:E:51:ILE:HG13	1:E:58:THR:HG22	1.48	0.94
1:C:20:VAL:HG13	1:C:110:THR:HG21	1.48	0.94
1:F:4:LEU:CG	1:F:107:GLY:CA	2.35	0.93
1:A:61:SER:OG	1:B:103:PHE:CZ	2.22	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LYS:NZ	1:C:213:LYS:HZ3	1.65	0.93
1:C:146:LYS:CG	1:C:180:SER:OG	2.16	0.93
1:C:152:PRO:HG2	1:C:205:PRO:CG	1.97	0.92
1:F:5:VAL:CG1	1:F:23:LYS:CA	2.47	0.92
1:D:198:ILE:HG22	1:D:200:ASN:OD1	1.70	0.92
1:C:73:ASP:OD2	1:C:76:ALA:HB2	1.70	0.92
1:D:61:SER:O	1:D:65:LYS:HG3	1.67	0.92
1:B:99:THR:O	1:B:103:PHE:O	1.87	0.92
1:B:203:HIS:ND1	1:B:206:SER:OG	1.96	0.92
1:F:174:GLN:OE1	1:F:180:SER:OG	1.88	0.92
1:F:5:VAL:CG1	1:F:23:LYS:O	2.19	0.91
1:C:28:THR:HG21	1:E:102:ARG:HA	1.51	0.91
1:C:115:SER:HB3	1:C:149:PHE:HZ	1.35	0.91
1:E:120:LYS:O	1:E:203:HIS:HE1	1.55	0.90
1:D:150:PRO:CD	1:D:205:PRO:CG	2.48	0.90
1:C:151:GLU:N	1:C:152:PRO:HD2	1.87	0.90
1:C:168:THR:OG1	1:C:183:SER:OG	1.90	0.90
1:C:115:SER:HB3	1:C:149:PHE:CZ	2.07	0.89
1:A:151:GLU:HG3	1:A:152:PRO:HA	1.53	0.89
1:A:163:THR:O	1:A:166:VAL:HG12	1.70	0.89
1:C:43:GLN:OE1	1:C:43:GLN:N	2.06	0.88
1:C:157:TRP:HB2	1:C:162:LEU:CD1	2.02	0.88
1:A:184:VAL:HG11	1:B:144:LEU:CD2	1.99	0.88
1:D:188:PRO:HG2	1:D:191:SER:HG	1.36	0.87
1:E:189:SER:O	1:E:192:LEU:HD12	1.73	0.87
1:E:22:CYS:HG	1:E:96:CYS:HG	0.95	0.87
1:D:166:VAL:C	1:D:167:HIS:HD1	1.81	0.86
1:D:51:ILE:HG13	1:D:58:THR:HG22	1.57	0.86
1:D:126:PRO:CB	1:D:214:VAL:HG22	2.06	0.86
1:B:141:LEU:O	1:B:185:VAL:N	2.09	0.85
1:B:147:ASP:CB	1:B:178:LEU:HD13	2.06	0.85
1:E:198:ILE:HG23	1:E:212:LYS:O	1.77	0.84
1:F:51:ILE:HG13	1:F:58:THR:CG2	2.07	0.84
1:F:18:VAL:CG1	1:F:86:LEU:HD11	2.05	0.84
1:F:163:THR:O	1:F:166:VAL:HG12	1.77	0.84
1:E:202:ASN:O	1:E:208:THR:O	1.95	0.84
1:C:215:GLU:O	1:D:130:SER:OG	1.96	0.83
1:C:212:LYS:HZ3	1:C:213:LYS:HZ3	0.86	0.83
1:F:19:LYS:CD	1:F:82:GLU:OE1	2.26	0.83
1:A:151:GLU:HG2	1:A:152:PRO:CA	2.08	0.82
1:D:174:GLN:OE1	1:D:180:SER:OG	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ILE:CG1	1:E:58:THR:CG2	2.58	0.81
1:F:5:VAL:HG13	1:F:23:LYS:N	1.95	0.81
1:C:102:ARG:HA	1:E:28:THR:CG2	2.10	0.81
1:B:142:GLY:HA2	1:B:157:TRP:HZ2	1.44	0.81
1:D:4:LEU:HD22	1:D:22:CYS:SG	2.21	0.81
1:F:4:LEU:HD13	1:F:96:CYS:SG	2.21	0.81
1:F:23:LYS:HE2	1:F:78:THR:HG21	1.62	0.81
1:C:159:SER:N	1:C:200:ASN:HD21	1.79	0.80
1:B:147:ASP:HB2	1:B:178:LEU:HD13	1.63	0.80
1:B:173:LEU:HD13	1:B:179:TYR:CZ	2.16	0.80
1:E:87:ARG:O	1:E:114:VAL:HG11	1.82	0.80
1:C:33:GLY:O	1:C:98:GLY:HA2	1.82	0.79
1:C:18:VAL:HG12	1:C:86:LEU:HD11	1.63	0.79
1:C:152:PRO:CG	1:C:205:PRO:CG	2.57	0.79
1:B:52:TYR:HD2	1:B:55:ALA:H	1.29	0.79
1:E:4:LEU:HD23	1:E:22:CYS:HG	1.48	0.79
1:E:189:SER:CA	1:E:192:LEU:HD11	2.13	0.79
1:B:142:GLY:HA2	1:B:157:TRP:CH2	2.17	0.79
1:E:91:THR:HG23	1:E:113:THR:HA	1.64	0.79
1:C:20:VAL:CG1	1:C:110:THR:CG2	2.60	0.78
1:C:203:HIS:ND1	1:C:206:SER:HB2	1.98	0.78
1:E:51:ILE:CG1	1:E:58:THR:HG22	2.13	0.78
1:D:119:THR:CG2	1:D:149:PHE:O	2.32	0.78
1:D:91:THR:HG23	1:D:113:THR:HA	1.64	0.78
1:E:124:VAL:HG21	1:E:201:VAL:HG21	1.64	0.78
1:C:146:LYS:HG3	1:C:180:SER:HG	1.45	0.78
1:E:22:CYS:CB	1:E:96:CYS:SG	2.71	0.77
1:D:200:ASN:HD21	1:D:211:ASP:CB	1.95	0.77
1:E:51:ILE:HG13	1:E:58:THR:HG23	1.67	0.77
1:C:212:LYS:NZ	1:C:213:LYS:NZ	2.26	0.77
1:E:4:LEU:HD23	1:E:22:CYS:SG	2.25	0.77
1:F:5:VAL:HG12	1:F:23:LYS:C	2.08	0.77
1:C:138:THR:OG1	1:C:189:SER:OG	2.00	0.77
1:D:113:THR:HG21	1:D:179:TYR:OH	1.85	0.76
1:F:73:ASP:OD1	1:F:76:ALA:HB3	1.86	0.76
1:F:4:LEU:HD11	1:F:107:GLY:CA	2.10	0.76
1:A:174:GLN:OE1	1:A:180:SER:OG	2.04	0.76
1:C:149:PHE:N	1:C:150:PRO:CD	2.49	0.76
1:E:126:PRO:HG3	1:E:212:LYS:HE2	1.66	0.76
1:A:61:SER:OG	1:B:103:PHE:HE2	1.60	0.76
1:D:119:THR:HA	1:D:149:PHE:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:PRO:HD2	1:D:208:THR:HG21	1.68	0.76
1:C:150:PRO:O	1:C:152:PRO:N	2.18	0.75
1:C:157:TRP:HB3	1:C:162:LEU:HD11	1.67	0.75
1:C:99:THR:OG1	1:E:31:ASN:ND2	2.19	0.75
1:D:166:VAL:O	1:D:167:HIS:ND1	2.12	0.75
1:D:17:SER:HB2	1:D:84:SER:HA	1.69	0.75
1:E:22:CYS:CB	1:E:96:CYS:HG	1.98	0.74
1:F:4:LEU:CD1	1:F:107:GLY:N	2.49	0.74
1:D:150:PRO:CD	1:D:205:PRO:HG2	2.14	0.74
1:C:103:PHE:HE2	1:D:62:GLU:HG2	1.53	0.74
1:C:184:VAL:HG21	1:D:144:LEU:HD13	1.70	0.74
1:F:39:GLN:O	1:F:92:ALA:HB1	1.88	0.74
1:A:58:THR:C	1:A:59:ASP:OD1	2.31	0.73
1:D:198:ILE:CG2	1:D:200:ASN:OD1	2.36	0.73
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.24	0.73
1:E:6:GLN:H	1:E:108:GLN:HE21	0.74	0.73
1:F:5:VAL:CG1	1:F:23:LYS:HB3	1.82	0.73
1:C:149:PHE:N	1:C:150:PRO:HD2	2.04	0.73
1:E:40:ALA:O	1:E:43:GLN:HB2	1.89	0.73
1:F:23:LYS:HG3	1:F:78:THR:HG22	1.69	0.72
1:C:22:CYS:CB	1:C:96:CYS:HG	1.96	0.72
1:D:126:PRO:HB3	1:D:214:VAL:CG2	2.19	0.72
1:B:147:ASP:HB3	1:B:178:LEU:CB	2.20	0.72
1:C:102:ARG:CD	1:E:28:THR:HG22	2.19	0.72
1:C:163:THR:O	1:C:166:VAL:HG12	1.89	0.72
1:F:83:LEU:HD23	1:F:86:LEU:HD21	1.70	0.72
1:B:5:VAL:HB	1:B:23:LYS:HG2	1.71	0.72
1:C:53:ILE:HD13	1:C:53:ILE:N	2.04	0.71
1:F:213:LYS:HE3	1:F:215:GLU:HG2	1.72	0.71
1:B:168:THR:OG1	1:B:183:SER:OG	2.03	0.71
1:C:143:CYS:SG	1:C:199:CYS:CB	2.78	0.71
1:F:4:LEU:CB	1:F:107:GLY:HA2	2.21	0.71
1:E:120:LYS:O	1:E:203:HIS:CE1	2.42	0.71
1:C:126:PRO:HD3	1:C:212:LYS:HD3	1.73	0.70
1:F:67:ARG:NH2	1:F:90:ASP:CG	2.48	0.70
1:C:87:ARG:O	1:C:114:VAL:HG11	1.90	0.70
1:F:5:VAL:HG13	1:F:23:LYS:CA	2.17	0.70
1:F:73:ASP:OD1	1:F:76:ALA:CB	2.40	0.70
1:A:5:VAL:HG21	1:D:5:VAL:CG2	2.22	0.70
1:C:121:GLY:O	1:C:147:ASP:O	2.09	0.70
1:F:213:LYS:HE3	1:F:215:GLU:CG	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:THR:HA	1:C:104:VAL:HG22	1.74	0.69
1:B:147:ASP:HB3	1:B:178:LEU:CD1	2.21	0.69
1:D:150:PRO:HD2	1:D:205:PRO:HB2	1.71	0.69
1:F:68:ALA:HB2	1:F:83:LEU:CD1	2.16	0.69
1:C:150:PRO:O	1:C:151:GLU:C	2.33	0.69
1:F:98:GLY:HA3	1:F:105:TYR:HB2	1.75	0.69
1:C:150:PRO:O	1:C:152:PRO:CD	2.41	0.69
1:F:5:VAL:HG13	1:F:23:LYS:H	1.57	0.69
1:F:138:THR:HG1	1:F:189:SER:H	1.41	0.68
1:C:201:VAL:HG22	1:C:210:VAL:HG12	1.74	0.68
1:B:147:ASP:HB3	1:B:178:LEU:HD13	1.73	0.68
1:E:37:VAL:HG11	1:F:106:TRP:CZ2	2.29	0.68
1:F:23:LYS:HG3	1:F:78:THR:CG2	2.23	0.68
1:D:147:ASP:HB3	1:D:178:LEU:HD22	1.74	0.68
1:C:150:PRO:HB2	1:C:152:PRO:HG2	1.73	0.68
1:C:97:ALA:HB2	1:C:106:TRP:CE3	2.28	0.68
1:A:8:GLY:HA3	1:D:19:LYS:HG2	1.75	0.67
1:C:159:SER:H	1:C:200:ASN:HD21	1.42	0.67
1:D:200:ASN:HA	1:D:211:ASP:HA	1.76	0.67
1:E:148:TYR:HB2	1:E:203:HIS:CE1	2.29	0.67
1:F:155:VAL:HG22	1:F:201:VAL:HG13	1.76	0.67
1:C:124:VAL:CG1	1:C:212:LYS:HD2	2.23	0.67
1:A:4:LEU:HD23	1:A:22:CYS:SG	2.35	0.67
1:C:143:CYS:CB	1:C:199:CYS:HG	2.07	0.67
1:E:47:TRP:CD2	1:F:104:VAL:HG13	2.29	0.67
1:A:132:LYS:HG3	1:B:126:PRO:HG3	1.75	0.67
1:C:151:GLU:N	1:C:152:PRO:CD	2.56	0.67
1:A:31:ASN:O	1:A:31:ASN:ND2	2.28	0.66
1:B:115:SER:HB3	1:B:149:PHE:CZ	2.30	0.66
1:A:32:TYR:HE1	1:A:34:ILE:HD11	1.61	0.66
1:A:129:PRO:HG2	1:A:192:LEU:HD21	1.77	0.66
1:E:122:PRO:CD	1:E:203:HIS:ND1	2.43	0.66
1:A:32:TYR:CE1	1:A:34:ILE:HD11	2.30	0.66
1:B:196:THR:CG2	1:B:213:LYS:HE2	2.26	0.66
1:C:204:LYS:N	1:C:205:PRO:CD	2.58	0.66
1:C:76:ALA:C	1:C:77:SER:HG	2.00	0.65
1:C:31:ASN:HB2	1:E:101:THR:HG22	1.77	0.65
1:C:149:PHE:H	1:C:150:PRO:CD	2.08	0.65
1:E:51:ILE:CG1	1:E:58:THR:HG23	2.26	0.65
1:F:5:VAL:CG1	1:F:23:LYS:N	2.58	0.65
1:C:200:ASN:OD1	1:C:200:ASN:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LEU:HD11	1:D:140:ALA:O	1.97	0.65
1:D:29:PHE:HE2	1:D:74:THR:HA	1.61	0.65
1:F:174:GLN:CG	1:F:178:LEU:O	2.38	0.64
1:C:122:PRO:HA	1:C:146:LYS:O	1.98	0.64
1:E:124:VAL:CG2	1:E:201:VAL:HG21	2.27	0.64
1:C:6:GLN:HG2	1:C:110:THR:HG22	1.80	0.64
1:C:153:VAL:HG23	1:C:203:HIS:HD2	1.63	0.64
1:D:197:TYR:O	1:D:213:LYS:O	2.16	0.64
1:C:47:TRP:CG	1:D:104:VAL:HG22	2.32	0.64
1:D:199:CYS:SG	1:D:201:VAL:HG13	2.38	0.64
1:A:51:ILE:HG13	1:A:58:THR:HG22	1.79	0.64
1:F:4:LEU:HD11	1:F:107:GLY:HA3	1.61	0.63
1:C:126:PRO:HB3	1:C:212:LYS:HG2	1.80	0.63
1:B:144:LEU:O	1:B:144:LEU:HG	1.97	0.63
1:C:4:LEU:N	1:C:4:LEU:HD12	2.14	0.63
1:D:124:VAL:CG1	1:D:143:CYS:SG	2.86	0.63
1:F:4:LEU:HD11	1:F:96:CYS:O	1.98	0.63
1:F:39:GLN:C	1:F:92:ALA:HB1	2.24	0.63
1:D:199:CYS:SG	1:D:201:VAL:CG1	2.86	0.63
1:A:6:GLN:NE2	1:A:110:THR:HG22	2.14	0.63
1:B:34:ILE:HD12	1:B:34:ILE:N	2.13	0.63
1:C:127:LEU:O	1:C:214:VAL:HG12	1.98	0.63
1:F:4:LEU:HG	1:F:107:GLY:CA	2.14	0.63
1:A:67:ARG:O	1:A:83:LEU:HA	1.98	0.63
1:C:141:LEU:HD23	1:C:214:VAL:HB	1.80	0.63
1:C:151:GLU:OE2	1:C:179:TYR:CE2	2.50	0.63
1:F:126:PRO:CB	1:F:214:VAL:HG12	2.28	0.63
1:F:201:VAL:O	1:F:209:LYS:HG2	1.99	0.63
1:E:25:SER:O	1:E:25:SER:OG	2.14	0.62
1:F:163:THR:O	1:F:166:VAL:CG1	2.47	0.62
1:A:132:LYS:CG	1:B:126:PRO:HG3	2.30	0.62
1:B:203:HIS:CE1	1:B:206:SER:HG	2.17	0.62
1:F:5:VAL:CG1	1:F:23:LYS:H	2.12	0.62
1:C:152:PRO:O	1:C:203:HIS:CD2	2.52	0.62
1:C:20:VAL:HG13	1:C:110:THR:CG2	2.23	0.62
1:C:22:CYS:HB3	1:C:96:CYS:SG	2.37	0.62
1:E:34:ILE:HD13	1:E:96:CYS:SG	2.40	0.62
1:E:129:PRO:HD3	1:E:141:LEU:HD23	1.81	0.62
1:E:87:ARG:O	1:E:114:VAL:CG1	2.47	0.62
1:F:5:VAL:CG1	1:F:23:LYS:C	2.68	0.62
1:A:36:TRP:HD1	1:A:70:ILE:CD1	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:PHE:CE2	1:D:62:GLU:HG2	2.35	0.62
1:B:142:GLY:CA	1:B:157:TRP:CH2	2.83	0.61
1:F:51:ILE:CG1	1:F:58:THR:CG2	2.72	0.61
1:D:29:PHE:CE2	1:D:74:THR:HA	2.34	0.61
1:F:6:GLN:HA	1:F:21:SER:O	2.01	0.61
1:B:142:GLY:HA3	1:B:184:VAL:HA	1.82	0.61
1:F:198:ILE:HG22	1:F:212:LYS:O	2.00	0.61
1:E:47:TRP:CE3	1:F:104:VAL:CG1	2.78	0.61
1:E:192:LEU:HD12	1:E:192:LEU:N	2.07	0.61
1:A:188:PRO:O	1:A:191:SER:OG	2.18	0.60
1:B:142:GLY:HA3	1:B:183:SER:O	2.01	0.60
1:B:91:THR:HG23	1:B:113:THR:HA	1.83	0.60
1:C:99:THR:O	1:C:103:PHE:O	2.19	0.60
1:F:5:VAL:HG13	1:F:5:VAL:O	2.01	0.60
1:F:67:ARG:HD3	1:F:83:LEU:CD1	2.31	0.60
1:D:120:LYS:O	1:D:148:TYR:HA	2.01	0.60
1:C:90:ASP:O	1:C:94:TYR:OH	2.17	0.60
1:C:47:TRP:CD1	1:D:104:VAL:CG2	2.82	0.60
1:D:150:PRO:CG	1:D:205:PRO:CG	2.79	0.60
1:F:22:CYS:HG	1:F:96:CYS:HG	1.48	0.60
1:A:20:VAL:HG11	1:A:110:THR:HG23	1.84	0.59
1:E:130:SER:HB2	1:F:126:PRO:HG2	1.84	0.59
1:F:12:LYS:O	1:F:114:VAL:HA	2.03	0.59
1:F:76:ALA:CB	1:F:78:THR:HG23	2.33	0.59
1:F:138:THR:OG1	1:F:189:SER:N	2.33	0.59
1:C:103:PHE:N	1:C:103:PHE:CD1	2.71	0.59
1:C:150:PRO:CA	1:C:152:PRO:HD2	2.31	0.59
1:C:6:GLN:NE2	1:C:107:GLY:HA3	2.18	0.59
1:E:127:LEU:HD21	1:F:140:ALA:O	2.03	0.59
1:E:6:GLN:CA	1:E:108:GLN:NE2	2.65	0.58
1:F:126:PRO:HB2	1:F:214:VAL:HG12	1.85	0.58
1:D:196:THR:O	1:D:196:THR:OG1	2.21	0.58
1:E:214:VAL:HG12	1:E:214:VAL:O	2.03	0.58
1:F:22:CYS:SG	1:F:96:CYS:SG	3.01	0.58
1:A:129:PRO:HD3	1:A:141:LEU:CD2	2.33	0.58
1:C:28:THR:CG2	1:E:102:ARG:HA	2.31	0.58
1:E:192:LEU:H	1:E:192:LEU:CD1	2.07	0.58
1:B:53:ILE:N	1:B:53:ILE:HD13	2.18	0.58
1:E:133:SER:HB2	1:F:126:PRO:HG2	1.84	0.58
1:C:172:VAL:HG23	1:C:172:VAL:O	2.02	0.58
1:B:173:LEU:CD1	1:B:179:TYR:CZ	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:VAL:C	1:D:167:HIS:ND1	2.57	0.58
1:E:174:GLN:HG3	1:E:178:LEU:O	2.03	0.58
1:C:124:VAL:HB	1:C:212:LYS:CD	2.33	0.58
1:F:4:LEU:HD11	1:F:107:GLY:N	2.17	0.58
1:B:28:THR:HG22	1:B:77:SER:HB2	1.85	0.57
1:D:200:ASN:CG	1:D:211:ASP:CB	2.70	0.57
1:C:124:VAL:HB	1:C:212:LYS:HD2	1.85	0.57
1:F:91:THR:HG23	1:F:113:THR:HA	1.87	0.57
1:F:159:SER:H	1:F:200:ASN:ND2	2.02	0.57
1:A:40:ALA:HB3	1:A:43:GLN:HB2	1.87	0.57
1:A:166:VAL:HB	1:A:185:VAL:HG23	1.85	0.57
1:C:166:VAL:HG13	1:C:166:VAL:O	2.04	0.57
1:A:129:PRO:HD3	1:A:141:LEU:HD23	1.87	0.57
1:B:115:SER:CB	1:B:149:PHE:CZ	2.87	0.57
1:D:214:VAL:HG12	1:D:214:VAL:O	2.03	0.57
1:E:23:LYS:HA	1:E:78:THR:HB	1.87	0.57
1:E:37:VAL:HG11	1:F:106:TRP:HZ2	1.67	0.57
1:A:5:VAL:HG21	1:D:5:VAL:HG22	1.86	0.57
1:F:23:LYS:CG	1:F:78:THR:HG22	2.34	0.57
1:F:102:ARG:HG2	1:F:102:ARG:HH11	1.70	0.57
1:C:31:ASN:O	1:E:101:THR:CG2	2.52	0.57
1:C:152:PRO:CG	1:C:205:PRO:HG3	2.34	0.57
1:C:28:THR:HG21	1:E:102:ARG:HG2	1.87	0.57
1:C:33:GLY:O	1:C:98:GLY:CA	2.52	0.57
1:E:124:VAL:HG12	1:E:212:LYS:HG3	1.87	0.57
1:F:67:ARG:HD3	1:F:83:LEU:HD11	1.87	0.57
1:D:137:GLY:O	1:D:189:SER:OG	2.13	0.57
1:F:19:LYS:HG3	1:F:82:GLU:HB2	1.85	0.57
1:C:114:VAL:HG12	1:C:114:VAL:O	2.04	0.56
1:A:148:TYR:CZ	1:A:179:TYR:HB3	2.40	0.56
1:C:115:SER:CB	1:C:149:PHE:HZ	2.11	0.56
1:F:94:TYR:CD1	1:F:94:TYR:N	2.73	0.56
1:B:142:GLY:CA	1:B:183:SER:O	2.54	0.56
1:C:31:ASN:CB	1:E:101:THR:HG22	2.34	0.56
1:E:189:SER:C	1:E:192:LEU:CD1	2.78	0.56
1:B:147:ASP:HB3	1:B:178:LEU:HB3	1.87	0.55
1:F:51:ILE:HG12	1:F:58:THR:HG22	1.86	0.55
1:E:1:GLU:OE1	1:E:26:GLY:O	2.24	0.55
1:E:6:GLN:C	1:E:108:GLN:HE22	2.14	0.55
1:C:159:SER:HA	1:C:200:ASN:HD22	1.67	0.55
1:F:83:LEU:HD23	1:F:86:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:VAL:HG21	1:D:106:TRP:HE1	1.72	0.55
1:D:122:PRO:HB2	1:D:145:VAL:HG12	1.89	0.55
1:D:198:ILE:HG22	1:D:200:ASN:CG	2.32	0.55
1:E:127:LEU:CD2	1:F:140:ALA:O	2.55	0.55
1:C:97:ALA:HB2	1:C:106:TRP:CD2	2.42	0.55
1:D:43:GLN:O	1:D:43:GLN:HG3	2.06	0.55
1:C:159:SER:CA	1:C:200:ASN:ND2	2.44	0.54
1:E:6:GLN:N	1:E:108:GLN:HE22	1.97	0.54
1:C:53:ILE:N	1:C:53:ILE:CD1	2.71	0.54
1:E:64:PHE:N	1:E:64:PHE:CD1	2.75	0.54
1:B:196:THR:CG2	1:B:213:LYS:CE	2.85	0.54
1:D:6:GLN:HG3	1:D:108:GLN:HG3	1.90	0.54
1:D:187:VAL:HG11	1:D:197:TYR:CE2	2.43	0.54
1:E:35:ASN:ND2	1:F:103:PHE:CD2	2.76	0.54
1:E:184:VAL:HG11	1:F:144:LEU:HD22	1.89	0.54
1:D:119:THR:HA	1:D:149:PHE:O	2.08	0.54
1:F:18:VAL:HG12	1:F:86:LEU:CD1	2.18	0.54
1:A:6:GLN:NE2	1:A:110:THR:CG2	2.71	0.54
1:A:198:ILE:HG12	1:A:198:ILE:O	2.08	0.54
1:E:63:LYS:HB3	1:E:64:PHE:CD1	2.43	0.53
1:C:126:PRO:HG3	1:C:212:LYS:HE3	1.90	0.53
1:B:145:VAL:CG2	1:B:181:LEU:HB3	2.39	0.53
1:D:2:VAL:HG22	1:D:26:GLY:HA3	1.91	0.53
1:D:126:PRO:HG3	1:D:212:LYS:HD2	1.91	0.53
1:D:204:LYS:CB	1:D:204:LYS:NZ	2.71	0.53
1:A:141:LEU:HB2	1:A:185:VAL:HG12	1.90	0.53
1:C:32:TYR:CD2	1:C:34:ILE:HD11	2.43	0.53
1:D:200:ASN:HA	1:D:211:ASP:CA	2.37	0.53
1:E:189:SER:C	1:E:192:LEU:HD11	2.33	0.53
1:D:197:TYR:N	1:D:197:TYR:CD1	2.76	0.53
1:E:104:VAL:HB	1:F:47:TRP:CG	2.43	0.53
1:C:153:VAL:HG23	1:C:203:HIS:CD2	2.42	0.53
1:E:106:TRP:CZ3	1:F:45:LEU:HD12	2.44	0.52
1:F:76:ALA:C	1:F:78:THR:HG23	2.34	0.52
1:E:22:CYS:HB2	1:E:96:CYS:SG	2.50	0.52
1:C:103:PHE:N	1:C:103:PHE:HD1	2.07	0.52
1:C:146:LYS:HG3	1:C:180:SER:CB	2.33	0.52
1:F:67:ARG:CZ	1:F:90:ASP:OD2	2.49	0.52
1:B:151:GLU:N	1:B:152:PRO:CD	2.73	0.52
1:C:100:GLY:O	1:E:31:ASN:HB2	2.10	0.52
1:A:124:VAL:HG13	1:A:212:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HB	1:A:181:LEU:HB3	1.91	0.52
1:A:6:GLN:HA	1:A:21:SER:O	2.09	0.52
1:B:34:ILE:HD12	1:B:34:ILE:H	1.74	0.52
1:F:157:TRP:HE3	1:F:198:ILE:O	1.85	0.52
1:A:20:VAL:CG1	1:A:110:THR:HG21	2.39	0.52
1:C:201:VAL:HG22	1:C:210:VAL:CG1	2.40	0.52
1:D:143:CYS:CB	1:D:199:CYS:HG	2.17	0.52
1:E:124:VAL:HG21	1:E:201:VAL:CG2	2.39	0.52
1:A:20:VAL:CG1	1:A:110:THR:CG2	2.88	0.52
1:C:157:TRP:O	1:C:200:ASN:OD1	2.28	0.52
1:E:213:LYS:HE2	1:E:215:GLU:HG2	1.93	0.51
1:A:148:TYR:O	1:A:179:TYR:HB2	2.10	0.51
1:C:32:TYR:CE2	1:C:34:ILE:HD11	2.46	0.51
1:E:214:VAL:HA	1:F:130:SER:HB3	1.92	0.51
1:F:73:ASP:OD1	1:F:76:ALA:N	2.37	0.51
1:F:87:ARG:HD3	1:F:89:GLU:OE1	2.11	0.51
1:E:144:LEU:HD13	1:F:184:VAL:HG11	1.92	0.51
1:A:163:THR:O	1:A:166:VAL:CG1	2.51	0.51
1:A:120:LYS:HD2	1:A:147:ASP:O	2.10	0.51
1:E:189:SER:O	1:E:192:LEU:HD11	2.06	0.51
1:B:147:ASP:CB	1:B:178:LEU:CD1	2.80	0.50
1:C:28:THR:CG2	1:E:102:ARG:HG2	2.41	0.50
1:F:8:GLY:O	1:F:110:THR:HG23	2.11	0.50
1:B:115:SER:CB	1:B:149:PHE:HZ	2.25	0.50
1:B:147:ASP:HB3	1:B:178:LEU:HB2	1.93	0.50
1:A:130:SER:OG	1:B:215:GLU:C	2.54	0.50
1:A:204:LYS:N	1:A:205:PRO:CD	2.73	0.50
1:B:173:LEU:HD13	1:B:179:TYR:CE2	2.46	0.50
1:C:22:CYS:SG	1:C:36:TRP:CH2	3.04	0.50
1:B:147:ASP:OD1	1:B:174:GLN:NE2	2.44	0.50
1:C:33:GLY:HA2	1:C:51:ILE:O	2.12	0.50
1:E:128:ALA:N	1:F:128:ALA:O	2.41	0.50
1:A:12:LYS:HD3	1:A:18:VAL:HB	1.94	0.50
1:A:58:THR:O	1:A:59:ASP:OD1	2.29	0.50
1:B:192:LEU:CD1	1:B:192:LEU:N	2.75	0.50
1:D:29:PHE:O	1:D:32:TYR:HB2	2.11	0.50
1:D:124:VAL:HG13	1:D:143:CYS:SG	2.51	0.50
1:B:188:PRO:O	1:B:191:SER:OG	2.29	0.50
1:E:215:GLU:N	1:F:130:SER:OG	2.44	0.50
1:C:47:TRP:HB2	1:D:104:VAL:HG23	1.94	0.49
1:D:204:LYS:HG3	1:D:204:LYS:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ASP:HB2	1:B:78:THR:HB	1.93	0.49
1:C:103:PHE:HE2	1:D:62:GLU:CG	2.23	0.49
1:C:126:PRO:CD	1:C:212:LYS:HD3	2.41	0.49
1:D:200:ASN:CA	1:D:211:ASP:HA	2.41	0.49
1:D:149:PHE:H	1:D:203:HIS:CE1	2.31	0.49
1:B:31:ASN:H	1:B:53:ILE:HB	1.77	0.49
1:C:124:VAL:CB	1:C:212:LYS:HD2	2.42	0.49
1:D:150:PRO:CG	1:D:205:PRO:HG2	2.41	0.49
1:D:124:VAL:HG21	1:D:201:VAL:CG2	2.43	0.49
1:C:127:LEU:O	1:C:214:VAL:CG1	2.61	0.49
1:D:31:ASN:N	1:D:31:ASN:OD1	2.46	0.49
1:F:34:ILE:O	1:F:34:ILE:HG22	2.13	0.49
1:A:51:ILE:CG1	1:A:58:THR:HG22	2.42	0.49
1:A:78:THR:CG2	1:D:8:GLY:HA3	2.43	0.49
1:C:149:PHE:O	1:C:149:PHE:CD2	2.66	0.49
1:F:77:SER:O	1:F:77:SER:OG	2.09	0.49
1:B:4:LEU:HD13	1:B:105:TYR:HB2	1.95	0.48
1:B:215:GLU:C	1:B:215:GLU:CD	2.80	0.48
1:D:215:GLU:HG3	1:D:216:PRO:HD2	1.95	0.48
1:F:48:ILE:O	1:F:48:ILE:HG22	2.13	0.48
1:C:91:THR:HG23	1:C:113:THR:HA	1.94	0.48
1:C:148:TYR:HE2	1:C:153:VAL:HB	1.79	0.48
1:C:168:THR:HG23	1:C:181:LEU:HD21	1.95	0.48
1:E:108:GLN:H	1:E:108:GLN:HG3	1.36	0.48
1:E:120:LYS:HE3	1:E:178:LEU:HD21	1.95	0.48
1:F:32:TYR:N	1:F:32:TYR:CD1	2.77	0.48
1:A:174:GLN:HG3	1:A:178:LEU:O	2.12	0.48
1:A:130:SER:HG	1:B:215:GLU:C	2.22	0.48
1:D:200:ASN:H	1:D:211:ASP:HA	1.78	0.48
1:A:59:ASP:OD1	1:A:59:ASP:N	2.43	0.48
1:B:127:LEU:HB2	1:B:142:GLY:O	2.13	0.48
1:E:128:ALA:O	1:F:128:ALA:O	2.32	0.48
1:A:125:PHE:O	1:A:143:CYS:HA	2.13	0.48
1:C:148:TYR:CE2	1:C:153:VAL:HB	2.48	0.48
1:D:162:LEU:HD21	1:D:185:VAL:HG21	1.95	0.48
1:E:63:LYS:HB3	1:E:64:PHE:CE1	2.49	0.48
1:F:141:LEU:HB2	1:F:185:VAL:HG12	1.95	0.48
1:D:53:ILE:N	1:D:53:ILE:HD13	2.29	0.48
1:A:18:VAL:HG12	1:A:86:LEU:HD11	1.96	0.48
1:D:29:PHE:O	1:D:32:TYR:N	2.42	0.48
1:E:64:PHE:O	1:E:68:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LYS:N	1:B:205:PRO:CD	2.77	0.47
1:A:151:GLU:CG	1:A:152:PRO:CA	2.61	0.47
1:B:60:TYR:CE2	1:B:70:ILE:HD12	2.49	0.47
1:B:148:TYR:C	1:B:148:TYR:CD1	2.91	0.47
1:B:29:PHE:O	1:B:53:ILE:HG12	2.14	0.47
1:F:147:ASP:HA	1:F:178:LEU:HB3	1.95	0.47
1:D:96:CYS:SG	1:D:107:GLY:HA3	2.55	0.47
1:B:143:CYS:HG	1:B:199:CYS:CB	2.21	0.47
1:C:6:GLN:HB2	1:C:108:GLN:HG3	1.96	0.47
1:C:148:TYR:CD1	1:C:179:TYR:O	2.67	0.47
1:E:121:GLY:HA2	1:E:203:HIS:CE1	2.50	0.47
1:C:203:HIS:CE1	1:C:205:PRO:HB2	2.49	0.47
1:D:67:ARG:HD2	1:D:84:SER:O	2.14	0.47
1:E:6:GLN:HA	1:E:21:SER:O	2.15	0.47
1:A:132:LYS:HG3	1:A:132:LYS:O	2.15	0.47
1:C:138:THR:CB	1:C:189:SER:HG	2.23	0.47
1:F:126:PRO:HB3	1:F:214:VAL:HG12	1.97	0.47
1:C:20:VAL:HG12	1:C:110:THR:HG21	1.88	0.47
1:C:127:LEU:CD1	1:D:140:ALA:O	2.62	0.47
1:C:152:PRO:HB2	1:C:205:PRO:CG	2.44	0.47
1:C:34:ILE:HG13	1:C:79:VAL:HG21	1.97	0.46
1:C:178:LEU:HD12	1:C:178:LEU:H	1.81	0.46
1:D:150:PRO:HG2	1:D:205:PRO:HG2	1.97	0.46
1:E:67:ARG:CD	1:E:84:SER:O	2.52	0.46
1:F:19:LYS:HD2	1:F:82:GLU:HB2	1.97	0.46
1:B:99:THR:HA	1:B:104:VAL:HG22	1.97	0.46
1:E:85:SER:O	1:E:85:SER:OG	2.22	0.46
1:E:128:ALA:HB1	1:E:129:PRO:HD2	1.97	0.46
1:E:2:VAL:HG11	1:E:27:TYR:CZ	2.51	0.46
1:F:68:ALA:HA	1:F:82:GLU:O	2.15	0.46
1:C:203:HIS:HB3	1:C:208:THR:HB	1.98	0.46
1:D:41:PRO:HD3	1:D:91:THR:O	2.15	0.46
1:A:115:SER:HB3	1:A:149:PHE:CE2	2.51	0.46
1:D:150:PRO:HG2	1:D:152:PRO:HD2	1.98	0.46
1:F:94:TYR:N	1:F:94:TYR:HD1	2.14	0.46
1:F:128:ALA:HB1	1:F:129:PRO:CD	2.46	0.46
1:C:151:GLU:CD	1:C:179:TYR:CD2	2.81	0.46
1:C:162:LEU:O	1:C:162:LEU:HD12	2.15	0.46
1:F:53:ILE:HG22	1:F:72:SER:OG	2.15	0.46
1:A:35:ASN:HB2	1:A:97:ALA:HB3	1.97	0.46
1:A:120:LYS:HD3	1:A:121:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:LEU:O	1:F:22:CYS:SG	2.73	0.46
1:B:39:GLN:C	1:B:92:ALA:HB1	2.41	0.46
1:B:165:GLY:O	1:B:185:VAL:HA	2.15	0.46
1:D:150:PRO:HG2	1:D:205:PRO:CG	2.46	0.46
1:A:140:ALA:HB1	1:B:144:LEU:HD23	1.98	0.45
1:D:174:GLN:HE21	1:D:174:GLN:HB2	1.55	0.45
1:A:32:TYR:CD1	1:A:32:TYR:O	2.69	0.45
1:E:7:SER:O	1:E:110:THR:HG23	2.16	0.45
1:E:76:ALA:O	1:E:77:SER:OG	2.24	0.45
1:C:31:ASN:O	1:E:101:THR:HG22	2.16	0.45
1:F:141:LEU:HD11	1:F:197:TYR:CD2	2.51	0.45
1:A:60:TYR:HE1	1:A:70:ILE:HG13	1.81	0.45
1:C:102:ARG:HG3	1:C:102:ARG:HH21	1.81	0.45
1:D:38:ARG:HB3	1:D:48:ILE:HD11	1.97	0.45
1:D:143:CYS:CB	1:D:199:CYS:SG	3.03	0.45
1:F:102:ARG:HH11	1:F:102:ARG:CG	2.30	0.45
1:A:78:THR:HG21	1:D:8:GLY:HA3	1.97	0.45
1:A:146:LYS:HE3	1:A:147:ASP:OD2	2.16	0.45
1:E:69:THR:O	1:E:69:THR:HG22	2.17	0.45
1:C:52:TYR:CZ	1:E:52:TYR:CE1	3.05	0.45
1:C:62:GLU:OE2	1:C:62:GLU:HA	2.15	0.45
1:C:152:PRO:CB	1:C:205:PRO:CG	2.94	0.45
1:E:6:GLN:CA	1:E:108:GLN:HE22	2.27	0.45
1:F:155:VAL:HG13	1:F:201:VAL:HG22	1.98	0.45
1:D:86:LEU:HB3	1:D:114:VAL:HG11	1.97	0.45
1:D:103:PHE:C	1:D:104:VAL:CG1	2.89	0.45
1:D:122:PRO:CB	1:D:145:VAL:HG12	2.47	0.45
1:E:157:TRP:HB2	1:E:162:LEU:HB3	1.98	0.45
1:F:76:ALA:HB1	1:F:78:THR:HG23	1.99	0.45
1:C:169:PHE:CE1	1:D:182:SER:HB2	2.53	0.44
1:D:200:ASN:HA	1:D:211:ASP:CB	2.46	0.44
1:F:32:TYR:O	1:F:53:ILE:CG1	2.65	0.44
1:A:124:VAL:CG1	1:A:212:LYS:HG3	2.47	0.44
1:A:140:ALA:CB	1:B:144:LEU:HD23	2.48	0.44
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.88	0.44
1:C:149:PHE:H	1:C:150:PRO:HD3	1.82	0.44
1:B:77:SER:O	1:B:78:THR:OG1	2.34	0.44
1:C:6:GLN:HG2	1:C:110:THR:CG2	2.46	0.44
1:F:215:GLU:HA	1:F:216:PRO:HD2	1.72	0.44
1:B:148:TYR:CD1	1:B:148:TYR:O	2.70	0.44
1:A:5:VAL:HG21	1:D:5:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LYS:HB3	1:C:209:LYS:HE2	1.32	0.44
1:F:214:VAL:O	1:F:214:VAL:HG23	2.18	0.44
1:C:128:ALA:N	1:D:128:ALA:O	2.49	0.44
1:C:213:LYS:HD3	1:C:213:LYS:H	1.82	0.44
1:E:212:LYS:HA	1:E:212:LYS:HD2	1.55	0.44
1:E:149:PHE:CD1	1:E:150:PRO:HA	2.53	0.44
1:B:151:GLU:CD	1:B:151:GLU:O	2.61	0.43
1:C:148:TYR:CE1	1:C:179:TYR:O	2.71	0.43
1:B:4:LEU:HD12	1:B:4:LEU:N	2.34	0.43
1:B:143:CYS:HG	1:B:199:CYS:HG	0.59	0.43
1:D:122:PRO:HB3	1:D:148:TYR:HB3	1.99	0.43
1:C:204:LYS:N	1:C:205:PRO:HD3	2.33	0.43
1:D:158:ASN:HB3	1:D:161:ALA:HB3	2.00	0.43
1:F:32:TYR:O	1:F:53:ILE:HG12	2.19	0.43
1:F:204:LYS:N	1:F:205:PRO:CD	2.82	0.43
1:A:53:ILE:HD13	1:A:53:ILE:HA	1.59	0.43
1:C:6:GLN:NE2	1:C:109:GLY:H	2.17	0.43
1:A:140:ALA:HB1	1:B:144:LEU:CD2	2.49	0.43
1:A:6:GLN:HE21	1:A:6:GLN:HB3	1.57	0.43
1:A:103:PHE:N	1:A:103:PHE:CD1	2.84	0.43
1:A:6:GLN:HB3	1:A:110:THR:CG2	2.48	0.43
1:A:163:THR:C	1:A:166:VAL:HG12	2.42	0.43
1:C:122:PRO:CA	1:C:146:LYS:O	2.65	0.43
1:C:155:VAL:HG13	1:C:201:VAL:HG12	2.00	0.43
1:D:81:MET:HE3	1:D:81:MET:HB3	1.68	0.43
1:E:28:THR:O	1:E:28:THR:OG1	2.34	0.43
1:F:151:GLU:HB2	1:F:179:TYR:CE2	2.54	0.43
1:E:204:LYS:N	1:E:205:PRO:CD	2.81	0.43
1:F:46:GLU:CD	1:F:63:LYS:NZ	2.70	0.43
1:A:155:VAL:CG1	1:A:199:CYS:SG	3.07	0.42
1:A:157:TRP:HZ3	1:A:214:VAL:HG21	1.83	0.42
1:B:67:ARG:NH1	1:B:90:ASP:OD2	2.46	0.42
1:C:152:PRO:CB	1:C:205:PRO:HG2	2.48	0.42
1:E:5:VAL:O	1:E:5:VAL:HG23	2.18	0.42
1:F:13:LYS:HB3	1:F:13:LYS:HE2	1.55	0.42
1:C:102:ARG:CZ	1:C:102:ARG:HB3	2.48	0.42
1:D:124:VAL:CG2	1:D:201:VAL:HG21	2.49	0.42
1:E:172:VAL:HG23	1:F:169:PHE:CD1	2.55	0.42
1:D:103:PHE:C	1:D:104:VAL:HG13	2.45	0.42
1:A:169:PHE:HA	1:A:170:PRO:HD3	1.92	0.42
1:D:149:PHE:HE1	1:D:177:GLY:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ARG:C	1:C:114:VAL:HG11	2.45	0.42
1:B:11:VAL:HG13	1:B:113:THR:HB	2.01	0.42
1:B:141:LEU:N	1:B:185:VAL:O	2.45	0.42
1:D:202:ASN:OD1	1:D:208:THR:O	2.37	0.42
1:A:144:LEU:HD22	1:B:184:VAL:HG11	2.02	0.42
1:A:215:GLU:HA	1:A:216:PRO:HD3	1.89	0.42
1:C:20:VAL:HG11	1:C:110:THR:CG2	2.46	0.42
1:D:27:TYR:HB3	1:D:28:THR:H	1.63	0.42
1:D:51:ILE:O	1:D:51:ILE:HG23	2.20	0.42
1:D:124:VAL:HG21	1:D:201:VAL:HG21	2.01	0.42
1:E:33:GLY:HA3	1:E:50:TYR:CZ	2.55	0.42
1:A:32:TYR:OH	1:A:77:SER:O	2.26	0.42
1:E:53:ILE:O	1:E:53:ILE:CG1	2.68	0.42
1:C:6:GLN:OE1	1:C:95:TYR:HA	2.20	0.42
1:A:10:GLU:HG2	1:A:12:LYS:CE	2.49	0.41
1:A:20:VAL:HG11	1:A:110:THR:CG2	2.47	0.41
1:C:162:LEU:CD1	1:C:162:LEU:O	2.68	0.41
1:E:64:PHE:HB3	1:E:68:ALA:HB2	2.02	0.41
1:E:148:TYR:CE2	1:E:153:VAL:HG23	2.55	0.41
1:B:195:GLN:OE1	1:B:196:THR:N	2.53	0.41
1:D:3:GLN:HE21	1:D:3:GLN:HB2	1.65	0.41
1:E:124:VAL:HG12	1:E:212:LYS:CG	2.50	0.41
1:E:208:THR:O	1:E:208:THR:CG2	2.69	0.41
1:A:32:TYR:CD1	1:A:32:TYR:C	2.98	0.41
1:E:6:GLN:HE21	1:E:6:GLN:HB3	1.53	0.41
1:E:132:LYS:HD3	1:E:132:LYS:HA	1.68	0.41
1:A:67:ARG:HB3	1:A:84:SER:O	2.21	0.41
1:D:204:LYS:CB	1:D:204:LYS:HZ2	2.32	0.41
1:A:27:TYR:CE2	1:A:29:PHE:HB2	2.55	0.41
1:C:47:TRP:CG	1:D:104:VAL:CG2	3.02	0.41
1:F:38:ARG:HB2	1:F:48:ILE:HD11	2.03	0.41
1:A:6:GLN:HB3	1:A:110:THR:HG22	2.02	0.41
1:B:151:GLU:N	1:B:152:PRO:HD2	2.36	0.41
1:C:140:ALA:O	1:D:127:LEU:HD21	2.20	0.41
1:C:150:PRO:HB2	1:C:205:PRO:HG2	2.02	0.41
1:C:166:VAL:HA	1:C:185:VAL:HG22	2.03	0.41
1:D:200:ASN:N	1:D:211:ASP:HA	2.35	0.41
1:B:173:LEU:CD1	1:B:179:TYR:CE1	3.04	0.41
1:C:170:PRO:HD2	1:D:170:PRO:HD2	2.03	0.41
1:F:149:PHE:HB2	1:F:178:LEU:HD23	2.03	0.41
1:F:163:THR:C	1:F:166:VAL:HG12	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:HA	1:A:149:PHE:O	2.20	0.41
1:A:149:PHE:HA	1:A:150:PRO:HA	1.83	0.41
1:B:61:SER:HB3	1:B:64:PHE:HD2	1.86	0.41
1:C:126:PRO:HG3	1:C:212:LYS:CE	2.50	0.41
1:C:178:LEU:HD12	1:C:178:LEU:N	2.36	0.41
1:D:103:PHE:O	1:D:104:VAL:HG12	2.21	0.41
1:D:204:LYS:HZ2	1:D:204:LYS:HB2	1.85	0.41
1:E:18:VAL:O	1:E:18:VAL:HG13	2.21	0.41
1:E:102:ARG:HE	1:E:102:ARG:HB3	1.62	0.41
1:E:5:VAL:O	1:E:5:VAL:CG2	2.69	0.41
1:F:52:TYR:O	1:F:56:GLY:N	2.50	0.41
1:B:140:ALA:HA	1:B:186:THR:HA	2.02	0.40
1:C:40:ALA:HB3	1:C:43:GLN:HB2	2.04	0.40
1:C:166:VAL:O	1:C:166:VAL:CG1	2.69	0.40
1:D:168:THR:HG23	1:D:181:LEU:HD21	2.04	0.40
1:D:204:LYS:N	1:D:205:PRO:CD	2.84	0.40
1:F:76:ALA:HB1	1:F:78:THR:CG2	2.51	0.40
1:B:142:GLY:CA	1:B:157:TRP:HH2	2.32	0.40
1:B:51:ILE:O	1:B:51:ILE:HG23	2.21	0.40
1:C:73:ASP:OD2	1:C:76:ALA:N	2.53	0.40
1:C:122:PRO:HA	1:C:147:ASP:O	2.21	0.40
1:D:9:ALA:C	1:D:10:GLU:HG2	2.47	0.40
1:A:51:ILE:HG13	1:A:58:THR:CG2	2.49	0.40
1:C:201:VAL:HG23	1:C:201:VAL:O	2.20	0.40
1:C:97:ALA:HA	1:C:105:TYR:O	2.21	0.40
1:C:201:VAL:O	1:C:201:VAL:CG2	2.69	0.40

All (22) 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:B:23:LYS:CE	1:C:194:THR:CB[2_546]	0.36	1.84
1:B:25:SER:C	1:C:195:GLN:OE1[2_546]	0.50	1.70
1:B:23:LYS:NZ	1:C:194:THR:CA[2_546]	0.62	1.58
1:B:23:LYS:CD	1:C:194:THR:CG2[2_546]	0.73	1.47
1:B:23:LYS:NZ	1:C:194:THR:N[2_546]	0.99	1.21
1:B:25:SER:O	1:C:195:GLN:OE1[2_546]	1.00	1.20
1:B:23:LYS:CE	1:C:194:THR:OG1[2_546]	1.16	1.04
1:B:23:LYS:CE	1:C:194:THR:CA[2_546]	1.47	0.73
1:B:23:LYS:NZ	1:C:194:THR:CB[2_546]	1.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LYS:CE	1:C:194:THR:CG2[2_546]	1.55	0.65
1:B:23:LYS:CD	1:C:194:THR:CB[2_546]	1.55	0.65
1:B:25:SER:CA	1:C:195:GLN:OE1[2_546]	1.62	0.58
1:B:25:SER:C	1:C:195:GLN:CD[2_546]	1.65	0.55
1:B:89:GLU:OE2	1:C:85:SER:OG[4_546]	1.74	0.46
1:B:25:SER:O	1:C:195:GLN:CD[2_546]	1.87	0.33
1:B:76:ALA:CB	1:C:188:PRO:CG[2_546]	1.90	0.30
1:B:23:LYS:CD	1:C:194:THR:OG1[2_546]	1.96	0.24
1:B:89:GLU:CD	1:C:85:SER:OG[4_546]	1.99	0.21
1:B:23:LYS:NZ	1:C:193:GLY:C[2_546]	2.01	0.19
1:B:23:LYS:NZ	1:C:194:THR:C[2_546]	2.05	0.15
1:B:89:GLU:OE1	1:C:85:SER:OG[4_546]	2.13	0.07
1:B:23:LYS:NZ	1:C:194:THR:CG2[2_546]	2.15	0.05

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	209/448 (47%)	198 (95%)	10 (5%)	1 (0%)	24	53
1	B	195/448 (44%)	187 (96%)	8 (4%)	0	100	100
1	C	194/448 (43%)	180 (93%)	12 (6%)	2 (1%)	12	37
1	D	201/448 (45%)	183 (91%)	16 (8%)	2 (1%)	12	37
1	E	214/448 (48%)	198 (92%)	13 (6%)	3 (1%)	9	29
1	F	198/448 (44%)	182 (92%)	15 (8%)	1 (0%)	24	53
All	All	1211/2688 (45%)	1128 (93%)	74 (6%)	9 (1%)	18	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	147	ASP
1	D	30	THR

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Mol	Chain	Res	Type
1	E	135	SER
1	A	131	SER
1	E	136	GLY
1	C	151	GLU
1	E	54	GLY
1	C	149	PHE
1	F	5	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/376 (47%)	129 (72%)	49 (28%)	0	1
1	B	168/376 (45%)	137 (82%)	31 (18%)	1	5
1	C	168/376 (45%)	107 (64%)	61 (36%)	0	0
1	D	172/376 (46%)	132 (77%)	40 (23%)	1	2
1	E	180/376 (48%)	140 (78%)	40 (22%)	1	3
1	F	170/376 (45%)	125 (74%)	45 (26%)	0	1
All	All	1036/2256 (46%)	770 (74%)	266 (26%)	0	2

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	10	GLU
1	A	12	LYS
1	A	18	VAL
1	A	23	LYS
1	A	31	ASN
1	A	32	TYR
1	A	38	ARG
1	A	43	GLN
1	A	45	LEU
1	A	51	ILE

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Mol	Chain	Res	Type
1	A	53	ILE
1	A	57	ASP
1	A	59	ASP
1	A	62	GLU
1	A	63	LYS
1	A	65	LYS
1	A	67	ARG
1	A	70	ILE
1	A	71	THR
1	A	77	SER
1	A	85	SER
1	A	87	ARG
1	A	88	SER
1	A	93	VAL
1	A	99	THR
1	A	101	THR
1	A	102	ARG
1	A	110	THR
1	A	111	LEU
1	A	119	THR
1	A	120	LYS
1	A	130	SER
1	A	132	LYS
1	A	133	SER
1	A	138	THR
1	A	144	LEU
1	A	152	PRO
1	A	153	VAL
1	A	154	THR
1	A	163	THR
1	A	178	LEU
1	A	182	SER
1	A	192	LEU
1	A	195	GLN
1	A	198	ILE
1	A	212	LYS
1	A	213	LYS
1	A	214	VAL
1	B	11	VAL
1	B	13	LYS
1	B	23	LYS
1	B	25	SER

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Mol	Chain	Res	Type
1	B	43	GLN
1	B	51	ILE
1	B	53	ILE
1	B	59	ASP
1	B	61	SER
1	B	63	LYS
1	B	65	LYS
1	B	69	THR
1	B	88	SER
1	B	118	SER
1	B	123	SER
1	B	144	LEU
1	B	145	VAL
1	B	146	LYS
1	B	147	ASP
1	B	150	PRO
1	B	163	THR
1	B	176	SER
1	B	182	SER
1	B	183	SER
1	B	189	SER
1	B	194	THR
1	B	196	THR
1	B	198	ILE
1	B	205	PRO
1	B	206	SER
1	B	215	GLU
1	C	3	GLN
1	C	6	GLN
1	C	10	GLU
1	C	11	VAL
1	C	14	PRO
1	C	17	SER
1	C	18	VAL
1	C	20	VAL
1	C	23	LYS
1	C	25	SER
1	C	37	VAL
1	C	46	GLU
1	C	53	ILE
1	C	67	ARG
1	C	74	THR

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Mol	Chain	Res	Type
1	C	85	SER
1	C	87	ARG
1	C	88	SER
1	C	101	THR
1	C	102	ARG
1	C	103	PHE
1	C	108	GLN
1	C	110	THR
1	C	113	THR
1	C	115	SER
1	C	116	SER
1	C	119	THR
1	C	120	LYS
1	C	124	VAL
1	C	127	LEU
1	C	141	LEU
1	C	143	CYS
1	C	146	LYS
1	C	153	VAL
1	C	154	THR
1	C	159	SER
1	C	162	LEU
1	C	163	THR
1	C	164	SER
1	C	172	VAL
1	C	178	LEU
1	C	181	LEU
1	C	183	SER
1	C	184	VAL
1	C	189	SER
1	C	190	SER
1	C	192	LEU
1	C	194	THR
1	C	195	GLN
1	C	198	ILE
1	C	200	ASN
1	C	201	VAL
1	C	202	ASN
1	C	206	SER
1	C	209	LYS
1	C	210	VAL
1	C	211	ASP

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Mol	Chain	Res	Type
1	C	212	LYS
1	C	213	LYS
1	C	214	VAL
1	C	215	GLU
1	D	5	VAL
1	D	10	GLU
1	D	17	SER
1	D	28	THR
1	D	31	ASN
1	D	43	GLN
1	D	51	ILE
1	D	57	ASP
1	D	71	THR
1	D	74	THR
1	D	77	SER
1	D	81	MET
1	D	84	SER
1	D	99	THR
1	D	104	VAL
1	D	108	GLN
1	D	113	THR
1	D	115	SER
1	D	118	SER
1	D	144	LEU
1	D	146	LYS
1	D	153	VAL
1	D	154	THR
1	D	159	SER
1	D	162	LEU
1	D	172	VAL
1	D	181	LEU
1	D	183	SER
1	D	184	VAL
1	D	187	VAL
1	D	189	SER
1	D	191	SER
1	D	192	LEU
1	D	194	THR
1	D	196	THR
1	D	204	LYS
1	D	205	PRO
1	D	210	VAL

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Mol	Chain	Res	Type
1	D	213	LYS
1	D	215	GLU
1	E	12	LYS
1	E	13	LYS
1	E	19	LYS
1	E	24	THR
1	E	28	THR
1	E	34	ILE
1	E	43	GLN
1	E	51	ILE
1	E	53	ILE
1	E	57	ASP
1	E	64	PHE
1	E	71	THR
1	E	74	THR
1	E	78	THR
1	E	79	VAL
1	E	87	ARG
1	E	88	SER
1	E	99	THR
1	E	102	ARG
1	E	108	GLN
1	E	111	LEU
1	E	113	THR
1	E	129	PRO
1	E	130	SER
1	E	131	SER
1	E	132	LYS
1	E	134	THR
1	E	144	LEU
1	E	146	LYS
1	E	150	PRO
1	E	162	LEU
1	E	164	SER
1	E	194	THR
1	E	202	ASN
1	E	204	LYS
1	E	208	THR
1	E	209	LYS
1	E	212	LYS
1	E	213	LYS
1	E	215	GLU

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Mol	Chain	Res	Type
1	F	1	GLU
1	F	3	GLN
1	F	4	LEU
1	F	10	GLU
1	F	11	VAL
1	F	13	LYS
1	F	18	VAL
1	F	19	LYS
1	F	20	VAL
1	F	23	LYS
1	F	32	TYR
1	F	34	ILE
1	F	37	VAL
1	F	46	GLU
1	F	51	ILE
1	F	53	ILE
1	F	59	ASP
1	F	61	SER
1	F	62	GLU
1	F	63	LYS
1	F	65	LYS
1	F	67	ARG
1	F	72	SER
1	F	77	SER
1	F	88	SER
1	F	89	GLU
1	F	104	VAL
1	F	113	THR
1	F	118	SER
1	F	123	SER
1	F	130	SER
1	F	143	CYS
1	F	146	LYS
1	F	150	PRO
1	F	154	THR
1	F	166	VAL
1	F	174	GLN
1	F	175	SER
1	F	188	PRO
1	F	196	THR
1	F	198	ILE
1	F	199	CYS

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Mol	Chain	Res	Type
1	F	209	LYS
1	F	210	VAL
1	F	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	B	43	GLN
1	C	6	GLN
1	C	108	GLN
1	C	200	ASN
1	D	3	GLN
1	D	195	GLN
1	E	31	ASN
1	E	108	GLN
1	E	203	HIS
1	F	167	HIS
1	F	200	ASN
1	F	202	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	213/448 (47%)	0.39	16 (7%)	20 16	10, 32, 61, 76	0
1	B	203/448 (45%)	0.36	20 (9%)	13 11	14, 31, 57, 72	0
1	C	202/448 (45%)	0.67	21 (10%)	11 10	18, 45, 71, 100	0
1	D	207/448 (46%)	0.38	13 (6%)	26 20	14, 35, 79, 110	0
1	E	216/448 (48%)	0.46	9 (4%)	40 32	26, 43, 71, 90	0
1	F	204/448 (45%)	0.61	19 (9%)	14 12	25, 47, 75, 86	0
All	All	1245/2688 (46%)	0.48	98 (7%)	18 15	10, 39, 71, 110	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	PRO	6.0
1	A	28	THR	5.7
1	D	200	ASN	5.4
1	C	147	ASP	5.2
1	D	150	PRO	5.0
1	B	76	ALA	4.9
1	C	126	PRO	4.7
1	C	124	VAL	4.5
1	E	27	TYR	4.4
1	A	199	CYS	4.4
1	F	5	VAL	4.3
1	E	96	CYS	4.0
1	A	61	SER	4.0
1	B	145	VAL	4.0
1	A	31	ASN	3.9
1	F	106	TRP	3.8
1	D	199	CYS	3.7
1	A	118	SER	3.7
1	B	55	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	99	THR	3.6
1	C	100	GLY	3.5
1	C	150	PRO	3.4
1	B	164	SER	3.4
1	E	28	THR	3.4
1	B	75	SER	3.4
1	E	29	PHE	3.4
1	C	153	VAL	3.3
1	C	118	SER	3.3
1	C	149	PHE	3.3
1	E	30	THR	3.3
1	C	127	LEU	3.2
1	B	77	SER	3.2
1	C	125	PHE	3.2
1	A	54	GLY	3.1
1	B	144	LEU	3.1
1	F	199	CYS	3.1
1	B	151	GLU	3.1
1	C	151	GLU	3.1
1	E	203	HIS	3.0
1	B	56	GLY	3.0
1	E	214	VAL	3.0
1	A	32	TYR	2.9
1	B	22	CYS	2.9
1	A	30	THR	2.9
1	B	100	GLY	2.9
1	F	98	GLY	2.9
1	C	194	THR	2.9
1	A	29	PHE	2.8
1	F	200	ASN	2.8
1	E	53	ILE	2.8
1	D	143	CYS	2.8
1	B	126	PRO	2.8
1	B	54	GLY	2.7
1	B	152	PRO	2.7
1	C	146	LYS	2.7
1	C	101	THR	2.7
1	F	4	LEU	2.7
1	D	103	PHE	2.7
1	D	27	TYR	2.7
1	F	53	ILE	2.6
1	F	198	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	117	ALA	2.6
1	D	204	LYS	2.6
1	F	69	THR	2.6
1	F	97	ALA	2.5
1	A	130	SER	2.5
1	F	201	VAL	2.5
1	A	132	LYS	2.4
1	F	80	TYR	2.4
1	C	120	LYS	2.3
1	C	22	CYS	2.3
1	A	133	SER	2.3
1	A	148	TYR	2.3
1	F	108	GLN	2.3
1	F	99	THR	2.3
1	D	202	ASN	2.3
1	F	2	VAL	2.3
1	B	74	THR	2.3
1	D	214	VAL	2.3
1	F	62	GLU	2.2
1	B	73	ASP	2.2
1	B	147	ASP	2.2
1	C	119	THR	2.2
1	F	6	GLN	2.2
1	A	34	ILE	2.2
1	D	56	GLY	2.1
1	E	26	GLY	2.1
1	B	99	THR	2.1
1	A	62	GLU	2.1
1	D	149	PHE	2.1
1	D	28	THR	2.1
1	B	32	TYR	2.1
1	B	23	LYS	2.0
1	D	96	CYS	2.0
1	C	97	ALA	2.0
1	A	150	PRO	2.0
1	F	8	GLY	2.0
1	F	55	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.