



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:31 AM UTC

PDB ID : 2D40 / pdb_00002d40
Title : Crystal Structure of Z3393 from Escherichia coli O157:H7
Authors : Adams, M.A.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2005-10-05
Resolution : 2.41 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

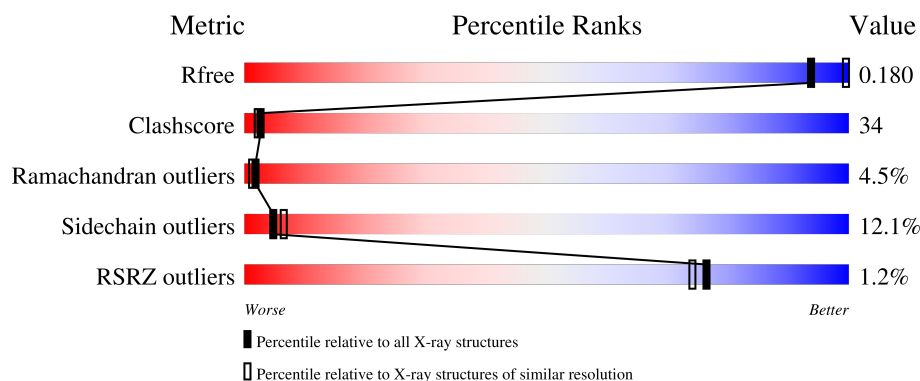
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	354	20% 39% 17% 6% 18%
1	B	354	20% 36% 16% 8% 20%
1	C	354	23% 32% 23% • 18%
1	D	354	22% 33% 19% 6% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9579 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 putative gentisate 1,2-dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	Se	0	0	0
			2280	1447	399	426	2	6			
1	B	284	Total	C	N	O	S	Se	0	0	0
			2235	1418	392	417	2	6			
1	C	289	Total	C	N	O	S	Se	0	0	0
			2281	1447	399	427	2	6			
1	D	287	Total	C	N	O	S	Se	0	0	0
			2263	1437	396	422	2	6			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q8X655
A	-10	GLY	-	expression tag	UNP Q8X655
A	-9	SER	-	expression tag	UNP Q8X655
A	-8	SER	-	expression tag	UNP Q8X655
A	-7	HIS	-	expression tag	UNP Q8X655
A	-6	HIS	-	expression tag	UNP Q8X655
A	-5	HIS	-	expression tag	UNP Q8X655
A	-4	HIS	-	expression tag	UNP Q8X655
A	-3	HIS	-	expression tag	UNP Q8X655
A	-2	HIS	-	expression tag	UNP Q8X655
A	-1	GLY	-	expression tag	UNP Q8X655
A	0	SER	-	expression tag	UNP Q8X655
A	1	MSE	MET	modified residue	UNP Q8X655
A	96	MSE	MET	modified residue	UNP Q8X655
A	131	MSE	MET	modified residue	UNP Q8X655
A	199	MSE	MET	modified residue	UNP Q8X655
A	241	MSE	MET	modified residue	UNP Q8X655
A	253	MSE	MET	modified residue	UNP Q8X655
A	256	MSE	MET	modified residue	UNP Q8X655
B	-11	MSE	-	expression tag	UNP Q8X655
B	-10	GLY	-	expression tag	UNP Q8X655

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	expression tag	UNP Q8X655
B	-8	SER	-	expression tag	UNP Q8X655
B	-7	HIS	-	expression tag	UNP Q8X655
B	-6	HIS	-	expression tag	UNP Q8X655
B	-5	HIS	-	expression tag	UNP Q8X655
B	-4	HIS	-	expression tag	UNP Q8X655
B	-3	HIS	-	expression tag	UNP Q8X655
B	-2	HIS	-	expression tag	UNP Q8X655
B	-1	GLY	-	expression tag	UNP Q8X655
B	0	SER	-	expression tag	UNP Q8X655
B	1	MSE	MET	modified residue	UNP Q8X655
B	96	MSE	MET	modified residue	UNP Q8X655
B	131	MSE	MET	modified residue	UNP Q8X655
B	199	MSE	MET	modified residue	UNP Q8X655
B	241	MSE	MET	modified residue	UNP Q8X655
B	253	MSE	MET	modified residue	UNP Q8X655
B	256	MSE	MET	modified residue	UNP Q8X655
C	-11	MSE	-	expression tag	UNP Q8X655
C	-10	GLY	-	expression tag	UNP Q8X655
C	-9	SER	-	expression tag	UNP Q8X655
C	-8	SER	-	expression tag	UNP Q8X655
C	-7	HIS	-	expression tag	UNP Q8X655
C	-6	HIS	-	expression tag	UNP Q8X655
C	-5	HIS	-	expression tag	UNP Q8X655
C	-4	HIS	-	expression tag	UNP Q8X655
C	-3	HIS	-	expression tag	UNP Q8X655
C	-2	HIS	-	expression tag	UNP Q8X655
C	-1	GLY	-	expression tag	UNP Q8X655
C	0	SER	-	expression tag	UNP Q8X655
C	1	MSE	MET	modified residue	UNP Q8X655
C	96	MSE	MET	modified residue	UNP Q8X655
C	131	MSE	MET	modified residue	UNP Q8X655
C	199	MSE	MET	modified residue	UNP Q8X655
C	241	MSE	MET	modified residue	UNP Q8X655
C	253	MSE	MET	modified residue	UNP Q8X655
C	256	MSE	MET	modified residue	UNP Q8X655
D	-11	MSE	-	expression tag	UNP Q8X655
D	-10	GLY	-	expression tag	UNP Q8X655
D	-9	SER	-	expression tag	UNP Q8X655
D	-8	SER	-	expression tag	UNP Q8X655
D	-7	HIS	-	expression tag	UNP Q8X655
D	-6	HIS	-	expression tag	UNP Q8X655

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP Q8X655
D	-4	HIS	-	expression tag	UNP Q8X655
D	-3	HIS	-	expression tag	UNP Q8X655
D	-2	HIS	-	expression tag	UNP Q8X655
D	-1	GLY	-	expression tag	UNP Q8X655
D	0	SER	-	expression tag	UNP Q8X655
D	1	MSE	MET	modified residue	UNP Q8X655
D	96	MSE	MET	modified residue	UNP Q8X655
D	131	MSE	MET	modified residue	UNP Q8X655
D	199	MSE	MET	modified residue	UNP Q8X655
D	241	MSE	MET	modified residue	UNP Q8X655
D	253	MSE	MET	modified residue	UNP Q8X655
D	256	MSE	MET	modified residue	UNP Q8X655

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

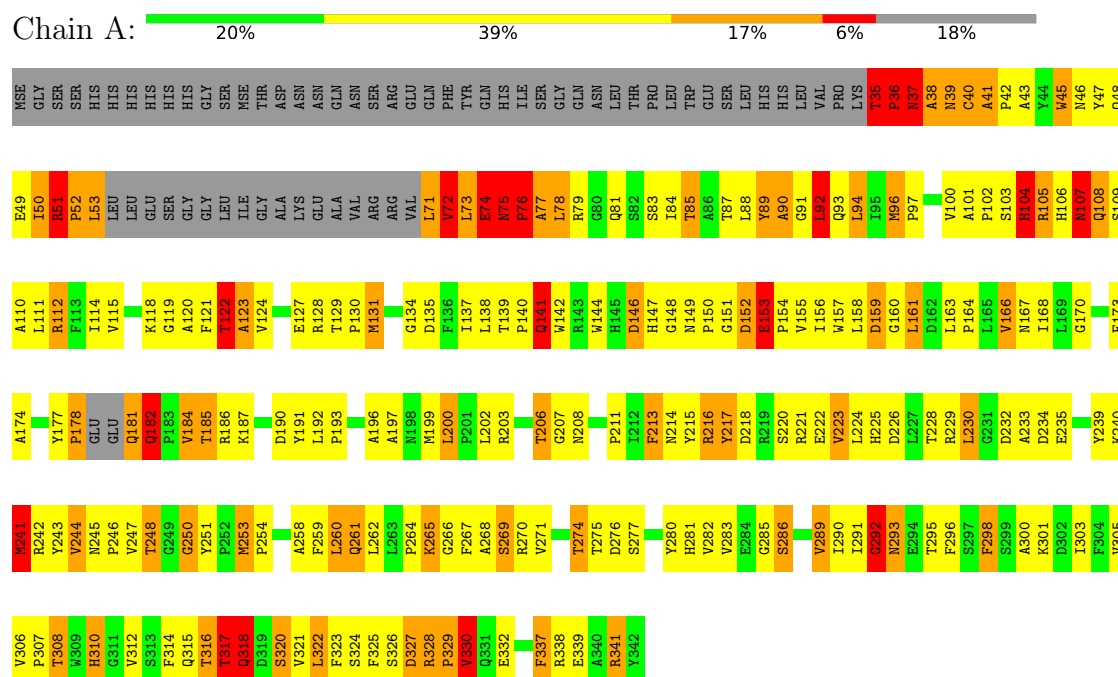
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	110	Total O 110 110	0	0
3	B	129	Total O 129 129	0	0
3	C	130	Total O 130 130	0	0
3	D	147	Total O 147 147	0	0

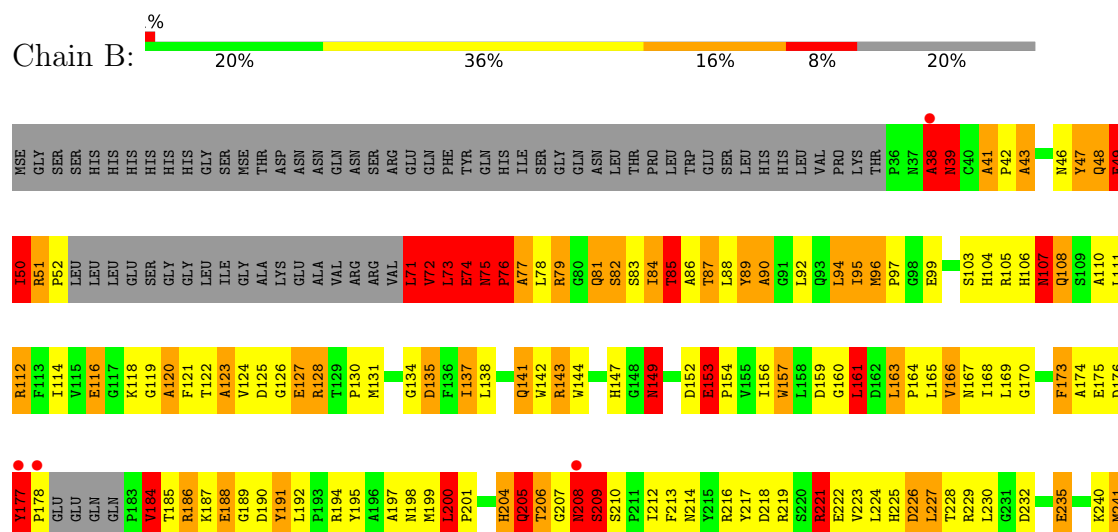
3 Residue-property plots

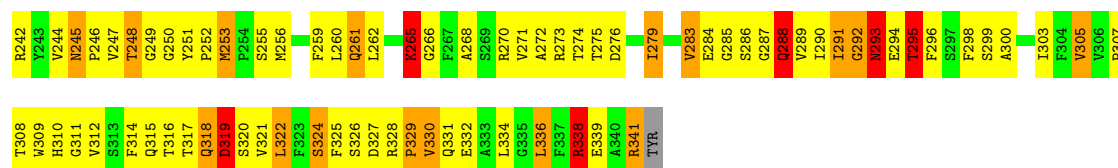
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: putative gentisate 1,2-dioxygenase

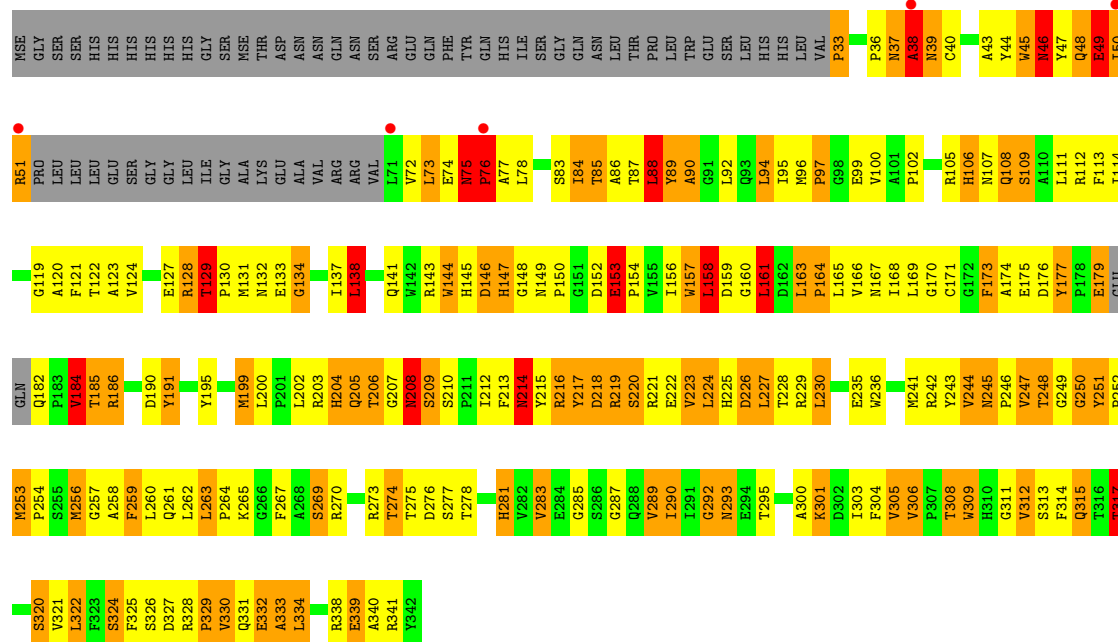
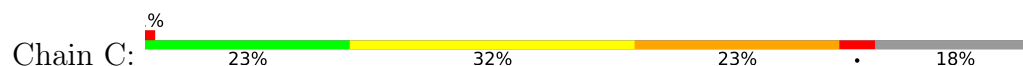


- Molecule 1: putative gentisate 1,2-dioxygenase

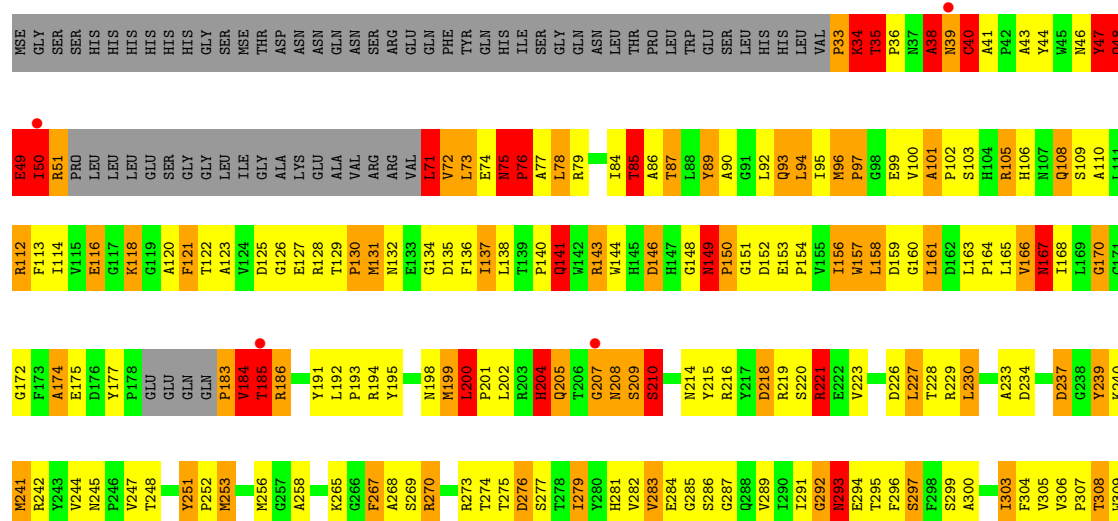
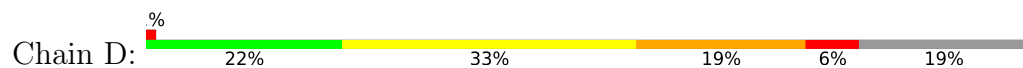




• Molecule 1: putative gentisate 1,2-dioxygenase



• Molecule 1: putative gentisate 1,2-dioxygenase



H310	G311	V312	S313	F314	Q315	T316	T317	Q318	D319	S320	V321	L322	F323	S324		D327	R328	P329	V330	Q331	E332	A333	L334	G335	L336	F337	R338	E339	A340	R341	Y342

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.13Å 76.08Å 85.46Å 114.08° 94.93° 108.11°	Depositor
Resolution (Å)	34.50 – 2.41 34.50 – 2.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.50-2.41) 93.6 (34.50-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.71 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.173 , 0.249 0.188 , 0.180	Depositor DCC
R_{free} test set	2054 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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: FE

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	2.92	201/2340 (8.6%)	1.88	36/3182 (1.1%)
1	B	2.80	176/2294 (7.7%)	1.88	42/3118 (1.3%)
1	C	2.84	189/2341 (8.1%)	1.95	69/3181 (2.2%)
1	D	2.93	202/2323 (8.7%)	1.93	68/3156 (2.2%)
All	All	2.87	768/9298 (8.3%)	1.91	215/12637 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	2
All	All	0	5

All (768) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	ILE	CA-CB	21.08	1.83	1.54
1	A	77	ALA	CA-CB	-19.15	1.21	1.53
1	D	96	MSE	SE-CE	16.07	2.43	1.95
1	A	40	CYS	C-O	15.22	1.43	1.24
1	D	50	ILE	N-CA	15.21	1.65	1.46
1	D	76	PRO	CA-CB	15.03	1.75	1.53
1	B	321	VAL	CA-CB	-14.94	1.36	1.54
1	D	100	VAL	C-O	-14.19	1.08	1.23
1	B	298	PHE	CA-C	-13.45	1.35	1.52
1	A	206	THR	CA-CB	12.31	1.71	1.53
1	A	90	ALA	CA-CB	-12.30	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	ARG	C-O	-12.13	1.12	1.24
1	D	101	ALA	CA-CB	12.01	1.71	1.54
1	B	41	ALA	CA-CB	11.88	1.70	1.53
1	A	152	ASP	C-O	11.83	1.37	1.23
1	C	50	ILE	CA-CB	-11.71	1.40	1.54
1	B	326	SER	C-O	-11.62	1.11	1.23
1	A	300	ALA	C-O	-11.60	1.09	1.23
1	D	144	TRP	C-O	-11.56	1.10	1.23
1	C	223	VAL	CA-CB	11.47	1.67	1.54
1	A	96	MSE	SE-CE	11.43	2.29	1.95
1	A	39	ASN	CA-C	11.34	1.65	1.52
1	C	77	ALA	N-CA	11.33	1.56	1.46
1	A	321	VAL	CA-CB	-11.14	1.40	1.53
1	C	85	THR	CA-CB	11.12	1.68	1.53
1	C	199	MSE	SE-CE	-10.97	1.62	1.95
1	A	77	ALA	CA-C	10.90	1.67	1.52
1	B	188	GLU	C-O	10.84	1.37	1.23
1	B	130	PRO	C-O	-10.80	1.10	1.23
1	C	156	ILE	CA-CB	10.79	1.68	1.54
1	A	124	VAL	C-O	-10.65	1.12	1.24
1	B	274	THR	C-O	-10.33	1.10	1.23
1	B	298	PHE	C-O	-10.18	1.11	1.23
1	B	77	ALA	CA-C	10.03	1.66	1.52
1	C	254	PRO	C-O	-10.02	1.12	1.24
1	B	206	THR	CA-CB	10.00	1.69	1.53
1	D	204	HIS	C-O	10.00	1.36	1.24
1	A	76	PRO	CA-CB	9.98	1.68	1.53
1	D	312	VAL	CA-CB	-9.92	1.40	1.54
1	C	49	GLU	CA-C	9.90	1.66	1.52
1	B	192	LEU	C-O	-9.89	1.15	1.24
1	B	38	ALA	CA-CB	9.88	1.70	1.53
1	A	330	VAL	CA-CB	9.86	1.67	1.54
1	A	137	ILE	CA-CB	9.79	1.68	1.54
1	B	157	TRP	C-O	-9.77	1.11	1.23
1	D	268	ALA	C-O	-9.76	1.12	1.23
1	D	33	PRO	N-CA	9.74	1.61	1.47
1	A	37	ASN	C-O	9.73	1.36	1.24
1	C	130	PRO	C-O	-9.60	1.11	1.23
1	A	75	ASN	CA-C	-9.60	1.40	1.52
1	D	253	MSE	SE-CE	9.55	2.24	1.95
1	C	76	PRO	CA-CB	9.50	1.67	1.53
1	D	200	LEU	N-CA	-9.43	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	185	THR	CA-CB	9.34	1.69	1.53
1	B	39	ASN	CB-CG	9.33	1.75	1.52
1	B	249	GLY	C-O	9.32	1.36	1.24
1	C	39	ASN	C-O	-9.29	1.13	1.23
1	A	341	ARG	CD-NE	-9.23	1.33	1.46
1	D	112	ARG	NE-CZ	-9.22	1.23	1.33
1	D	313	SER	CA-C	-9.17	1.41	1.52
1	D	39	ASN	CB-CG	9.15	1.75	1.52
1	D	105	ARG	NE-CZ	9.15	1.43	1.33
1	B	124	VAL	C-O	-9.14	1.14	1.24
1	A	112	ARG	C-O	-9.04	1.13	1.23
1	D	110	ALA	C-O	-9.01	1.12	1.23
1	D	299	SER	C-O	-8.97	1.12	1.24
1	A	316	THR	C-O	-8.97	1.12	1.24
1	B	169	LEU	N-CA	8.96	1.57	1.46
1	B	123	ALA	CA-C	8.93	1.63	1.52
1	D	48	GLN	N-CA	8.93	1.58	1.46
1	B	135	ASP	CA-C	8.91	1.64	1.52
1	B	245	ASN	CA-C	-8.90	1.42	1.52
1	C	47	TYR	CA-C	8.87	1.63	1.53
1	D	177	TYR	CA-C	8.87	1.62	1.53
1	A	185	THR	N-CA	8.86	1.57	1.46
1	C	185	THR	N-CA	8.83	1.57	1.46
1	D	209	SER	C-O	-8.81	1.12	1.24
1	D	110	ALA	CA-CB	-8.80	1.38	1.53
1	B	90	ALA	CA-CB	-8.79	1.35	1.54
1	A	157	TRP	C-O	-8.78	1.12	1.23
1	C	95	ILE	C-O	-8.73	1.14	1.24
1	C	38	ALA	CA-CB	8.69	1.68	1.53
1	C	75	ASN	CG-ND2	8.68	1.51	1.33
1	C	152	ASP	C-O	8.68	1.33	1.23
1	B	38	ALA	CA-C	8.61	1.64	1.52
1	C	219	ARG	C-O	-8.60	1.13	1.24
1	C	285	GLY	C-O	-8.58	1.12	1.24
1	C	320	SER	C-O	-8.47	1.12	1.23
1	B	166	VAL	CA-CB	-8.44	1.42	1.54
1	A	247	VAL	C-O	-8.44	1.12	1.24
1	A	203	ARG	C-O	8.43	1.33	1.23
1	A	196	ALA	C-O	-8.42	1.12	1.24
1	C	249	GLY	C-O	-8.42	1.12	1.24
1	C	133	GLU	C-O	-8.41	1.13	1.24
1	D	218	ASP	C-O	-8.41	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	GLN	C-O	-8.34	1.14	1.24
1	B	77	ALA	N-CA	8.32	1.56	1.46
1	D	156	ILE	C-O	-8.30	1.15	1.24
1	B	290	ILE	C-O	-8.30	1.15	1.24
1	D	201	PRO	CA-C	8.29	1.62	1.52
1	D	97	PRO	C-O	-8.29	1.14	1.23
1	A	326	SER	C-O	-8.28	1.16	1.24
1	B	165	LEU	C-O	-8.28	1.14	1.24
1	D	265	LYS	C-O	-8.28	1.13	1.23
1	B	73	LEU	CA-C	-8.24	1.42	1.52
1	B	149	ASN	CB-CG	-8.23	1.31	1.52
1	B	43	ALA	CA-CB	-8.19	1.39	1.53
1	A	104	HIS	C-O	-8.17	1.14	1.23
1	B	210	SER	CA-C	8.16	1.61	1.52
1	D	199	MSE	N-CA	-8.15	1.35	1.45
1	C	208	ASN	C-O	-8.14	1.13	1.24
1	D	297	SER	CA-CB	8.13	1.65	1.53
1	B	128	ARG	C-O	-8.13	1.13	1.23
1	A	139	THR	C-O	-8.12	1.16	1.24
1	A	123	ALA	C-O	-8.11	1.14	1.23
1	B	241	MSE	C-O	-8.11	1.12	1.23
1	A	139	THR	CA-C	-8.10	1.42	1.52
1	C	311	GLY	C-O	-8.10	1.12	1.23
1	D	205	GLN	CA-C	8.10	1.63	1.52
1	A	322	LEU	CA-CB	-8.09	1.42	1.53
1	C	165	LEU	C-O	-8.08	1.14	1.24
1	D	328	ARG	N-CA	-8.04	1.39	1.46
1	B	77	ALA	CA-CB	-8.04	1.39	1.53
1	A	271	VAL	CA-CB	-8.03	1.44	1.54
1	C	124	VAL	CA-C	-8.02	1.42	1.52
1	D	168	ILE	CA-CB	7.99	1.64	1.54
1	A	253	MSE	SE-CE	7.99	2.19	1.95
1	C	262	LEU	CA-CB	-7.98	1.41	1.53
1	B	141	GLN	N-CA	-7.98	1.36	1.46
1	C	76	PRO	CA-C	7.97	1.63	1.52
1	C	128	ARG	N-CA	-7.95	1.36	1.45
1	B	72	VAL	N-CA	7.95	1.55	1.46
1	D	328	ARG	C-O	-7.94	1.16	1.24
1	A	226	ASP	N-CA	7.92	1.55	1.46
1	C	290	ILE	CA-C	7.91	1.61	1.52
1	D	198	ASN	N-CA	7.89	1.56	1.46
1	A	206	THR	N-CA	7.88	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	GLN	CA-C	7.88	1.63	1.52
1	D	227	LEU	N-CA	-7.87	1.36	1.46
1	B	103	SER	N-CA	-7.86	1.36	1.46
1	A	37	ASN	N-CA	7.86	1.56	1.46
1	C	124	VAL	CA-CB	7.85	1.64	1.54
1	D	247	VAL	CA-CB	7.85	1.65	1.54
1	D	312	VAL	C-O	7.84	1.31	1.24
1	A	45	TRP	C-O	-7.84	1.15	1.23
1	A	42	PRO	C-O	-7.83	1.14	1.23
1	B	163	LEU	C-O	-7.82	1.17	1.24
1	A	36	PRO	N-CA	7.82	1.57	1.47
1	A	232	ASP	N-CA	-7.81	1.36	1.46
1	A	241	MSE	SE-CE	-7.80	1.72	1.95
1	B	114	ILE	C-O	7.80	1.31	1.24
1	A	270	ARG	CA-C	7.80	1.63	1.53
1	B	289	VAL	N-CA	-7.79	1.37	1.46
1	D	158	LEU	CA-C	-7.79	1.43	1.52
1	A	293	ASN	CB-CG	7.77	1.71	1.52
1	A	52	PRO	CA-C	7.76	1.63	1.52
1	C	43	ALA	CA-CB	-7.76	1.40	1.53
1	C	89	TYR	C-O	-7.76	1.14	1.23
1	A	245	ASN	CA-C	-7.73	1.44	1.52
1	A	122	THR	CA-C	-7.72	1.43	1.52
1	A	253	MSE	CG-SE	7.70	2.18	1.95
1	D	253	MSE	C-O	-7.69	1.17	1.24
1	A	217	TYR	C-O	-7.66	1.14	1.24
1	D	293	ASN	N-CA	7.64	1.56	1.46
1	A	196	ALA	CA-CB	-7.63	1.41	1.53
1	A	229	ARG	C-O	-7.62	1.13	1.24
1	A	100	VAL	CA-CB	-7.62	1.44	1.54
1	A	108	GLN	C-O	-7.60	1.14	1.24
1	A	248	THR	CA-CB	-7.60	1.43	1.54
1	C	218	ASP	C-O	-7.59	1.15	1.24
1	B	324	SER	CA-C	-7.58	1.42	1.52
1	A	318	GLN	C-O	-7.58	1.14	1.24
1	B	208	ASN	C-O	7.57	1.34	1.23
1	C	51	ARG	NE-CZ	-7.56	1.24	1.33
1	C	141	GLN	CD-OE1	7.56	1.38	1.23
1	B	316	THR	N-CA	-7.54	1.36	1.45
1	C	243	TYR	C-O	-7.49	1.14	1.23
1	C	177	TYR	CA-C	7.48	1.61	1.53
1	A	107	ASN	CB-CG	-7.48	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	PRO	C-O	7.48	1.32	1.24
1	B	39	ASN	CA-CB	7.47	1.62	1.52
1	A	215	TYR	CZ-OH	7.45	1.53	1.38
1	C	111	LEU	C-O	-7.45	1.14	1.23
1	D	274	THR	C-O	-7.43	1.14	1.23
1	C	216	ARG	NE-CZ	-7.42	1.24	1.33
1	D	297	SER	C-O	-7.42	1.14	1.23
1	C	217	TYR	C-O	-7.42	1.15	1.24
1	B	288	GLN	C-O	-7.41	1.14	1.23
1	B	289	VAL	C-O	-7.39	1.16	1.24
1	B	289	VAL	CB-CG2	-7.36	1.28	1.52
1	A	300	ALA	CA-C	-7.36	1.43	1.52
1	B	262	LEU	CA-C	7.34	1.61	1.52
1	C	209	SER	CA-CB	7.34	1.67	1.53
1	C	163	LEU	C-O	7.31	1.33	1.24
1	C	258	ALA	C-O	-7.30	1.15	1.23
1	D	177	TYR	C-O	-7.30	1.14	1.24
1	A	260	LEU	CG-CD2	-7.29	1.28	1.52
1	D	87	THR	CA-C	-7.25	1.43	1.52
1	B	75	ASN	CA-C	7.22	1.61	1.52
1	A	261	GLN	C-O	-7.22	1.15	1.23
1	B	287	GLY	C-O	-7.21	1.14	1.23
1	D	251	TYR	N-CA	7.20	1.55	1.45
1	C	128	ARG	C-O	-7.20	1.14	1.23
1	B	200	LEU	C-O	-7.18	1.16	1.24
1	B	153	GLU	C-O	-7.18	1.15	1.24
1	A	192	LEU	C-O	-7.17	1.17	1.24
1	C	195	TYR	CA-CB	7.17	1.64	1.54
1	C	313	SER	CA-C	-7.17	1.43	1.52
1	C	50	ILE	CB-CG2	7.15	1.76	1.52
1	C	241	MSE	CA-C	7.14	1.61	1.52
1	D	131	MSE	CA-CB	-7.13	1.43	1.53
1	D	274	THR	CA-CB	-7.13	1.40	1.54
1	B	319	ASP	CB-CG	-7.12	1.34	1.52
1	C	143	ARG	CG-CD	7.12	1.73	1.52
1	D	267	PHE	CD2-CE2	-7.10	1.17	1.38
1	D	286	SER	C-O	-7.10	1.16	1.23
1	D	316	THR	C-O	-7.10	1.15	1.23
1	C	78	LEU	CA-CB	7.10	1.62	1.53
1	D	323	PHE	CA-C	-7.10	1.44	1.52
1	A	159	ASP	CA-C	-7.09	1.43	1.52
1	D	128	ARG	C-O	-7.09	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	GLN	C-O	-7.08	1.15	1.24
1	C	333	ALA	CA-CB	-7.08	1.42	1.53
1	C	73	LEU	CA-CB	-7.07	1.42	1.53
1	A	314	PHE	C-O	7.05	1.33	1.23
1	A	155	VAL	C-O	-7.04	1.16	1.24
1	D	230	LEU	C-O	-7.03	1.15	1.23
1	D	113	PHE	C-O	7.03	1.32	1.24
1	D	96	MSE	CA-C	-7.02	1.43	1.52
1	C	332	GLU	N-CA	-7.01	1.37	1.46
1	C	247	VAL	CA-CB	7.01	1.63	1.54
1	D	128	ARG	CZ-NH2	-7.00	1.24	1.33
1	A	262	LEU	C-O	6.99	1.32	1.24
1	C	220	SER	C-O	-6.99	1.15	1.24
1	C	245	ASN	CA-C	-6.99	1.45	1.52
1	C	203	ARG	NE-CZ	6.99	1.40	1.33
1	A	274	THR	CA-CB	-6.98	1.40	1.54
1	C	169	LEU	CA-C	-6.98	1.43	1.52
1	A	286	SER	C-O	6.97	1.32	1.23
1	B	116	GLU	CA-C	-6.97	1.44	1.52
1	B	94	LEU	N-CA	6.96	1.54	1.46
1	C	340	ALA	C-O	-6.96	1.15	1.24
1	C	206	THR	CA-CB	6.95	1.68	1.54
1	D	320	SER	N-CA	-6.95	1.37	1.46
1	A	105	ARG	CA-C	6.92	1.61	1.52
1	D	329	PRO	C-O	-6.90	1.15	1.24
1	C	164	PRO	C-O	-6.90	1.14	1.24
1	B	305	VAL	C-O	-6.89	1.16	1.24
1	A	51	ARG	C-O	-6.89	1.17	1.24
1	B	273	ARG	C-O	-6.88	1.15	1.23
1	D	210	SER	C-O	-6.87	1.15	1.24
1	C	224	LEU	CG-CD2	-6.86	1.29	1.52
1	B	86	ALA	C-O	6.85	1.32	1.24
1	C	244	VAL	C-O	6.84	1.30	1.24
1	A	128	ARG	C-O	6.83	1.31	1.23
1	C	190	ASP	C-O	-6.83	1.16	1.24
1	C	259	PHE	C-O	-6.83	1.15	1.23
1	C	290	ILE	C-O	6.83	1.32	1.24
1	D	337	PHE	C-O	-6.82	1.15	1.23
1	C	45	TRP	N-CA	-6.81	1.38	1.46
1	B	85	THR	CB-CG2	-6.80	1.30	1.52
1	B	262	LEU	N-CA	-6.79	1.38	1.46
1	C	269	SER	CA-C	-6.79	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	ASN	CA-C	-6.78	1.44	1.52
1	A	289	VAL	CA-C	-6.78	1.44	1.52
1	A	322	LEU	C-O	-6.76	1.16	1.24
1	B	194	ARG	C-O	6.76	1.32	1.24
1	B	200	LEU	N-CA	-6.75	1.37	1.46
1	C	97	PRO	C-O	-6.75	1.15	1.24
1	C	111	LEU	CA-C	-6.75	1.44	1.52
1	B	223	VAL	CA-CB	6.75	1.61	1.54
1	C	48	GLN	N-CA	6.75	1.54	1.46
1	D	304	PHE	C-O	-6.74	1.15	1.23
1	D	125	ASP	CG-OD2	6.73	1.38	1.25
1	D	314	PHE	N-CA	-6.73	1.37	1.46
1	B	143	ARG	CZ-NH1	6.72	1.42	1.32
1	A	339	GLU	CA-C	6.71	1.60	1.52
1	C	128	ARG	CA-C	-6.71	1.44	1.52
1	C	295	THR	C-O	-6.71	1.15	1.23
1	B	227	LEU	CG-CD2	6.71	1.74	1.52
1	B	118	LYS	CA-CB	6.70	1.64	1.53
1	A	45	TRP	CA-CB	-6.70	1.42	1.53
1	A	41	ALA	CA-CB	-6.70	1.42	1.53
1	B	168	ILE	CA-C	-6.70	1.43	1.52
1	B	204	HIS	C-O	6.70	1.32	1.24
1	D	237	ASP	N-CA	-6.70	1.36	1.45
1	B	329	PRO	CA-CB	-6.69	1.43	1.53
1	D	195	TYR	C-O	-6.69	1.15	1.24
1	B	198	ASN	CA-CB	-6.69	1.43	1.53
1	D	159	ASP	CG-OD2	6.69	1.38	1.25
1	C	75	ASN	CG-OD1	6.67	1.36	1.23
1	A	76	PRO	N-CA	6.66	1.55	1.47
1	B	296	PHE	C-O	-6.66	1.15	1.23
1	A	139	THR	C-N	-6.66	1.25	1.33
1	A	223	VAL	CA-CB	-6.66	1.47	1.54
1	A	310	HIS	C-O	-6.66	1.16	1.24
1	C	253	MSE	SE-CE	6.65	2.15	1.95
1	D	85	THR	CB-CG2	-6.63	1.30	1.52
1	C	339	GLU	CA-C	6.62	1.60	1.52
1	D	307	PRO	CA-C	-6.62	1.44	1.52
1	A	293	ASN	CA-CB	6.60	1.62	1.54
1	B	270	ARG	CA-C	6.60	1.62	1.53
1	D	209	SER	CA-CB	6.60	1.64	1.53
1	C	149	ASN	N-CA	-6.59	1.39	1.46
1	A	84	ILE	C-O	-6.59	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	ARG	NE-CZ	6.58	1.40	1.33
1	C	147	HIS	CA-C	6.58	1.60	1.52
1	A	213	PHE	C-O	-6.58	1.14	1.23
1	D	74	GLU	CA-C	-6.57	1.45	1.52
1	D	108	GLN	CG-CD	6.57	1.68	1.52
1	D	265	LYS	CG-CD	6.55	1.72	1.52
1	A	233	ALA	N-CA	-6.54	1.37	1.46
1	A	40	CYS	N-CA	-6.54	1.37	1.46
1	C	274	THR	C-O	-6.54	1.15	1.23
1	A	268	ALA	CA-C	-6.54	1.46	1.53
1	D	149	ASN	CA-C	-6.53	1.45	1.52
1	A	229	ARG	NE-CZ	6.53	1.40	1.33
1	D	49	GLU	C-N	6.53	1.42	1.33
1	B	141	GLN	C-O	-6.52	1.15	1.23
1	A	92	LEU	N-CA	-6.51	1.38	1.46
1	D	105	ARG	CB-CG	-6.51	1.32	1.52
1	B	120	ALA	C-O	-6.51	1.15	1.24
1	D	143	ARG	CD-NE	6.51	1.55	1.46
1	D	170	GLY	C-O	-6.50	1.15	1.23
1	B	322	LEU	CG-CD1	-6.50	1.31	1.52
1	D	303	ILE	CB-CG1	-6.49	1.40	1.53
1	A	190	ASP	C-O	6.48	1.31	1.24
1	D	128	ARG	N-CA	-6.48	1.38	1.45
1	B	76	PRO	CA-CB	6.47	1.62	1.53
1	D	73	LEU	C-O	-6.47	1.15	1.23
1	C	113	PHE	N-CA	-6.46	1.38	1.46
1	B	299	SER	C-O	6.46	1.31	1.23
1	D	242	ARG	CA-C	-6.45	1.45	1.52
1	C	78	LEU	C-O	-6.45	1.14	1.23
1	A	258	ALA	CA-CB	-6.42	1.41	1.53
1	D	279	ILE	CA-CB	-6.42	1.46	1.53
1	C	38	ALA	N-CA	-6.42	1.38	1.46
1	A	152	ASP	CA-CB	-6.42	1.44	1.53
1	D	258	ALA	CA-C	-6.42	1.44	1.52
1	D	94	LEU	C-O	-6.41	1.16	1.24
1	D	204	HIS	CA-C	6.41	1.61	1.52
1	C	334	LEU	C-O	6.40	1.31	1.23
1	C	210	SER	C-O	-6.40	1.16	1.24
1	B	138	LEU	CB-CG	-6.39	1.40	1.53
1	B	90	ALA	CA-C	6.39	1.60	1.52
1	A	120	ALA	CA-CB	-6.39	1.42	1.53
1	A	246	PRO	C-O	6.39	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	HIS	CA-CB	-6.39	1.42	1.53
1	B	166	VAL	N-CA	-6.35	1.38	1.46
1	B	51	ARG	NE-CZ	6.35	1.40	1.33
1	B	127	GLU	CA-C	-6.34	1.45	1.52
1	A	94	LEU	CA-C	-6.33	1.44	1.52
1	D	321	VAL	C-O	-6.31	1.17	1.24
1	A	83	SER	C-O	-6.31	1.16	1.23
1	C	114	ILE	C-O	-6.31	1.16	1.24
1	D	336	LEU	CA-C	6.31	1.60	1.52
1	D	118	LYS	C-O	6.29	1.32	1.23
1	B	242	ARG	CA-CB	-6.28	1.42	1.53
1	C	312	VAL	CA-CB	-6.28	1.45	1.54
1	A	106	HIS	N-CA	-6.27	1.38	1.46
1	B	286	SER	C-N	-6.27	1.27	1.33
1	C	205	GLN	C-O	6.27	1.31	1.24
1	A	105	ARG	N-CA	-6.27	1.38	1.45
1	D	209	SER	N-CA	6.25	1.54	1.46
1	C	138	LEU	CB-CG	-6.25	1.41	1.53
1	D	319	ASP	C-O	-6.25	1.16	1.24
1	D	184	VAL	C-O	-6.24	1.16	1.24
1	C	96	MSE	SE-CE	6.24	2.14	1.95
1	C	73	LEU	C-O	-6.24	1.15	1.23
1	C	48	GLN	C-O	-6.23	1.17	1.24
1	A	242	ARG	C-O	6.23	1.31	1.24
1	D	132	ASN	CA-C	6.23	1.60	1.52
1	D	229	ARG	CG-CD	6.23	1.71	1.52
1	D	270	ARG	CZ-NH2	-6.23	1.25	1.33
1	D	226	ASP	N-CA	6.23	1.54	1.46
1	D	234	ASP	CA-CB	6.23	1.62	1.53
1	D	41	ALA	CA-CB	-6.22	1.44	1.53
1	A	100	VAL	CA-C	6.21	1.60	1.52
1	A	296	PHE	N-CA	-6.21	1.38	1.46
1	B	123	ALA	CA-CB	-6.21	1.42	1.53
1	A	153	GLU	C-O	-6.21	1.16	1.24
1	D	340	ALA	CA-C	-6.20	1.45	1.52
1	D	72	VAL	CA-CB	-6.20	1.45	1.54
1	C	85	THR	C-O	6.20	1.30	1.23
1	B	253	MSE	SE-CE	6.19	2.14	1.95
1	A	242	ARG	N-CA	-6.18	1.38	1.46
1	A	317	THR	C-N	-6.18	1.25	1.33
1	B	222	GLU	N-CA	-6.18	1.38	1.46
1	B	286	SER	N-CA	-6.18	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	328	ARG	CA-C	-6.18	1.45	1.52
1	C	215	TYR	N-CA	6.17	1.54	1.46
1	B	209	SER	CA-CB	6.16	1.63	1.53
1	A	247	VAL	N-CA	6.16	1.54	1.46
1	B	295	THR	C-O	-6.15	1.16	1.24
1	C	281	HIS	CA-CB	-6.15	1.43	1.53
1	C	182	GLN	N-CA	6.14	1.57	1.46
1	C	202	LEU	CA-C	6.14	1.61	1.52
1	D	273	ARG	C-O	6.13	1.31	1.23
1	A	253	MSE	CA-C	-6.13	1.46	1.52
1	A	220	SER	C-O	-6.13	1.16	1.24
1	B	273	ARG	CG-CD	-6.13	1.34	1.52
1	A	213	PHE	CE2-CZ	-6.12	1.20	1.38
1	C	144	TRP	C-O	-6.12	1.16	1.23
1	B	86	ALA	CA-CB	-6.11	1.42	1.53
1	D	35	THR	CB-CG2	6.10	1.72	1.52
1	B	246	PRO	C-O	6.10	1.32	1.24
1	A	325	PHE	CA-C	-6.09	1.45	1.52
1	A	51	ARG	CA-CB	-6.09	1.48	1.54
1	D	150	PRO	CA-CB	-6.08	1.45	1.53
1	A	225	HIS	CA-C	-6.07	1.44	1.52
1	A	259	PHE	C-O	6.07	1.31	1.23
1	C	84	ILE	CA-CB	-6.07	1.46	1.54
1	B	338	ARG	C-O	-6.07	1.16	1.23
1	A	155	VAL	CA-CB	-6.06	1.46	1.54
1	D	291	ILE	CA-CB	-6.04	1.46	1.54
1	A	110	ALA	CA-C	-6.04	1.45	1.52
1	B	212	ILE	N-CA	6.04	1.53	1.46
1	C	253	MSE	CA-CB	-6.03	1.46	1.54
1	B	191	TYR	CZ-OH	-6.03	1.25	1.38
1	D	332	GLU	N-CA	-6.03	1.38	1.46
1	D	323	PHE	C-O	-6.02	1.16	1.24
1	A	52	PRO	C-O	-6.02	1.16	1.24
1	A	130	PRO	CA-CB	-6.02	1.45	1.53
1	B	223	VAL	C-O	-6.02	1.17	1.24
1	D	87	THR	CB-OG1	-6.01	1.34	1.43
1	C	108	GLN	CA-C	6.01	1.61	1.52
1	D	153	GLU	CA-C	-6.01	1.47	1.52
1	C	204	HIS	CA-C	6.00	1.60	1.52
1	D	44	TYR	C-O	6.00	1.30	1.23
1	D	283	VAL	CB-CG1	-6.00	1.32	1.52
1	D	306	VAL	CA-CB	-5.97	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	ASP	N-CA	-5.97	1.39	1.46
1	C	224	LEU	C-O	-5.96	1.17	1.24
1	C	270	ARG	N-CA	5.96	1.53	1.45
1	C	263	LEU	N-CA	5.96	1.53	1.46
1	A	184	VAL	CA-CB	5.96	1.61	1.54
1	D	72	VAL	C-O	5.95	1.30	1.24
1	D	315	GLN	N-CA	5.95	1.53	1.46
1	B	317	THR	C-O	-5.95	1.15	1.24
1	D	114	ILE	CA-C	5.94	1.59	1.52
1	A	90	ALA	CA-C	5.93	1.59	1.52
1	B	212	ILE	C-O	-5.93	1.17	1.24
1	C	312	VAL	CB-CG1	5.93	1.72	1.52
1	A	221	ARG	C-O	-5.92	1.16	1.24
1	C	236	TRP	CA-C	5.92	1.60	1.52
1	C	273	ARG	CA-C	-5.92	1.45	1.52
1	D	140	PRO	CA-CB	-5.91	1.45	1.53
1	C	315	GLN	CA-CB	5.91	1.60	1.52
1	A	315	GLN	CA-C	-5.90	1.45	1.52
1	D	167	ASN	CB-CG	-5.90	1.37	1.52
1	D	282	VAL	CA-C	-5.90	1.46	1.52
1	D	252	PRO	CB-CG	-5.89	1.20	1.49
1	D	99	GLU	C-O	-5.88	1.16	1.23
1	B	291	ILE	C-O	-5.88	1.17	1.24
1	B	71	LEU	CG-CD2	5.88	1.72	1.52
1	C	161	LEU	CA-C	-5.88	1.45	1.52
1	D	233	ALA	N-CA	-5.87	1.38	1.46
1	D	131	MSE	SE-CE	5.87	2.13	1.95
1	B	271	VAL	CA-CB	-5.87	1.47	1.54
1	A	182	GLN	CA-C	-5.87	1.45	1.52
1	C	43	ALA	N-CA	5.86	1.53	1.45
1	B	142	TRP	C-O	-5.86	1.16	1.23
1	C	39	ASN	N-CA	-5.86	1.38	1.46
1	B	137	ILE	CA-CB	5.86	1.62	1.54
1	C	157	TRP	CA-CB	-5.85	1.42	1.54
1	B	314	PHE	CG-CD1	5.85	1.51	1.38
1	C	94	LEU	CG-CD1	-5.85	1.33	1.52
1	C	33	PRO	CB-CG	5.84	1.78	1.49
1	D	313	SER	C-O	-5.83	1.16	1.23
1	A	90	ALA	C-O	-5.83	1.16	1.23
1	B	131	MSE	SE-CE	-5.83	1.77	1.95
1	C	226	ASP	CG-OD1	5.83	1.36	1.25
1	D	300	ALA	CA-C	-5.83	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	GLU	CD-OE1	5.82	1.36	1.25
1	A	149	ASN	N-CA	-5.82	1.39	1.46
1	B	205	GLN	CA-C	5.82	1.60	1.52
1	D	49	GLU	CA-C	5.82	1.61	1.53
1	D	95	ILE	C-O	-5.81	1.17	1.24
1	D	327	ASP	C-O	-5.81	1.16	1.24
1	C	301	LYS	CA-C	5.81	1.63	1.53
1	C	45	TRP	CA-C	5.81	1.58	1.52
1	B	208	ASN	CB-CG	5.81	1.66	1.52
1	C	146	ASP	C-N	-5.80	1.25	1.33
1	D	150	PRO	CA-C	5.80	1.60	1.52
1	A	140	PRO	CA-C	5.80	1.59	1.52
1	A	148	GLY	C-O	-5.78	1.17	1.24
1	D	110	ALA	N-CA	-5.78	1.39	1.46
1	C	146	ASP	CA-C	-5.78	1.45	1.52
1	B	95	ILE	CA-CB	-5.78	1.46	1.54
1	D	48	GLN	CA-CB	-5.78	1.45	1.53
1	A	226	ASP	C-O	-5.77	1.17	1.24
1	D	289	VAL	CA-C	-5.77	1.45	1.52
1	C	287	GLY	C-O	-5.77	1.16	1.23
1	A	251	TYR	CE2-CZ	5.77	1.52	1.38
1	B	184	VAL	CA-CB	-5.76	1.46	1.54
1	A	131	MSE	N-CA	-5.76	1.39	1.46
1	D	202	LEU	CG-CD2	-5.74	1.33	1.52
1	A	71	LEU	N-CA	5.74	1.57	1.46
1	D	293	ASN	C-O	5.74	1.31	1.24
1	A	161	LEU	CA-C	-5.74	1.45	1.52
1	B	156	ILE	C-O	-5.73	1.16	1.24
1	D	334	LEU	N-CA	5.72	1.53	1.45
1	B	290	ILE	N-CA	-5.71	1.39	1.46
1	D	321	VAL	CA-C	-5.71	1.45	1.52
1	A	114	ILE	N-CA	-5.71	1.39	1.46
1	D	87	THR	N-CA	-5.70	1.39	1.46
1	A	119	GLY	C-O	-5.68	1.16	1.24
1	D	237	ASP	C-O	5.68	1.31	1.24
1	B	325	PHE	C-O	5.67	1.30	1.23
1	C	168	ILE	N-CA	-5.67	1.39	1.46
1	B	107	ASN	CA-C	5.67	1.60	1.52
1	B	261	GLN	CB-CG	-5.67	1.35	1.52
1	D	143	ARG	C-O	-5.67	1.17	1.24
1	D	285	GLY	CA-C	-5.67	1.44	1.52
1	D	123	ALA	CA-CB	5.66	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	143	ARG	NE-CZ	5.66	1.39	1.33
1	C	216	ARG	C-O	-5.65	1.17	1.23
1	D	183	PRO	CA-CB	-5.65	1.42	1.53
1	D	341	ARG	CA-C	5.64	1.59	1.53
1	C	277	SER	C-O	-5.64	1.17	1.24
1	A	339	GLU	C-O	-5.64	1.16	1.24
1	A	295	THR	C-O	-5.63	1.17	1.23
1	A	197	ALA	C-O	-5.62	1.16	1.23
1	D	209	SER	CA-C	-5.62	1.45	1.52
1	A	131	MSE	CG-SE	5.62	2.12	1.95
1	D	174	ALA	CA-C	-5.61	1.45	1.52
1	B	315	GLN	CG-CD	5.61	1.66	1.52
1	C	330	VAL	CB-CG2	-5.61	1.34	1.52
1	A	264	PRO	CA-CB	5.61	1.61	1.53
1	D	251	TYR	CA-CB	-5.61	1.44	1.53
1	C	293	ASN	N-CA	5.60	1.52	1.46
1	A	221	ARG	CA-C	5.59	1.60	1.52
1	C	46	ASN	CA-C	-5.59	1.45	1.52
1	D	121	PHE	C-O	-5.59	1.16	1.23
1	A	91	GLY	N-CA	-5.59	1.39	1.45
1	C	306	VAL	N-CA	5.59	1.53	1.46
1	C	303	ILE	CB-CG2	5.58	1.71	1.52
1	D	75	ASN	N-CA	5.58	1.52	1.45
1	D	128	ARG	NE-CZ	5.58	1.39	1.33
1	D	157	TRP	CA-CB	-5.58	1.43	1.54
1	B	96	MSE	C-O	-5.58	1.16	1.23
1	C	129	THR	CA-C	5.58	1.57	1.52
1	B	341	ARG	CD-NE	-5.57	1.38	1.46
1	B	86	ALA	N-CA	5.57	1.53	1.46
1	D	241	MSE	N-CA	-5.57	1.38	1.45
1	A	122	THR	C-O	-5.56	1.17	1.23
1	B	279	ILE	C-O	5.56	1.30	1.24
1	B	204	HIS	CA-C	5.56	1.60	1.52
1	C	128	ARG	CB-CG	-5.54	1.35	1.52
1	D	330	VAL	N-CA	-5.54	1.39	1.46
1	B	265	LYS	C-O	5.53	1.30	1.24
1	C	158	LEU	CG-CD1	-5.53	1.34	1.52
1	C	46	ASN	CG-ND2	-5.53	1.21	1.33
1	B	341	ARG	NE-CZ	-5.52	1.26	1.33
1	B	268	ALA	CA-C	5.52	1.58	1.53
1	A	298	PHE	C-O	-5.51	1.16	1.23
1	C	167	ASN	CG-ND2	5.51	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	137	ILE	CA-C	5.51	1.59	1.52
1	D	321	VAL	CA-CB	-5.50	1.46	1.53
1	C	90	ALA	CA-CB	-5.50	1.44	1.53
1	B	330	VAL	C-N	-5.49	1.26	1.33
1	C	308	THR	CB-OG1	-5.49	1.34	1.43
1	C	169	LEU	C-O	-5.49	1.17	1.24
1	A	146	ASP	CA-C	-5.48	1.46	1.52
1	C	229	ARG	C-O	5.48	1.31	1.24
1	D	205	GLN	C-O	5.48	1.30	1.24
1	D	165	LEU	C-O	-5.48	1.17	1.24
1	A	85	THR	C-O	5.47	1.31	1.23
1	A	115	VAL	CA-CB	-5.47	1.48	1.54
1	B	161	LEU	C-O	5.47	1.30	1.23
1	B	177	TYR	CA-C	-5.47	1.46	1.52
1	B	84	ILE	CA-CB	-5.47	1.46	1.54
1	A	35	THR	CA-C	-5.46	1.41	1.52
1	A	230	LEU	CG-CD1	-5.46	1.34	1.52
1	C	235	GLU	C-O	-5.46	1.17	1.24
1	A	138	LEU	CA-C	5.46	1.59	1.52
1	C	324	SER	CB-OG	5.46	1.53	1.42
1	A	303	ILE	N-CA	-5.46	1.39	1.46
1	C	222	GLU	CA-C	-5.45	1.45	1.52
1	B	315	GLN	CB-CG	5.45	1.68	1.52
1	D	274	THR	CA-C	-5.45	1.45	1.52
1	A	324	SER	CA-C	-5.45	1.45	1.52
1	B	103	SER	C-O	5.44	1.30	1.23
1	D	93	GLN	CA-C	5.44	1.59	1.52
1	C	276	ASP	CA-C	-5.44	1.46	1.52
1	C	228	THR	C-N	-5.43	1.25	1.33
1	C	164	PRO	N-CA	5.43	1.54	1.47
1	C	229	ARG	CZ-NH1	5.43	1.40	1.32
1	D	84	ILE	CA-C	-5.43	1.46	1.52
1	A	84	ILE	CB-CG2	-5.42	1.34	1.52
1	B	156	ILE	CB-CG2	5.42	1.70	1.52
1	B	194	ARG	NE-CZ	5.41	1.39	1.33
1	D	121	PHE	N-CA	-5.41	1.39	1.45
1	B	157	TRP	CA-C	-5.41	1.45	1.52
1	D	184	VAL	CA-C	-5.41	1.45	1.52
1	B	226	ASP	CA-C	-5.40	1.45	1.52
1	A	216	ARG	NE-CZ	-5.40	1.27	1.33
1	D	76	PRO	C-N	5.40	1.41	1.33
1	A	332	GLU	C-O	-5.39	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	PHE	CA-C	5.39	1.59	1.52
1	D	109	SER	CA-C	5.39	1.59	1.52
1	B	318	GLN	C-N	-5.39	1.26	1.33
1	B	184	VAL	N-CA	5.39	1.53	1.46
1	B	50	ILE	CA-CB	5.38	1.61	1.54
1	C	199	MSE	N-CA	-5.38	1.39	1.45
1	D	118	LYS	CE-NZ	5.38	1.65	1.49
1	A	47	TYR	N-CA	-5.38	1.39	1.46
1	B	303	ILE	CB-CG1	-5.38	1.42	1.53
1	C	174	ALA	CA-CB	-5.38	1.43	1.53
1	C	134	GLY	C-N	5.38	1.40	1.33
1	A	156	ILE	C-O	-5.38	1.18	1.24
1	B	184	VAL	CB-CG2	5.38	1.70	1.52
1	A	328	ARG	CA-C	-5.37	1.45	1.52
1	D	296	PHE	CG-CD1	-5.37	1.27	1.38
1	B	138	LEU	C-O	-5.36	1.17	1.24
1	A	181	GLN	CD-OE1	5.36	1.33	1.23
1	A	226	ASP	CA-C	-5.36	1.45	1.52
1	C	143	ARG	CA-C	-5.36	1.46	1.52
1	A	337	PHE	CA-C	-5.36	1.45	1.52
1	D	116	GLU	N-CA	5.36	1.52	1.46
1	B	305	VAL	CA-C	-5.36	1.46	1.52
1	C	75	ASN	C-O	-5.34	1.16	1.24
1	B	248	THR	CA-C	-5.34	1.45	1.52
1	B	268	ALA	C-O	-5.34	1.17	1.23
1	A	323	PHE	C-O	-5.34	1.17	1.23
1	A	321	VAL	C-O	-5.33	1.18	1.24
1	D	112	ARG	C-O	-5.33	1.18	1.24
1	A	208	ASN	CA-C	5.33	1.60	1.52
1	C	76	PRO	N-CA	5.32	1.54	1.47
1	C	219	ARG	NE-CZ	5.32	1.39	1.33
1	C	171	CYS	N-CA	5.32	1.52	1.46
1	D	89	TYR	CE2-CZ	-5.31	1.25	1.38
1	C	225	HIS	N-CA	5.31	1.52	1.46
1	D	90	ALA	CA-CB	-5.30	1.43	1.54
1	A	84	ILE	CA-CB	-5.29	1.46	1.54
1	A	72	VAL	CA-CB	-5.29	1.46	1.53
1	A	156	ILE	CA-CB	5.29	1.62	1.55
1	D	208	ASN	C-O	5.29	1.30	1.23
1	D	90	ALA	N-CA	-5.28	1.39	1.45
1	A	156	ILE	CA-C	5.28	1.59	1.52
1	C	244	VAL	CB-CG1	-5.28	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	317	THR	CA-C	5.28	1.59	1.52
1	B	174	ALA	CA-CB	-5.27	1.45	1.53
1	D	130	PRO	C-O	-5.27	1.17	1.23
1	C	173	PHE	CA-C	-5.27	1.46	1.52
1	D	51	ARG	CZ-NH2	5.27	1.40	1.33
1	C	329	PRO	CA-C	-5.26	1.43	1.52
1	C	36	PRO	CA-C	5.26	1.58	1.52
1	D	248	THR	CA-CB	5.26	1.62	1.54
1	B	116	GLU	C-O	5.26	1.30	1.23
1	A	100	VAL	C-O	-5.25	1.18	1.24
1	B	307	PRO	C-O	-5.25	1.17	1.23
1	D	194	ARG	CD-NE	-5.25	1.38	1.46
1	A	154	PRO	CA-CB	5.25	1.60	1.53
1	A	320	SER	N-CA	-5.25	1.39	1.46
1	B	82	SER	CA-C	5.25	1.59	1.53
1	C	165	LEU	N-CA	5.25	1.52	1.46
1	D	341	ARG	C-O	-5.24	1.16	1.23
1	D	282	VAL	CB-CG2	-5.24	1.35	1.52
1	D	94	LEU	CA-C	-5.23	1.46	1.52
1	A	329	PRO	CG-CD	5.23	1.68	1.50
1	A	109	SER	C-O	5.23	1.30	1.23
1	B	88	LEU	N-CA	-5.23	1.39	1.45
1	B	321	VAL	C-O	-5.23	1.18	1.24
1	B	84	ILE	N-CA	-5.23	1.38	1.46
1	B	232	ASP	CA-CB	5.23	1.62	1.53
1	A	135	ASP	CA-C	5.22	1.59	1.52
1	D	144	TRP	CA-C	-5.22	1.46	1.52
1	C	305	VAL	CB-CG1	-5.22	1.35	1.52
1	A	94	LEU	N-CA	5.22	1.52	1.46
1	A	250	GLY	N-CA	5.22	1.50	1.45
1	A	265	LYS	CA-CB	-5.21	1.44	1.53
1	A	306	VAL	C-O	-5.21	1.17	1.24
1	B	223	VAL	CA-C	-5.21	1.46	1.52
1	C	102	PRO	CA-C	-5.21	1.47	1.52
1	A	327	ASP	N-CA	5.20	1.51	1.46
1	A	215	TYR	CA-C	-5.20	1.46	1.53
1	A	243	TYR	C-O	-5.20	1.17	1.23
1	A	229	ARG	CA-C	-5.20	1.44	1.52
1	A	233	ALA	CA-CB	-5.20	1.45	1.53
1	D	35	THR	CA-CB	5.20	1.61	1.53
1	A	307	PRO	C-O	5.19	1.29	1.23
1	B	336	LEU	C-O	5.19	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	214	ASN	N-CA	-5.19	1.40	1.46
1	D	229	ARG	N-CA	5.19	1.53	1.46
1	C	168	ILE	CA-CB	-5.19	1.47	1.54
1	A	235	GLU	CA-CB	5.18	1.62	1.53
1	B	168	ILE	CA-CB	-5.17	1.47	1.54
1	A	74	GLU	N-CA	-5.17	1.39	1.46
1	C	90	ALA	C-O	-5.17	1.18	1.23
1	A	242	ARG	CZ-NH1	-5.17	1.25	1.32
1	C	289	VAL	CA-C	-5.16	1.46	1.52
1	A	155	VAL	CB-CG2	5.16	1.69	1.52
1	A	223	VAL	N-CA	-5.16	1.40	1.46
1	D	166	VAL	N-CA	-5.15	1.39	1.46
1	D	315	GLN	CA-C	-5.15	1.46	1.52
1	C	174	ALA	CA-C	5.14	1.58	1.52
1	A	327	ASP	CB-CG	5.14	1.64	1.52
1	B	318	GLN	CA-C	5.14	1.59	1.52
1	C	262	LEU	CG-CD2	-5.14	1.35	1.52
1	C	304	PHE	C-O	5.14	1.30	1.23
1	C	261	GLN	CD-OE1	5.14	1.33	1.23
1	C	312	VAL	C-O	-5.14	1.18	1.24
1	A	72	VAL	CB-CG2	-5.13	1.35	1.52
1	B	255	SER	C-O	5.13	1.30	1.24
1	B	284	GLU	CA-C	5.13	1.59	1.52
1	C	259	PHE	CA-C	-5.12	1.46	1.52
1	D	116	GLU	CA-C	-5.12	1.45	1.52
1	B	300	ALA	C-O	-5.12	1.17	1.24
1	D	335	GLY	N-CA	5.12	1.52	1.45
1	C	153	GLU	CA-C	5.12	1.59	1.52
1	C	191	TYR	C-N	-5.12	1.26	1.34
1	B	229	ARG	C-O	5.12	1.30	1.23
1	B	186	ARG	CZ-NH2	-5.11	1.26	1.33
1	A	217	TYR	N-CA	-5.11	1.39	1.46
1	B	187	LYS	CB-CG	5.11	1.67	1.52
1	C	132	ASN	C-O	-5.11	1.17	1.23
1	D	157	TRP	CA-C	-5.11	1.46	1.52
1	D	148	GLY	CA-C	-5.10	1.46	1.51
1	A	337	PHE	CA-CB	-5.10	1.44	1.53
1	A	137	ILE	C-N	-5.10	1.25	1.33
1	B	286	SER	C-O	-5.09	1.17	1.23
1	C	72	VAL	N-CA	5.09	1.52	1.46
1	A	254	PRO	CA-C	5.09	1.59	1.52
1	D	310	HIS	CA-C	-5.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	TRP	C-O	-5.09	1.15	1.24
1	A	141	GLN	C-N	-5.09	1.26	1.33
1	A	280	TYR	CE1-CZ	-5.09	1.26	1.38
1	C	145	HIS	CA-C	5.08	1.58	1.52
1	D	87	THR	CA-CB	5.08	1.61	1.53
1	D	199	MSE	SE-CE	-5.07	1.80	1.95
1	C	120	ALA	C-O	-5.07	1.17	1.23
1	B	78	LEU	C-O	-5.07	1.16	1.23
1	C	314	PHE	C-O	-5.07	1.17	1.23
1	D	112	ARG	CD-NE	-5.07	1.39	1.46
1	B	312	VAL	C-O	-5.07	1.19	1.24
1	C	264	PRO	CA-C	-5.07	1.45	1.52
1	D	72	VAL	N-CA	5.06	1.53	1.46
1	C	341	ARG	NE-CZ	-5.06	1.27	1.33
1	A	187	LYS	C-O	5.05	1.29	1.23
1	C	309	TRP	N-CA	5.05	1.54	1.46
1	D	74	GLU	CA-CB	-5.05	1.45	1.53
1	C	148	GLY	C-O	-5.05	1.18	1.23
1	D	207	GLY	N-CA	5.05	1.52	1.45
1	A	277	SER	CA-CB	5.05	1.61	1.53
1	B	74	GLU	CA-C	-5.05	1.46	1.53
1	B	339	GLU	CA-C	5.05	1.58	1.52
1	D	265	LYS	N-CA	-5.05	1.39	1.46
1	B	124	VAL	CA-C	-5.04	1.46	1.52
1	D	245	ASN	C-O	-5.04	1.17	1.24
1	C	263	LEU	CA-CB	5.04	1.60	1.53
1	D	239	TYR	CA-CB	-5.04	1.45	1.52
1	A	197	ALA	N-CA	5.04	1.53	1.46
1	A	36	PRO	CB-CG	5.04	1.74	1.49
1	D	233	ALA	C-O	-5.04	1.17	1.23
1	C	83	SER	CA-CB	-5.03	1.44	1.53
1	C	72	VAL	CB-CG2	5.03	1.69	1.52
1	D	41	ALA	N-CA	-5.03	1.37	1.45
1	A	112	ARG	NE-CZ	-5.02	1.27	1.33
1	B	293	ASN	C-N	-5.02	1.26	1.33
1	B	262	LEU	C-O	-5.02	1.18	1.24
1	C	130	PRO	CB-CG	-5.02	1.24	1.49
1	C	195	TYR	CA-C	5.02	1.59	1.52
1	B	195	TYR	C-O	5.01	1.31	1.23
1	C	97	PRO	CA-C	-5.01	1.45	1.52
1	B	74	GLU	N-CA	-5.01	1.40	1.46
1	B	128	ARG	CA-C	-5.01	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	330	VAL	C-O	5.00	1.30	1.24

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	CYS	N-CA-C	-13.13	82.83	110.80
1	C	76	PRO	CA-C-N	10.04	137.00	120.23
1	C	76	PRO	C-N-CA	10.04	137.00	120.23
1	B	81	GLN	N-CA-C	-9.75	101.38	113.18
1	C	128	ARG	NE-CZ-NH2	9.67	127.91	119.20
1	C	128	ARG	NE-CZ-NH1	-9.59	111.91	121.50
1	A	184	VAL	N-CA-C	9.56	120.39	110.36
1	B	49	GLU	N-CA-C	-9.41	90.77	110.80
1	D	208	ASN	N-CA-C	-9.40	94.17	109.96
1	A	292	GLY	CA-C-N	-9.37	112.15	126.86
1	A	292	GLY	C-N-CA	-9.37	112.15	126.86
1	B	208	ASN	N-CA-C	-9.31	98.72	111.28
1	C	73	LEU	N-CA-C	9.20	124.07	110.46
1	D	334	LEU	N-CA-C	-8.60	99.83	110.41
1	C	85	THR	OG1-CB-CG2	-8.46	92.38	109.30
1	D	50	ILE	CA-CB-CG2	8.46	124.88	110.50
1	B	319	ASP	N-CA-C	-7.96	93.85	110.80
1	C	50	ILE	N-CA-C	7.92	120.27	108.54
1	B	72	VAL	CB-CA-C	-7.81	98.92	110.33
1	A	39	ASN	N-CA-C	7.79	121.05	107.49
1	C	48	GLN	CB-CA-C	-7.76	98.95	109.28
1	D	34	LYS	N-CA-C	-7.68	97.06	109.96
1	B	122	THR	OG1-CB-CG2	-7.67	93.97	109.30
1	B	73	LEU	CB-CA-C	-7.65	96.91	109.53
1	B	87	THR	N-CA-C	7.59	123.69	113.97
1	A	77	ALA	CA-C-O	7.41	131.11	120.51
1	D	49	GLU	CA-C-N	7.36	135.22	121.97
1	D	49	GLU	C-N-CA	7.36	135.22	121.97
1	D	87	THR	N-CA-C	7.30	122.25	113.12
1	A	84	ILE	N-CA-C	-7.26	102.12	112.35
1	D	303	ILE	CA-CB-CG2	7.26	122.83	110.50
1	C	51	ARG	NE-CZ-NH1	-7.23	114.27	121.50
1	D	310	HIS	CA-C-N	-7.21	113.25	120.10
1	D	310	HIS	C-N-CA	-7.21	113.25	120.10
1	D	299	SER	N-CA-C	-7.18	98.73	108.86
1	D	330	VAL	N-CA-C	-7.13	103.52	110.72
1	A	78	LEU	N-CA-C	-7.01	102.11	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	GLY	CA-C-N	7.00	130.12	120.39
1	C	250	GLY	C-N-CA	7.00	130.12	120.39
1	C	152	ASP	N-CA-C	-6.99	99.03	109.86
1	B	293	ASN	CA-C-N	-6.97	112.10	122.07
1	B	293	ASN	C-N-CA	-6.97	112.10	122.07
1	A	295	THR	OG1-CB-CG2	-6.92	95.46	109.30
1	D	287	GLY	CA-C-O	-6.87	116.17	120.91
1	C	48	GLN	N-CA-C	-6.86	106.80	114.62
1	D	48	GLN	N-CA-C	6.83	121.06	113.21
1	C	277	SER	CA-C-O	-6.82	112.66	120.58
1	C	186	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	D	141	GLN	CA-C-N	-6.79	111.78	121.83
1	D	141	GLN	C-N-CA	-6.79	111.78	121.83
1	A	317	THR	O-C-N	-6.79	114.59	123.21
1	C	248	THR	OG1-CB-CG2	-6.76	95.78	109.30
1	C	205	GLN	CA-C-N	-6.75	112.00	122.59
1	C	205	GLN	C-N-CA	-6.75	112.00	122.59
1	D	134	GLY	N-CA-C	-6.74	106.16	114.92
1	B	332	GLU	N-CA-C	-6.73	104.03	111.36
1	D	105	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	C	157	TRP	N-CA-C	6.69	119.34	109.24
1	D	210	SER	CA-CB-OG	-6.68	97.73	111.10
1	C	119	GLY	N-CA-C	6.63	122.72	114.37
1	B	107	ASN	CB-CA-C	6.63	121.94	110.01
1	B	206	THR	N-CA-C	-6.61	99.46	108.38
1	C	220	SER	N-CA-C	6.59	118.54	111.36
1	D	227	LEU	CA-C-O	-6.55	113.60	120.55
1	A	303	ILE	CA-CB-CG2	6.55	121.63	110.50
1	A	341	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	B	175	GLU	N-CA-C	6.49	119.48	108.90
1	A	41	ALA	N-CA-C	6.37	123.90	109.81
1	D	78	LEU	N-CA-C	-6.35	102.75	110.88
1	C	256	MSE	N-CA-C	6.35	119.74	109.40
1	D	132	ASN	N-CA-C	6.34	119.96	110.14
1	A	141	GLN	O-C-N	-6.33	114.17	122.59
1	D	286	SER	N-CA-C	6.33	117.77	108.14
1	C	49	GLU	N-CA-C	6.31	124.23	110.80
1	D	332	GLU	N-CA-C	-6.29	104.52	111.82
1	D	308	THR	OG1-CB-CG2	-6.29	96.73	109.30
1	A	308	THR	N-CA-C	6.28	119.59	110.42
1	B	303	ILE	N-CA-C	6.28	117.82	108.46
1	C	262	LEU	CD1-CG-CD2	-6.27	97.00	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	THR	N-CA-CB	-6.26	101.48	111.62
1	C	179	GLU	CA-C-O	-6.21	110.24	120.80
1	C	102	PRO	N-CA-C	-6.21	101.88	111.13
1	C	72	VAL	CA-C-N	-6.19	111.95	122.67
1	C	72	VAL	C-N-CA	-6.19	111.95	122.67
1	D	76	PRO	CA-C-O	-6.19	109.33	120.60
1	D	338	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	B	86	ALA	N-CA-C	6.15	120.39	113.01
1	A	152	ASP	N-CA-C	-6.14	100.20	109.60
1	B	153	GLU	N-CA-C	6.14	123.38	109.81
1	C	51	ARG	NH1-CZ-NH2	6.13	127.27	119.30
1	A	308	THR	OG1-CB-CG2	-6.12	97.06	109.30
1	C	128	ARG	CA-CB-CG	6.12	126.33	114.10
1	D	216	ARG	N-CA-C	6.12	119.23	110.24
1	B	76	PRO	CA-C-O	-6.06	109.57	120.60
1	B	289	VAL	CB-CA-C	-6.06	101.17	110.50
1	C	47	TYR	CA-C-N	6.03	133.14	121.63
1	C	47	TYR	C-N-CA	6.03	133.14	121.63
1	C	99	GLU	N-CA-C	6.02	118.54	110.35
1	D	341	ARG	N-CA-C	6.01	118.63	109.62
1	D	75	ASN	CA-C-O	-6.00	113.67	120.46
1	A	329	PRO	N-CD-CG	-5.97	94.25	103.20
1	C	212	ILE	CA-C-N	-5.96	112.70	122.54
1	C	212	ILE	C-N-CA	-5.96	112.70	122.54
1	B	168	ILE	N-CA-C	-5.95	103.61	111.05
1	B	96	MSE	CG-SE-CE	5.94	111.99	98.92
1	C	51	ARG	CG-CD-NE	-5.93	98.94	112.00
1	B	77	ALA	N-CA-C	5.93	123.43	110.80
1	C	143	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	B	317	THR	OG1-CB-CG2	-5.88	97.53	109.30
1	A	269	SER	N-CA-CB	-5.87	102.04	110.44
1	D	73	LEU	N-CA-C	5.87	118.34	110.35
1	D	148	GLY	CA-C-O	-5.87	115.86	121.49
1	C	326	SER	CA-CB-OG	-5.87	99.37	111.10
1	B	47	TYR	CA-C-N	-5.86	110.35	121.54
1	B	47	TYR	C-N-CA	-5.86	110.35	121.54
1	C	109	SER	N-CA-C	-5.85	102.81	110.53
1	D	299	SER	CA-C-N	5.82	129.37	121.05
1	D	299	SER	C-N-CA	5.82	129.37	121.05
1	D	221	ARG	N-CA-C	-5.81	105.03	111.36
1	D	334	LEU	CA-C-N	-5.79	110.06	121.41
1	D	334	LEU	C-N-CA	-5.79	110.06	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLN	CA-CB-CG	5.77	125.65	114.10
1	C	50	ILE	N-CA-CB	-5.76	104.49	110.95
1	A	341	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	D	183	PRO	N-CD-CG	-5.74	94.59	103.20
1	A	138	LEU	N-CA-C	5.74	118.56	109.50
1	C	76	PRO	N-CA-C	5.71	124.23	112.47
1	A	289	VAL	CB-CA-C	-5.71	100.49	110.71
1	C	253	MSE	CA-CB-CG	-5.70	102.71	114.10
1	B	142	TRP	N-CA-C	5.68	119.27	111.54
1	C	185	THR	N-CA-C	5.68	122.89	110.80
1	C	150	PRO	CA-C-N	5.67	128.15	122.30
1	C	150	PRO	C-N-CA	5.67	128.15	122.30
1	C	308	THR	CB-CA-C	-5.67	99.14	110.42
1	B	120	ALA	N-CA-C	5.64	122.82	110.80
1	C	100	VAL	CA-C-O	-5.64	114.57	120.27
1	D	334	LEU	O-C-N	-5.64	115.77	122.65
1	D	34	LYS	CA-C-O	-5.64	114.44	120.92
1	C	88	LEU	CB-CG-CD1	5.61	127.53	110.70
1	B	246	PRO	CA-C-O	5.59	126.57	118.86
1	C	147	HIS	N-CA-C	5.57	116.43	108.74
1	A	182	GLN	N-CA-C	-5.57	97.50	109.81
1	D	157	TRP	N-CA-C	5.56	117.64	109.24
1	B	116	GLU	CB-CA-C	-5.55	101.11	110.43
1	B	184	VAL	CB-CA-C	-5.55	102.19	111.29
1	B	48	GLN	CA-CB-CG	-5.53	103.03	114.10
1	D	330	VAL	CG1-CB-CG2	-5.53	98.63	110.80
1	D	76	PRO	CB-CA-C	-5.52	102.46	111.56
1	D	72	VAL	N-CA-C	5.50	116.49	107.24
1	A	178	PRO	N-CD-CG	5.50	111.45	103.20
1	C	97	PRO	CA-C-O	-5.50	110.59	120.60
1	C	184	VAL	CB-CA-C	-5.50	102.27	111.29
1	D	247	VAL	N-CA-C	5.50	119.73	112.04
1	B	206	THR	OG1-CB-CG2	-5.49	98.31	109.30
1	D	252	PRO	N-CD-CG	-5.48	94.97	103.20
1	A	242	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	D	276	ASP	N-CA-C	5.47	117.63	107.99
1	B	221	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	D	209	SER	CA-C-N	5.46	135.13	121.80
1	D	209	SER	C-N-CA	5.46	135.13	121.80
1	D	248	THR	CA-C-O	5.46	125.25	118.43
1	D	342	TYR	CA-CB-CG	-5.46	104.08	113.90
1	D	140	PRO	CA-C-O	-5.45	115.14	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	PHE	O-C-N	-5.45	117.21	123.42
1	D	85	THR	N-CA-CB	-5.44	102.62	111.22
1	C	119	GLY	CA-C-O	5.44	124.76	119.27
1	C	113	PHE	N-CA-C	-5.42	99.58	108.41
1	C	186	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	C	102	PRO	CA-C-O	-5.35	115.08	122.15
1	C	290	ILE	N-CA-C	-5.35	99.25	106.85
1	C	251	TYR	O-C-N	5.34	126.80	121.30
1	D	244	VAL	N-CA-C	5.33	116.15	108.48
1	D	159	ASP	N-CA-C	-5.31	101.50	109.95
1	C	50	ILE	CG1-CB-CG2	5.31	126.63	110.70
1	A	241	MSE	N-CA-CB	-5.30	101.72	111.37
1	D	318	GLN	N-CA-C	5.30	117.92	109.81
1	A	105	ARG	N-CA-C	-5.30	100.67	108.99
1	C	301	LYS	N-CA-CB	-5.27	108.16	114.17
1	B	303	ILE	CA-CB-CG2	5.26	119.44	110.50
1	D	342	TYR	CB-CA-C	-5.26	100.11	110.10
1	C	186	ARG	CG-CD-NE	-5.25	100.45	112.00
1	D	38	ALA	O-C-N	-5.24	115.62	122.59
1	D	150	PRO	CA-C-N	5.22	127.08	122.43
1	D	150	PRO	C-N-CA	5.22	127.08	122.43
1	A	222	GLU	N-CA-C	5.21	117.86	111.82
1	D	227	LEU	N-CA-C	5.19	116.94	111.28
1	B	119	GLY	N-CA-C	-5.18	102.94	112.62
1	B	47	TYR	O-C-N	-5.17	116.71	122.75
1	C	51	ARG	CA-CB-CG	-5.16	103.78	114.10
1	C	75	ASN	CA-C-O	-5.16	113.99	120.23
1	A	244	VAL	CB-CA-C	-5.16	102.56	110.50
1	D	48	GLN	CB-CG-CD	5.16	121.36	112.60
1	A	72	VAL	CA-C-O	-5.15	115.10	120.51
1	C	334	LEU	N-CA-C	-5.15	102.06	110.20
1	A	291	ILE	N-CA-C	5.15	114.16	106.85
1	A	146	ASP	CA-C-O	-5.14	115.78	121.28
1	D	93	GLN	CA-C-N	5.14	130.24	122.99
1	D	93	GLN	C-N-CA	5.14	130.24	122.99
1	A	72	VAL	CB-CA-C	-5.13	105.39	111.09
1	C	175	GLU	CA-C-O	5.13	125.90	120.36
1	C	205	GLN	CA-C-O	5.12	125.84	120.36
1	B	177	TYR	O-C-N	5.12	127.21	121.32
1	A	211	PRO	N-CA-C	-5.11	107.37	114.27
1	A	75	ASN	CA-C-O	-5.11	114.33	120.41
1	C	311	GLY	N-CA-C	-5.11	106.06	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	THR	CA-C-O	-5.08	112.17	120.80
1	C	148	GLY	N-CA-C	5.07	120.52	110.83
1	A	266	GLY	N-CA-C	-5.06	108.14	115.27
1	D	105	ARG	CG-CD-NE	5.05	123.12	112.00
1	C	184	VAL	N-CA-C	5.05	119.84	109.34
1	B	71	LEU	N-CA-CB	-5.04	101.93	110.50
1	B	47	TYR	N-CA-C	-5.04	103.83	110.43
1	D	318	GLN	N-CA-CB	-5.04	103.49	111.05
1	D	146	ASP	CA-C-O	-5.02	115.78	121.25
1	D	71	LEU	CB-CG-CD2	-5.01	95.66	110.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	ASN	Peptide
1	B	39	ASN	Peptide
1	B	76	PRO	Peptide
1	D	149	ASN	Mainchain
1	D	47	TYR	Peptide

5.2 Too-close contacts [i](#)

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	2280	0	2134	139	0
1	B	2235	0	2093	185	0
1	C	2281	0	2135	145	0
1	D	2263	0	2122	150	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	110	0	0	9	0
3	B	129	0	0	26	0
3	C	130	0	0	22	0
3	D	147	0	0	25	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9579	0	8484	593	2

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 34.

All (593) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:PRO:CB	1:D:76:PRO:CA	1.75	1.61
1:B:227:LEU:CG	1:B:227:LEU:CD2	1.74	1.59
1:C:50:ILE:CB	1:C:50:ILE:CG2	1.76	1.59
1:D:39:ASN:CG	1:D:39:ASN:CB	1.74	1.56
1:D:50:ILE:CA	1:D:50:ILE:CB	1.83	1.56
1:C:33:PRO:CG	1:C:33:PRO:CB	1.78	1.53
1:B:39:ASN:CB	1:B:39:ASN:CG	1.75	1.52
1:C:253:MSE:SE	1:C:253:MSE:CE	2.15	1.44
1:A:36:PRO:CG	1:A:36:PRO:CB	1.74	1.44
1:A:253:MSE:SE	1:A:253:MSE:CG	2.18	1.41
1:A:253:MSE:SE	1:A:253:MSE:CE	2.19	1.40
1:D:253:MSE:SE	1:D:253:MSE:CE	2.24	1.35
1:A:96:MSE:SE	1:A:96:MSE:CE	2.29	1.29
1:C:209:SER:HA	3:C:1103:HOH:O	1.31	1.28
1:D:185:THR:HG21	3:D:1049:HOH:O	1.42	1.17
1:D:96:MSE:SE	1:D:96:MSE:CE	2.43	1.16
1:B:149:ASN:N	1:B:149:ASN:HD22	1.37	1.15
1:A:241:MSE:HE2	1:B:201:PRO:HA	1.28	1.14
1:A:240:LYS:O	1:A:241:MSE:HE3	1.42	1.14
1:B:39:ASN:HB3	3:B:1111:HOH:O	1.49	1.13
1:D:71:LEU:HD22	1:D:72:VAL:N	1.68	1.09
1:B:265:LYS:HG2	1:B:266:GLY:H	0.98	1.07
1:C:85:THR:HB	3:C:1069:HOH:O	1.57	1.04
1:B:265:LYS:HG2	1:B:266:GLY:N	1.70	1.04
1:D:209:SER:N	3:D:1078:HOH:O	1.58	1.03
1:B:207:GLY:HA2	3:B:1070:HOH:O	1.56	1.01
1:B:120:ALA:HB2	1:B:149:ASN:HB3	1.40	1.01
1:D:207:GLY:C	3:D:1079:HOH:O	2.02	1.01
1:D:71:LEU:HD22	1:D:71:LEU:C	1.82	1.01
1:D:75:ASN:H	1:D:75:ASN:HD22	1.08	1.00
1:B:149:ASN:H	1:B:149:ASN:ND2	1.61	0.97
1:C:331:GLN:O	1:C:334:LEU:O	1.83	0.96
1:D:85:THR:HG22	1:D:87:THR:H	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ASN:N	1:B:149:ASN:ND2	2.11	0.96
1:B:248:THR:HG23	1:B:250:GLY:H	1.30	0.96
1:C:37:ASN:O	1:C:38:ALA:O	1.84	0.96
1:A:248:THR:HG21	3:A:1041:HOH:O	1.67	0.94
1:B:38:ALA:HB2	1:B:308:THR:HB	1.50	0.92
1:B:319:ASP:N	3:B:1043:HOH:O	2.02	0.92
1:C:50:ILE:CG2	1:C:50:ILE:CA	2.49	0.91
1:C:275:THR:HA	1:C:308:THR:HG23	1.52	0.90
1:B:106:HIS:HB2	1:B:108:GLN:NE2	1.86	0.90
1:B:275:THR:HA	1:B:308:THR:HG23	1.53	0.90
1:A:40:CYS:O	1:A:76:PRO:HB2	1.72	0.89
1:A:142:TRP:N	3:A:1043:HOH:O	2.03	0.89
1:B:184:VAL:HG23	1:B:185:THR:H	1.33	0.89
1:B:96:MSE:HE3	1:B:97:PRO:HD2	1.53	0.89
1:B:227:LEU:CD2	1:B:227:LEU:CD1	2.51	0.88
1:C:248:THR:HG23	1:C:250:GLY:H	1.36	0.88
1:B:49:GLU:O	1:B:50:ILE:HB	1.74	0.87
1:B:96:MSE:HE3	1:B:97:PRO:CD	2.05	0.86
1:C:108:GLN:HG3	1:C:166:VAL:HG21	1.55	0.86
1:A:40:CYS:O	1:A:76:PRO:CB	2.24	0.85
1:D:49:GLU:O	1:D:51:ARG:HG3	1.79	0.83
1:B:108:GLN:H	1:B:108:GLN:HE21	1.23	0.83
1:A:73:LEU:HD12	1:A:73:LEU:H	1.43	0.83
1:A:317:THR:O	1:A:318:GLN:HB2	1.76	0.82
1:B:149:ASN:HD22	1:B:149:ASN:H	0.86	0.82
1:D:208:ASN:C	3:D:1079:HOH:O	2.22	0.81
1:C:51:ARG:C	3:C:1130:HOH:O	2.24	0.80
1:D:75:ASN:HD22	1:D:75:ASN:N	1.69	0.80
1:D:127:GLU:HB2	1:D:186:ARG:HG2	1.63	0.80
1:B:207:GLY:CA	3:B:1070:HOH:O	2.20	0.80
1:B:227:LEU:CD2	1:B:227:LEU:CB	2.60	0.80
1:B:327:ASP:O	1:B:330:VAL:HG22	1.80	0.80
1:C:206:THR:HG21	1:C:247:VAL:HG11	1.63	0.79
1:B:99:GLU:HB2	3:B:1088:HOH:O	1.82	0.79
1:C:105:ARG:HG2	1:C:144:TRP:CZ3	2.18	0.78
1:B:240:LYS:HG3	1:B:261:GLN:HB3	1.66	0.78
1:A:38:ALA:O	1:A:39:ASN:OD1	2.02	0.78
1:A:160:GLY:C	1:A:161:LEU:HD12	2.09	0.77
1:B:75:ASN:ND2	1:B:83:SER:H	1.81	0.77
1:D:208:ASN:O	3:D:1079:HOH:O	2.01	0.77
1:B:38:ALA:CB	1:B:308:THR:HB	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:THR:HG23	1:B:250:GLY:N	2.00	0.77
1:A:163:LEU:HB2	1:A:164:PRO:HD3	1.67	0.76
1:A:327:ASP:O	1:A:330:VAL:HG22	1.85	0.76
1:A:89:TYR:CD1	1:A:89:TYR:C	2.62	0.76
1:D:76:PRO:CB	1:D:76:PRO:C	2.59	0.76
1:A:191:TYR:OH	1:A:214:ASN:HB3	1.86	0.76
1:B:160:GLY:C	1:B:161:LEU:HD23	2.10	0.75
1:B:47:TYR:O	1:B:48:GLN:HB2	1.86	0.75
1:B:85:THR:HG22	1:B:87:THR:H	1.52	0.75
1:D:267:PHE:CE2	1:D:269:SER:HB3	2.22	0.75
1:B:73:LEU:HD11	1:B:89:TYR:CE2	2.23	0.74
1:B:208:ASN:O	1:B:209:SER:HB3	1.86	0.74
1:D:208:ASN:HA	3:D:1102:HOH:O	1.86	0.74
1:D:149:ASN:HD22	1:D:149:ASN:H	1.35	0.74
1:B:265:LYS:HA	1:B:318:GLN:O	1.88	0.74
1:D:50:ILE:CA	1:D:50:ILE:HB	2.10	0.74
1:D:270:ARG:HH21	1:D:342:TYR:HE1	1.35	0.73
1:C:223:VAL:HG21	1:D:199:MSE:HE3	1.69	0.73
1:A:241:MSE:HE2	1:B:201:PRO:CA	2.14	0.73
1:A:103:SER:OG	1:A:181:GLN:O	2.05	0.73
1:A:105:ARG:HB2	1:A:144:TRP:CE3	2.24	0.72
1:B:76:PRO:HD3	1:B:84:ILE:HA	1.71	0.72
1:A:181:GLN:O	1:A:182:GLN:HB2	1.89	0.72
1:B:49:GLU:O	1:B:50:ILE:CB	2.38	0.71
1:B:120:ALA:CB	1:B:149:ASN:HB3	2.20	0.71
1:B:160:GLY:O	1:B:161:LEU:HD23	1.91	0.71
1:D:106:HIS:O	1:D:141:GLN:O	2.06	0.71
1:B:216:ARG:HD3	1:B:219:ARG:HD2	1.71	0.71
1:D:75:ASN:H	1:D:75:ASN:ND2	1.85	0.71
1:D:327:ASP:O	1:D:330:VAL:HG12	1.90	0.71
1:C:184:VAL:O	1:C:185:THR:HB	1.92	0.70
1:D:135:ASP:HB3	1:D:214:ASN:HD21	1.56	0.70
1:B:206:THR:HG23	3:B:1070:HOH:O	1.92	0.69
1:B:265:LYS:CG	1:B:266:GLY:H	1.89	0.69
1:B:116:GLU:HA	3:B:1052:HOH:O	1.91	0.69
1:B:208:ASN:O	1:B:208:ASN:CG	2.34	0.69
1:C:33:PRO:N	3:C:1080:HOH:O	2.25	0.69
1:C:220:SER:HA	1:D:199:MSE:HE1	1.75	0.69
1:D:167:ASN:OD1	3:D:1031:HOH:O	2.09	0.69
1:A:85:THR:HG22	1:A:88:LEU:H	1.57	0.69
1:D:79:ARG:NE	3:D:1146:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:N	3:D:1079:HOH:O	2.22	0.69
1:B:71:LEU:N	3:B:1027:HOH:O	2.26	0.69
1:C:248:THR:HG21	3:C:1034:HOH:O	1.92	0.69
1:A:292:GLY:O	1:A:293:ASN:HB2	1.92	0.68
1:D:79:ARG:HG3	1:D:79:ARG:HH11	1.58	0.68
1:A:317:THR:O	1:A:318:GLN:CB	2.36	0.68
1:D:126:GLY:O	1:D:186:ARG:HB3	1.94	0.68
1:C:51:ARG:HH22	1:C:94:LEU:HB2	1.58	0.68
1:B:76:PRO:HA	3:B:1042:HOH:O	1.92	0.68
1:D:270:ARG:NH2	1:D:342:TYR:OH	2.27	0.68
1:D:305:VAL:HG21	3:D:1126:HOH:O	1.92	0.68
1:A:73:LEU:HD12	1:A:73:LEU:N	2.09	0.68
1:A:308:THR:HG21	1:D:170:GLY:O	1.94	0.68
1:B:184:VAL:CG2	1:B:185:THR:H	2.05	0.68
1:B:245:ASN:HB3	1:B:248:THR:HG22	1.76	0.68
1:B:108:GLN:NE2	1:B:108:GLN:H	1.90	0.67
1:D:85:THR:HG22	1:D:87:THR:N	2.08	0.67
1:D:149:ASN:HD22	1:D:149:ASN:N	1.87	0.67
1:A:75:ASN:ND2	3:A:1049:HOH:O	2.26	0.67
1:D:184:VAL:HG23	3:D:1059:HOH:O	1.93	0.67
1:B:47:TYR:O	1:B:48:GLN:CB	2.37	0.67
1:C:208:ASN:C	3:C:1097:HOH:O	2.37	0.67
1:C:163:LEU:HB2	1:C:164:PRO:HD3	1.77	0.67
1:D:43:ALA:HB3	1:D:305:VAL:CG1	2.24	0.67
1:D:208:ASN:HB3	3:D:1109:HOH:O	1.94	0.67
1:C:161:LEU:HD12	1:C:163:LEU:CD1	2.25	0.66
1:B:170:GLY:HA2	3:C:1108:HOH:O	1.96	0.66
1:B:184:VAL:HG23	1:B:185:THR:N	2.09	0.66
1:D:183:PRO:HD2	3:D:1085:HOH:O	1.95	0.66
1:D:85:THR:HG21	3:D:1068:HOH:O	1.94	0.66
1:B:126:GLY:O	1:B:184:VAL:O	2.13	0.66
1:D:49:GLU:O	1:D:51:ARG:CG	2.44	0.66
1:D:50:ILE:CB	1:D:50:ILE:C	2.65	0.66
1:C:226:ASP:O	1:C:230:LEU:HD22	1.95	0.65
1:B:52:PRO:O	3:B:1057:HOH:O	2.14	0.65
1:A:85:THR:CG2	1:A:88:LEU:H	2.09	0.65
1:B:338:ARG:HB2	1:B:338:ARG:HH21	1.61	0.65
1:A:46:ASN:HB3	1:A:49:GLU:CG	2.27	0.65
1:D:75:ASN:N	1:D:75:ASN:ND2	2.35	0.65
1:C:275:THR:CA	1:C:308:THR:HG23	2.27	0.65
1:D:108:GLN:HG2	1:D:163:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HG2	1:A:163:LEU:HD23	1.78	0.65
1:A:240:LYS:O	1:A:241:MSE:CE	2.33	0.64
1:C:46:ASN:ND2	1:C:48:GLN:HB3	2.11	0.64
1:A:45:TRP:CZ2	1:A:74:GLU:HB2	2.32	0.64
1:D:163:LEU:HB2	1:D:164:PRO:HD3	1.80	0.64
1:B:127:GLU:HB3	1:B:186:ARG:HB3	1.80	0.64
1:A:240:LYS:HG3	1:A:261:GLN:HB3	1.80	0.63
1:C:85:THR:HG22	1:C:88:LEU:HB2	1.80	0.63
1:B:106:HIS:HB2	1:B:108:GLN:HE21	1.62	0.63
1:C:206:THR:CG2	1:C:247:VAL:HG11	2.28	0.63
1:A:127:GLU:HG3	1:A:213:PHE:HZ	1.64	0.63
1:B:75:ASN:HD21	1:B:83:SER:H	1.44	0.62
1:B:235:GLU:HG2	3:B:1048:HOH:O	2.00	0.62
1:B:92:LEU:HD22	1:B:92:LEU:N	2.14	0.62
1:B:248:THR:CG2	1:B:250:GLY:H	2.10	0.62
1:C:204:HIS:NE2	1:C:206:THR:HB	2.14	0.61
1:D:191:TYR:OH	1:D:214:ASN:HB3	2.00	0.61
1:B:308:THR:HG21	1:C:170:GLY:O	2.00	0.61
1:B:209:SER:HA	3:B:1114:HOH:O	2.00	0.61
1:D:39:ASN:CG	1:D:39:ASN:CA	2.69	0.61
1:A:46:ASN:HB3	1:A:49:GLU:HG3	1.81	0.61
1:A:230:LEU:HD21	1:B:190:ASP:HA	1.81	0.61
1:D:79:ARG:HA	3:D:1150:HOH:O	2.00	0.61
1:A:248:THR:HG23	1:A:250:GLY:H	1.66	0.61
1:B:279:ILE:O	1:B:324:SER:HA	1.99	0.61
1:A:199:MSE:HE2	1:B:241:MSE:HB3	1.83	0.61
1:C:248:THR:HG23	1:C:250:GLY:N	2.13	0.61
1:D:137:ILE:C	1:D:138:LEU:HD12	2.24	0.61
1:C:50:ILE:CG2	1:C:50:ILE:HB	2.16	0.61
1:C:292:GLY:O	1:C:293:ASN:HB2	2.01	0.61
1:C:37:ASN:O	1:C:38:ALA:C	2.44	0.60
1:B:216:ARG:HB3	1:B:218:ASP:OD1	1.99	0.60
1:C:184:VAL:O	1:C:185:THR:CB	2.48	0.60
1:B:84:ILE:HG21	1:B:90:ALA:CB	2.31	0.60
1:D:108:GLN:HG3	1:D:166:VAL:HG21	1.83	0.60
1:B:330:VAL:HG23	1:B:331:GLN:N	2.15	0.60
1:C:45:TRP:O	1:C:46:ASN:HB3	2.01	0.60
1:B:111:LEU:C	1:B:111:LEU:HD12	2.26	0.60
1:B:89:TYR:CD1	1:B:89:TYR:C	2.80	0.60
1:A:267:PHE:CE2	1:A:269:SER:HB3	2.37	0.59
1:C:85:THR:CG2	1:C:88:LEU:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LEU:HD12	1:C:138:LEU:N	2.18	0.59
1:C:38:ALA:CB	1:C:308:THR:HB	2.32	0.59
1:A:181:GLN:O	1:A:182:GLN:CB	2.51	0.59
1:B:288:GLN:NE2	1:B:295:THR:OG1	2.34	0.59
1:B:293:ASN:O	1:B:294:GLU:C	2.46	0.59
1:D:48:GLN:O	1:D:48:GLN:CG	2.50	0.59
1:D:135:ASP:HB3	1:D:214:ASN:ND2	2.18	0.58
1:D:192:LEU:HB2	1:D:193:PRO:CD	2.34	0.58
1:C:244:VAL:HG21	1:D:200:LEU:HD22	1.85	0.58
1:A:78:LEU:O	1:A:81:GLN:HB2	2.04	0.58
1:B:224:LEU:HD11	1:B:260:LEU:HG	1.85	0.58
1:A:73:LEU:H	1:A:73:LEU:CD1	2.14	0.58
1:A:244:VAL:HG21	1:B:200:LEU:HB2	1.86	0.58
1:B:104:HIS:HD2	3:B:1095:HOH:O	1.85	0.58
1:B:127:GLU:HG3	1:B:213:PHE:HZ	1.69	0.58
1:B:96:MSE:HE3	1:B:97:PRO:HD3	1.85	0.58
1:C:199:MSE:HE3	1:D:223:VAL:HG21	1.86	0.58
1:A:230:LEU:CD2	1:B:190:ASP:HA	2.34	0.58
1:C:245:ASN:HB3	1:C:248:THR:HG22	1.86	0.57
1:D:160:GLY:O	1:D:161:LEU:HD23	2.04	0.57
1:A:228:THR:HG22	1:A:239:TYR:CE1	2.39	0.57
1:D:341:ARG:O	1:D:342:TYR:CG	2.57	0.57
1:B:318:GLN:C	3:B:1043:HOH:O	2.43	0.57
1:D:214:ASN:C	1:D:214:ASN:HD22	2.11	0.57
1:C:208:ASN:C	1:C:208:ASN:HD22	2.12	0.57
1:D:48:GLN:O	1:D:48:GLN:HG2	2.04	0.57
1:B:253:MSE:CE	1:B:256:MSE:HE3	2.35	0.56
1:A:38:ALA:CB	1:A:308:THR:HB	2.36	0.56
1:A:244:VAL:HG21	1:B:200:LEU:HD22	1.86	0.56
1:A:53:LEU:HG	1:A:72:VAL:CG2	2.35	0.56
3:B:1128:HOH:O	1:C:208:ASN:HB3	2.04	0.56
1:B:48:GLN:O	1:B:49:GLU:HB2	2.03	0.56
1:C:121:PHE:CE1	1:C:128:ARG:HD2	2.41	0.56
1:C:161:LEU:HD12	1:C:163:LEU:HD12	1.88	0.56
1:D:101:ALA:HB1	1:D:102:PRO:HD2	1.87	0.56
1:B:338:ARG:HH21	1:B:338:ARG:CB	2.19	0.56
1:A:49:GLU:O	1:A:50:ILE:HB	2.04	0.56
1:D:43:ALA:HB3	1:D:305:VAL:HG12	1.87	0.56
1:D:76:PRO:C	1:D:78:LEU:H	2.13	0.56
1:B:226:ASP:O	1:B:230:LEU:HD13	2.06	0.56
1:B:76:PRO:CA	3:B:1042:HOH:O	2.51	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ARG:HG2	1:C:216:ARG:NH2	2.21	0.55
1:C:121:PHE:CD1	1:C:121:PHE:C	2.83	0.55
1:D:267:PHE:HE2	1:D:269:SER:HB3	1.67	0.55
1:A:275:THR:HA	1:A:308:THR:HG23	1.88	0.55
1:C:129:THR:HG22	1:C:213:PHE:CE2	2.41	0.55
1:A:37:ASN:CG	1:A:38:ALA:H	2.13	0.55
1:A:40:CYS:O	1:A:76:PRO:CG	2.54	0.55
1:B:208:ASN:O	1:B:209:SER:CB	2.52	0.55
1:D:160:GLY:C	1:D:161:LEU:HD23	2.31	0.55
1:D:275:THR:HA	1:D:308:THR:HG23	1.88	0.55
1:D:143:ARG:HA	3:D:1125:HOH:O	2.05	0.55
1:B:85:THR:HG21	3:B:1017:HOH:O	2.06	0.55
1:D:184:VAL:O	1:D:185:THR:C	2.46	0.55
1:B:272:ALA:O	1:B:311:GLY:HA2	2.07	0.55
1:B:285:GLY:HA3	1:B:320:SER:HB3	1.89	0.55
1:D:183:PRO:CG	3:D:1085:HOH:O	2.53	0.55
1:C:191:TYR:OH	1:C:214:ASN:HB3	2.06	0.55
1:C:308:THR:HG22	1:C:309:TRP:N	2.21	0.55
1:A:89:TYR:CD1	1:A:90:ALA:N	2.75	0.54
1:B:253:MSE:HE3	1:B:256:MSE:HE3	1.89	0.54
1:A:184:VAL:O	1:A:185:THR:HB	2.07	0.54
1:D:183:PRO:CD	3:D:1085:HOH:O	2.52	0.54
1:D:106:HIS:HB2	1:D:108:GLN:OE1	2.06	0.54
1:A:76:PRO:HG2	1:A:78:LEU:HG	1.89	0.54
1:D:223:VAL:O	1:D:227:LEU:HG	2.07	0.54
1:B:84:ILE:HG21	1:B:90:ALA:HB3	1.89	0.54
1:C:107:ASN:ND2	1:C:173:PHE:HB2	2.22	0.54
1:A:248:THR:HG23	1:A:250:GLY:N	2.23	0.54
1:C:281:HIS:HE1	3:C:1052:HOH:O	1.91	0.54
1:D:50:ILE:CA	1:D:50:ILE:CG1	2.81	0.54
1:D:105:ARG:HH11	1:D:175:GLU:CD	2.16	0.54
1:C:163:LEU:CB	1:C:164:PRO:HD3	2.38	0.54
1:C:129:THR:HG22	1:C:213:PHE:HE2	1.73	0.54
1:A:248:THR:CG2	1:A:250:GLY:H	2.21	0.53
1:A:85:THR:HG23	1:A:87:THR:H	1.73	0.53
1:B:39:ASN:CB	1:B:39:ASN:ND2	2.64	0.53
1:D:308:THR:O	1:D:310:HIS:HD2	1.90	0.53
1:A:35:THR:N	1:D:174:ALA:H	2.06	0.53
1:B:46:ASN:ND2	1:B:47:TYR:O	2.42	0.53
1:B:334:LEU:HB2	1:B:336:LEU:HD12	1.91	0.53
1:C:127:GLU:HB2	1:C:186:ARG:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TYR:CD1	1:A:178:PRO:HD2	2.44	0.53
1:C:109:SER:HB2	1:C:256:MSE:HE2	1.90	0.53
1:D:85:THR:HG22	1:D:86:ALA:N	2.22	0.53
1:D:240:LYS:C	1:D:241:MSE:HG2	2.33	0.53
1:A:94:LEU:HD21	1:A:96:MSE:SE	2.59	0.53
1:A:274:THR:HB	1:A:276:ASP:OD1	2.09	0.53
1:C:214:ASN:C	1:C:214:ASN:HD22	2.17	0.53
1:A:328:ARG:N	1:A:329:PRO:CD	2.71	0.52
1:B:127:GLU:OE1	1:B:186:ARG:NH2	2.42	0.52
1:D:292:GLY:O	1:D:293:ASN:HB2	2.09	0.52
1:A:97:PRO:HB3	1:A:151:GLY:O	2.08	0.52
1:B:265:LYS:CG	1:B:266:GLY:N	2.52	0.52
1:A:289:VAL:HG23	1:A:298:PHE:CD2	2.45	0.52
1:C:251:TYR:CG	1:C:329:PRO:HG3	2.44	0.52
1:A:85:THR:HG22	1:A:88:LEU:HB2	1.91	0.52
1:A:111:LEU:C	1:A:111:LEU:HD12	2.35	0.52
3:A:1088:HOH:O	1:B:227:LEU:HD13	2.08	0.52
1:B:184:VAL:CG2	1:B:185:THR:N	2.72	0.52
1:D:103:SER:HA	1:D:146:ASP:HB3	1.92	0.52
1:A:104:HIS:C	1:A:104:HIS:CD2	2.87	0.52
1:B:106:HIS:HB2	1:B:108:GLN:HE22	1.68	0.52
1:B:328:ARG:N	1:B:329:PRO:CD	2.73	0.52
1:D:85:THR:CG2	1:D:86:ALA:N	2.73	0.52
1:D:267:PHE:O	1:D:315:GLN:HA	2.10	0.52
1:C:89:TYR:CD1	1:C:89:TYR:C	2.87	0.52
1:A:123:ALA:HB3	1:A:146:ASP:OD1	2.10	0.51
1:C:50:ILE:O	1:C:50:ILE:CG1	2.57	0.51
1:C:338:ARG:CD	3:C:1027:HOH:O	2.58	0.51
1:A:170:GLY:O	1:D:308:THR:HG21	2.11	0.51
1:C:283:VAL:HG22	1:C:321:VAL:HB	1.91	0.51
1:D:78:LEU:O	1:D:79:ARG:C	2.53	0.51
1:A:127:GLU:HG3	1:A:213:PHE:CZ	2.45	0.51
1:A:253:MSE:SE	1:A:253:MSE:CB	3.04	0.51
1:B:163:LEU:HB2	1:B:164:PRO:HD3	1.93	0.51
1:B:305:VAL:HG13	1:B:305:VAL:O	2.11	0.51
1:C:94:LEU:HD11	1:C:154:PRO:HB3	1.92	0.51
1:D:138:LEU:HD12	1:D:138:LEU:N	2.26	0.51
1:C:163:LEU:HD23	3:C:1096:HOH:O	2.10	0.51
1:B:188:GLU:HG2	1:B:189:GLY:N	2.25	0.51
1:B:197:ALA:O	1:B:199:MSE:HG3	2.09	0.51
1:C:208:ASN:HA	3:C:1097:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:TYR:O	1:C:218:ASP:C	2.51	0.51
1:D:89:TYR:O	1:D:160:GLY:HA2	2.11	0.51
1:C:134:GLY:C	1:C:217:TYR:HB2	2.36	0.51
1:D:328:ARG:N	1:D:329:PRO:CD	2.74	0.51
1:B:121:PHE:CD1	1:B:121:PHE:C	2.89	0.50
1:B:275:THR:CA	1:B:308:THR:HG23	2.35	0.50
1:C:161:LEU:HD12	1:C:163:LEU:HD11	1.93	0.50
1:C:208:ASN:N	3:C:1081:HOH:O	2.43	0.50
1:B:72:VAL:HG23	3:B:1124:HOH:O	2.10	0.50
1:B:123:ALA:HB2	1:B:128:ARG:HB3	1.93	0.50
1:C:90:ALA:HA	1:C:159:ASP:O	2.11	0.50
1:B:207:GLY:O	1:B:208:ASN:C	2.54	0.50
1:C:137:ILE:HA	1:C:213:PHE:O	2.11	0.50
1:C:45:TRP:O	1:C:46:ASN:CB	2.58	0.50
1:C:112:ARG:HH22	1:C:147:HIS:CD2	2.28	0.50
1:A:107:ASN:C	1:A:107:ASN:HD22	2.15	0.50
1:B:112:ARG:HH21	1:B:147:HIS:HD2	1.59	0.50
1:B:161:LEU:HD12	1:B:163:LEU:HD12	1.94	0.50
1:D:149:ASN:N	1:D:149:ASN:ND2	2.58	0.50
1:B:134:GLY:C	1:B:217:TYR:HB2	2.37	0.50
1:B:308:THR:O	1:B:310:HIS:HD2	1.95	0.50
1:D:136:PHE:HB3	1:D:215:TYR:HB2	1.93	0.50
1:B:75:ASN:HD21	1:B:82:SER:CA	2.24	0.49
1:C:251:TYR:CD1	1:C:329:PRO:HG3	2.47	0.49
1:B:90:ALA:HA	1:B:159:ASP:O	2.13	0.49
1:A:206:THR:HG23	1:A:207:GLY:N	2.26	0.49
1:C:257:GLY:O	1:C:325:PHE:HA	2.12	0.49
1:C:275:THR:HA	1:C:308:THR:CG2	2.33	0.49
1:C:332:GLU:HG2	3:C:1110:HOH:O	2.12	0.49
1:B:75:ASN:ND2	1:B:83:SER:N	2.57	0.49
1:D:228:THR:HG22	1:D:239:TYR:CE1	2.46	0.49
1:B:75:ASN:HD21	1:B:83:SER:N	2.10	0.49
1:D:112:ARG:HD3	1:D:131:MSE:CE	2.43	0.49
1:D:192:LEU:CB	1:D:193:PRO:CD	2.91	0.49
1:A:292:GLY:O	1:A:293:ASN:CB	2.55	0.49
1:C:199:MSE:HE1	1:D:220:SER:HA	1.95	0.49
1:D:46:ASN:O	1:D:48:GLN:N	2.44	0.49
1:D:79:ARG:HG3	1:D:79:ARG:NH1	2.27	0.49
1:B:178:PRO:HA	3:B:1035:HOH:O	2.13	0.48
1:D:39:ASN:CB	1:D:39:ASN:ND2	2.66	0.48
1:D:163:LEU:O	1:D:167:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:N	3:A:1038:HOH:O	2.45	0.48
1:A:228:THR:HA	1:A:239:TYR:CZ	2.48	0.48
1:C:45:TRP:CE2	1:C:74:GLU:HG3	2.49	0.48
1:C:106:HIS:HB2	1:C:108:GLN:OE1	2.13	0.48
1:D:97:PRO:HB3	1:D:151:GLY:O	2.12	0.48
1:D:305:VAL:CG2	3:D:1126:HOH:O	2.57	0.48
1:A:173:PHE:CE2	1:D:338:ARG:HD3	2.49	0.48
1:B:207:GLY:C	3:B:1070:HOH:O	2.53	0.48
1:A:85:THR:HG21	3:A:1021:HOH:O	2.14	0.48
1:D:328:ARG:HB3	1:D:329:PRO:HD3	1.96	0.48
1:A:53:LEU:HG	1:A:72:VAL:HG21	1.95	0.48
1:B:43:ALA:HB3	1:B:305:VAL:HG12	1.96	0.48
1:C:85:THR:HG23	1:C:87:THR:H	1.79	0.48
1:B:105:ARG:HD3	1:B:144:TRP:CE2	2.49	0.48
1:C:267:PHE:O	1:C:315:GLN:HA	2.14	0.47
1:D:108:GLN:HG2	1:D:163:LEU:CD2	2.42	0.47
1:D:228:THR:HA	1:D:239:TYR:CZ	2.49	0.47
1:C:76:PRO:HG3	1:C:84:ILE:O	2.14	0.47
1:D:214:ASN:ND2	1:D:214:ASN:C	2.72	0.47
1:A:289:VAL:HG23	1:A:298:PHE:HD2	1.79	0.47
1:B:73:LEU:HD11	1:B:89:TYR:HE2	1.70	0.47
1:D:208:ASN:CA	3:D:1078:HOH:O	2.61	0.47
1:A:38:ALA:O	1:A:39:ASN:CG	2.57	0.47
1:A:164:PRO:O	1:A:168:ILE:HG23	2.14	0.47
1:B:73:LEU:CD1	1:B:89:TYR:CE2	2.97	0.47
1:C:216:ARG:HG2	1:C:216:ARG:HH21	1.79	0.47
1:C:224:LEU:HD11	1:C:260:LEU:HG	1.95	0.47
1:D:50:ILE:CG1	1:D:72:VAL:HG21	2.45	0.47
1:B:330:VAL:CG2	1:B:331:GLN:N	2.78	0.47
1:D:151:GLY:HA3	3:D:1010:HOH:O	2.13	0.47
1:C:38:ALA:HB3	1:C:308:THR:HB	1.96	0.47
1:C:123:ALA:HB2	1:C:128:ARG:HB3	1.96	0.47
1:C:177:TYR:HB3	3:C:1116:HOH:O	2.13	0.47
1:B:251:TYR:CD2	1:B:329:PRO:HG3	2.50	0.47
1:C:138:LEU:N	1:C:138:LEU:CD1	2.78	0.47
1:D:221:ARG:NH2	1:D:284:GLU:OE1	2.44	0.47
1:D:251:TYR:OH	1:D:332:GLU:OE2	2.27	0.47
1:B:265:LYS:HA	1:B:318:GLN:C	2.40	0.47
1:D:276:ASP:O	1:D:277:SER:C	2.53	0.46
1:D:341:ARG:O	1:D:342:TYR:CD1	2.68	0.46
1:C:129:THR:HB	3:C:1021:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD12	1:A:93:GLN:HG3	1.97	0.46
1:B:217:TYR:CE2	1:B:283:VAL:HG21	2.51	0.46
1:B:41:ALA:HB1	1:B:42:PRO:HD2	1.97	0.46
1:B:127:GLU:HG3	1:B:213:PHE:CZ	2.48	0.46
1:B:137:ILE:HA	1:B:213:PHE:O	2.16	0.46
1:B:276:ASP:OD1	1:B:276:ASP:N	2.42	0.46
1:B:293:ASN:OD1	1:B:293:ASN:C	2.58	0.46
1:A:90:ALA:HA	1:A:159:ASP:O	2.15	0.46
1:A:96:MSE:O	1:A:97:PRO:C	2.59	0.46
1:B:205:GLN:NE2	3:B:1108:HOH:O	2.48	0.46
1:D:157:TRP:CD1	1:D:157:TRP:C	2.94	0.46
1:D:183:PRO:HB3	3:D:1106:HOH:O	2.15	0.46
1:A:240:LYS:C	1:A:241:MSE:HE3	2.31	0.46
1:A:216:ARG:HD2	3:A:1105:HOH:O	2.15	0.46
1:A:108:GLN:HE21	1:A:166:VAL:HG21	1.81	0.45
1:B:84:ILE:HG21	1:B:90:ALA:HB2	1.98	0.45
1:B:184:VAL:O	1:B:185:THR:HB	2.16	0.45
1:C:51:ARG:H	1:C:51:ARG:HG2	1.32	0.45
1:C:158:LEU:HD13	1:C:159:ASP:N	2.31	0.45
1:C:204:HIS:HE2	1:C:206:THR:HB	1.81	0.45
1:C:246:PRO:HB2	3:C:1075:HOH:O	2.15	0.45
1:D:221:ARG:NH1	3:D:1092:HOH:O	2.49	0.45
1:B:291:ILE:O	1:B:293:ASN:O	2.34	0.45
1:C:207:GLY:CA	3:C:1081:HOH:O	2.64	0.45
1:A:51:ARG:O	1:A:53:LEU:N	2.48	0.45
1:C:219:ARG:CZ	3:C:1032:HOH:O	2.65	0.45
1:D:143:ARG:NH1	3:D:1098:HOH:O	2.47	0.45
1:A:161:LEU:HD12	1:A:161:LEU:N	2.31	0.45
1:D:105:ARG:NH1	1:D:175:GLU:OE2	2.45	0.45
1:A:71:LEU:CD1	1:A:93:GLN:HG3	2.46	0.45
1:B:143:ARG:NH1	3:B:1112:HOH:O	2.40	0.45
1:B:144:TRP:HZ3	1:B:177:TYR:H	1.65	0.45
1:B:216:ARG:CD	1:B:219:ARG:HD2	2.45	0.45
1:B:338:ARG:HD2	1:C:173:PHE:CZ	2.52	0.45
1:C:158:LEU:HD13	1:C:158:LEU:C	2.41	0.45
1:C:219:ARG:NH1	3:C:1065:HOH:O	2.49	0.45
1:A:282:VAL:HG21	1:A:298:PHE:CD1	2.51	0.45
1:B:191:TYR:CD1	1:B:191:TYR:C	2.95	0.45
1:B:338:ARG:HB2	1:B:338:ARG:NH2	2.28	0.45
1:A:127:GLU:HB3	1:A:186:ARG:HB2	1.99	0.45
1:B:51:ARG:N	1:B:52:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:TRP:HZ2	1:C:75:ASN:O	2.00	0.45
1:A:223:VAL:O	1:A:224:LEU:C	2.58	0.45
1:C:89:TYR:CD1	1:C:90:ALA:N	2.84	0.45
1:C:265:LYS:HG3	1:C:317:THR:O	2.17	0.45
1:C:44:TYR:CE2	1:C:46:ASN:HB2	2.52	0.44
1:C:216:ARG:HH21	1:C:216:ARG:CG	2.30	0.44
1:D:46:ASN:C	1:D:48:GLN:N	2.75	0.44
1:A:36:PRO:HA	1:D:172:GLY:O	2.17	0.44
1:A:103:SER:HB2	1:A:177:TYR:HB2	1.98	0.44
1:C:108:GLN:CG	1:C:166:VAL:HG21	2.37	0.44
1:A:129:THR:HG22	1:A:213:PHE:HE2	1.82	0.44
1:A:202:LEU:N	1:A:202:LEU:HD12	2.32	0.44
1:A:337:PHE:N	3:A:1018:HOH:O	2.49	0.44
1:B:74:GLU:HB2	1:B:90:ALA:O	2.17	0.44
1:B:291:ILE:O	1:B:292:GLY:C	2.59	0.44
1:D:39:ASN:O	1:D:40:CYS:CB	2.66	0.44
1:B:105:ARG:NE	1:B:144:TRP:CZ2	2.86	0.44
1:D:112:ARG:HD3	1:D:131:MSE:HE1	2.00	0.44
1:A:199:MSE:CE	1:B:241:MSE:HB3	2.46	0.44
1:A:38:ALA:C	1:A:39:ASN:CG	2.86	0.44
1:C:134:GLY:HA3	1:C:217:TYR:CG	2.53	0.44
1:C:121:PHE:O	1:C:147:HIS:HB2	2.18	0.44
1:A:290:ILE:O	1:A:312:VAL:HA	2.18	0.44
1:B:107:ASN:ND2	1:B:173:PHE:H	2.16	0.44
1:D:39:ASN:O	1:D:40:CYS:HB3	2.18	0.44
1:A:241:MSE:HB3	1:B:199:MSE:HE2	1.99	0.43
1:A:214:ASN:HD22	1:A:214:ASN:C	2.26	0.43
1:A:285:GLY:HA3	1:A:320:SER:HA	1.99	0.43
1:C:263:LEU:HB2	1:C:320:SER:HB2	2.00	0.43
1:C:267:PHE:CE2	1:C:269:SER:HB3	2.53	0.43
1:C:278:THR:CG2	1:C:324:SER:HB2	2.48	0.43
1:B:206:THR:HG22	1:B:247:VAL:HG11	2.00	0.43
1:C:252:PRO:C	1:C:253:MSE:HG3	2.43	0.43
1:D:38:ALA:O	1:D:39:ASN:C	2.58	0.43
1:D:94:LEU:HD11	1:D:154:PRO:HB3	2.00	0.43
1:D:270:ARG:NH2	1:D:342:TYR:CZ	2.87	0.43
1:A:289:VAL:HG12	1:A:290:ILE:N	2.31	0.43
1:C:33:PRO:CA	3:C:1080:HOH:O	2.67	0.43
1:C:160:GLY:O	1:C:161:LEU:HD23	2.19	0.43
1:C:46:ASN:HD22	1:C:48:GLN:HB3	1.82	0.43
1:D:120:ALA:HA	1:D:149:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HH22	1:A:147:HIS:HD2	1.66	0.43
1:A:163:LEU:CB	1:A:164:PRO:HD3	2.43	0.43
1:B:293:ASN:CG	1:B:294:GLU:N	2.77	0.43
1:B:104:HIS:CD2	3:B:1095:HOH:O	2.64	0.43
1:B:221:ARG:HG2	1:B:221:ARG:HH21	1.83	0.43
1:D:121:PHE:CD1	1:D:121:PHE:C	2.97	0.43
1:D:281:HIS:HD2	1:D:303:ILE:HG22	1.82	0.43
1:C:199:MSE:CE	1:D:223:VAL:HG21	2.48	0.43
1:A:122:THR:HG22	1:A:123:ALA:N	2.33	0.43
1:B:48:GLN:O	1:B:49:GLU:CB	2.67	0.43
1:C:221:ARG:HH21	1:C:221:ARG:HG2	1.84	0.43
1:C:259:PHE:CD1	1:C:259:PHE:N	2.86	0.43
1:D:138:LEU:N	1:D:138:LEU:CD1	2.82	0.43
1:A:85:THR:HG22	1:A:88:LEU:N	2.30	0.42
1:A:122:THR:OG1	1:A:131:MSE:HE3	2.19	0.42
1:A:308:THR:O	1:A:310:HIS:HD2	2.02	0.42
1:B:166:VAL:HG23	1:B:167:ASN:N	2.34	0.42
1:C:274:THR:HG22	1:C:339:GLU:HB3	2.00	0.42
1:A:202:LEU:N	1:A:202:LEU:CD1	2.82	0.42
1:B:184:VAL:O	1:B:185:THR:CB	2.66	0.42
1:C:122:THR:OG1	1:C:131:MSE:HE3	2.19	0.42
1:D:46:ASN:OD1	1:D:48:GLN:HB3	2.19	0.42
1:A:267:PHE:HE2	1:A:269:SER:HB3	1.80	0.42
1:C:49:GLU:C	1:C:49:GLU:OE1	2.63	0.42
1:C:224:LEU:O	1:C:227:LEU:HB2	2.19	0.42
1:C:290:ILE:O	1:C:312:VAL:HA	2.19	0.42
1:A:43:ALA:HB3	1:A:305:VAL:HG12	2.01	0.42
1:B:294:GLU:O	1:B:295:THR:O	2.36	0.42
1:D:209:SER:HB2	1:D:210:SER:H	1.35	0.42
1:A:121:PHE:CD1	1:A:121:PHE:C	2.98	0.42
1:B:141:GLN:CD	1:B:208:ASN:HD21	2.28	0.42
1:C:332:GLU:O	1:C:333:ALA:C	2.61	0.42
1:D:89:TYR:CD1	1:D:89:TYR:C	2.97	0.42
1:B:143:ARG:HA	3:B:1059:HOH:O	2.19	0.42
1:C:38:ALA:N	3:C:1108:HOH:O	2.38	0.42
1:B:94:LEU:HD11	1:B:154:PRO:HB3	2.02	0.42
1:B:288:GLN:NE2	1:B:295:THR:HG1	2.17	0.42
1:B:330:VAL:O	1:B:334:LEU:HG	2.19	0.42
1:A:112:ARG:HA	1:A:158:LEU:O	2.19	0.42
1:A:118:LYS:HB2	1:A:118:LYS:HE3	1.84	0.42
1:B:318:GLN:CA	3:B:1043:HOH:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ILE:O	1:D:324:SER:HA	2.20	0.42
1:B:259:PHE:HB2	1:B:324:SER:HG	1.85	0.42
1:D:112:ARG:NH1	1:D:122:THR:CG2	2.83	0.42
1:D:270:ARG:NH2	1:D:342:TYR:CE1	2.79	0.42
1:A:141:GLN:HG2	1:A:142:TRP:N	2.35	0.41
1:A:152:ASP:O	1:A:153:GLU:HB2	2.20	0.41
1:C:221:ARG:HH21	1:C:221:ARG:CG	2.34	0.41
1:C:301:LYS:NZ	3:C:1052:HOH:O	2.50	0.41
1:D:204:HIS:CE1	3:D:1151:HOH:O	2.72	0.41
1:D:214:ASN:HD22	1:D:215:TYR:N	2.17	0.41
1:A:174:ALA:O	1:D:34:LYS:HG3	2.19	0.41
1:B:112:ARG:HB3	1:B:157:TRP:CD1	2.55	0.41
1:B:153:GLU:HA	1:B:154:PRO:HD3	1.82	0.41
1:C:263:LEU:HD11	1:C:322:LEU:HD22	2.02	0.41
1:C:306:VAL:HG21	1:C:312:VAL:HG21	2.02	0.41
1:A:103:SER:HB2	1:A:177:TYR:CB	2.50	0.41
1:A:166:VAL:HG23	1:A:167:ASN:N	2.34	0.41
1:B:95:ILE:CG1	1:B:157:TRP:CZ3	3.03	0.41
1:C:85:THR:OG1	1:C:86:ALA:N	2.54	0.41
1:B:252:PRO:HD3	3:B:1029:HOH:O	2.20	0.41
1:B:288:GLN:HE21	1:B:288:GLN:HB3	1.29	0.41
1:C:112:ARG:HH22	1:C:147:HIS:HD2	1.66	0.41
1:B:163:LEU:HA	1:B:166:VAL:HG22	2.03	0.41
1:B:217:TYR:CZ	1:B:283:VAL:HG21	2.56	0.41
1:C:85:THR:CG2	1:C:88:LEU:H	2.34	0.41
1:A:101:ALA:HA	1:A:102:PRO:HD2	1.84	0.41
1:A:200:LEU:HB2	1:B:244:VAL:HG11	2.02	0.41
1:D:46:ASN:C	1:D:48:GLN:H	2.28	0.41
1:D:253:MSE:CE	1:D:256:MSE:HE3	2.51	0.41
1:A:38:ALA:HB1	1:A:308:THR:HB	2.02	0.41
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.76	0.41
1:C:45:TRP:CE2	1:C:74:GLU:CG	3.04	0.41
1:C:112:ARG:HG2	1:C:157:TRP:NE1	2.36	0.41
1:C:242:ARG:HD2	1:C:251:TYR:CE1	2.55	0.41
1:C:247:VAL:O	1:C:247:VAL:HG12	2.21	0.41
1:C:300:ALA:O	1:C:301:LYS:HB2	2.20	0.41
1:D:129:THR:HA	1:D:130:PRO:HD3	1.92	0.41
1:D:313:SER:HB2	1:D:315:GLN:HE22	1.86	0.41
1:A:46:ASN:HB3	1:A:49:GLU:CD	2.46	0.41
1:A:53:LEU:HD13	1:A:53:LEU:C	2.45	0.41
1:A:241:MSE:HG3	1:B:200:LEU:C	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLY:O	1:C:308:THR:HG21	2.21	0.41
1:C:51:ARG:NH2	1:C:94:LEU:HB2	2.32	0.41
1:C:292:GLY:O	1:C:293:ASN:CB	2.66	0.41
1:A:118:LYS:HG3	3:A:1079:HOH:O	2.20	0.40
1:A:301:LYS:HD3	1:A:301:LYS:N	2.35	0.40
1:A:328:ARG:HB3	1:A:329:PRO:HD3	2.03	0.40
1:B:135:ASP:HB3	1:B:214:ASN:OD1	2.21	0.40
1:D:47:TYR:O	1:D:47:TYR:CG	2.74	0.40
1:D:256:MSE:C	1:D:329:PRO:HG2	2.46	0.40
1:A:265:LYS:HD2	1:A:318:GLN:H	1.86	0.40
1:B:248:THR:HG23	1:B:250:GLY:CA	2.51	0.40
1:C:49:GLU:OE1	1:C:49:GLU:CA	2.70	0.40
1:D:218:ASP:OD1	1:D:219:ARG:N	2.54	0.40
1:A:94:LEU:HD23	1:A:94:LEU:C	2.46	0.40
1:B:225:HIS:O	1:B:228:THR:OG1	2.36	0.40
1:D:35:THR:HA	1:D:36:PRO:HD3	1.85	0.40
1:D:93:GLN:O	1:D:156:ILE:HA	2.21	0.40
1:B:47:TYR:OH	1:B:116:GLU:OE2	2.21	0.40
1:B:110:ALA:HA	1:B:160:GLY:O	2.22	0.40
1:B:120:ALA:CA	1:B:149:ASN:HB3	2.51	0.40
1:C:216:ARG:NH2	1:C:216:ARG:CG	2.82	0.40
1:C:327:ASP:O	1:C:328:ARG:C	2.64	0.40
1:A:134:GLY:C	1:A:217:TYR:HB2	2.46	0.40
1:A:234:ASP:CG	1:A:341:ARG:HH22	2.30	0.40
1:B:75:ASN:HD21	1:B:82:SER:N	2.18	0.40
1:C:137:ILE:C	1:C:138:LEU:HD12	2.47	0.40
1:C:163:LEU:CB	1:C:164:PRO:CD	3.00	0.40

All (2) 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:D:35:THR:N	3:D:1122:HOH:O[1_455]	1.91	0.29
1:D:33:PRO:CB	3:D:1136:HOH:O[1_455]	1.98	0.22

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	283/354 (80%)	257 (91%)	13 (5%)	13 (5%)	2	1
1	B	278/354 (78%)	248 (89%)	15 (5%)	15 (5%)	1	1
1	C	283/354 (80%)	251 (89%)	25 (9%)	7 (2%)	4	4
1	D	281/354 (79%)	249 (89%)	16 (6%)	16 (6%)	1	0
All	All	1125/1416 (79%)	1005 (89%)	69 (6%)	51 (4%)	2	1

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	50	ILE
1	A	77	ALA
1	A	141	GLN
1	A	182	GLN
1	B	38	ALA
1	B	49	GLU
1	B	77	ALA
1	B	209	SER
1	B	265	LYS
1	B	295	THR
1	C	38	ALA
1	C	184	VAL
1	D	50	ILE
1	D	77	ALA
1	D	186	ARG
1	D	210	SER
1	A	292	GLY
1	B	184	VAL
1	B	204	HIS
1	B	205	GLN
1	B	292	GLY

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Mol	Chain	Res	Type
1	C	76	PRO
1	D	40	CYS
1	D	47	TYR
1	D	205	GLN
1	D	292	GLY
1	A	76	PRO
1	A	79	ARG
1	B	50	ILE
1	B	79	ARG
1	B	319	ASP
1	C	292	GLY
1	D	38	ALA
1	D	185	THR
1	D	293	ASN
1	D	319	ASP
1	A	36	PRO
1	A	41	ALA
1	A	52	PRO
1	A	153	GLU
1	B	153	GLU
1	B	177	TYR
1	C	46	ASN
1	C	153	GLU
1	D	76	PRO
1	D	184	VAL
1	C	97	PRO
1	D	35	THR
1	D	204	HIS
1	A	318	GLN

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	232/293 (79%)	207 (89%)	25 (11%)	6	9
1	B	227/293 (78%)	198 (87%)	29 (13%)	4	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	232/293 (79%)	204 (88%)	28 (12%)	5	6
1	D	230/293 (78%)	201 (87%)	29 (13%)	4	6
All	All	921/1172 (79%)	810 (88%)	111 (12%)	5	6

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	51	ARG
1	A	53	LEU
1	A	72	VAL
1	A	73	LEU
1	A	74	GLU
1	A	75	ASN
1	A	89	TYR
1	A	92	LEU
1	A	104	HIS
1	A	107	ASN
1	A	122	THR
1	A	141	GLN
1	A	150	PRO
1	A	166	VAL
1	A	200	LEU
1	A	241	MSE
1	A	260	LEU
1	A	283	VAL
1	A	286	SER
1	A	316	THR
1	A	317	THR
1	A	322	LEU
1	A	330	VAL
1	A	338	ARG
1	B	71	LEU
1	B	72	VAL
1	B	73	LEU
1	B	74	GLU
1	B	75	ASN
1	B	81	GLN
1	B	85	THR
1	B	89	TYR
1	B	107	ASN

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Mol	Chain	Res	Type
1	B	108	GLN
1	B	112	ARG
1	B	125	ASP
1	B	149	ASN
1	B	152	ASP
1	B	161	LEU
1	B	176	ASP
1	B	184	VAL
1	B	200	LEU
1	B	208	ASN
1	B	221	ARG
1	B	235	GLU
1	B	265	LYS
1	B	283	VAL
1	B	288	GLN
1	B	293	ASN
1	B	319	ASP
1	B	322	LEU
1	B	338	ARG
1	B	341	ARG
1	C	37	ASN
1	C	39	ASN
1	C	49	GLU
1	C	73	LEU
1	C	75	ASN
1	C	88	LEU
1	C	92	LEU
1	C	106	HIS
1	C	129	THR
1	C	138	LEU
1	C	146	ASP
1	C	153	GLU
1	C	158	LEU
1	C	161	LEU
1	C	176	ASP
1	C	179	GLU
1	C	200	LEU
1	C	205	GLN
1	C	208	ASN
1	C	214	ASN
1	C	227	LEU
1	C	230	LEU

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Mol	Chain	Res	Type
1	C	283	VAL
1	C	289	VAL
1	C	305	VAL
1	C	317	THR
1	C	322	LEU
1	C	330	VAL
1	D	34	LYS
1	D	40	CYS
1	D	48	GLN
1	D	49	GLU
1	D	71	LEU
1	D	73	LEU
1	D	75	ASN
1	D	85	THR
1	D	92	LEU
1	D	116	GLU
1	D	118	LYS
1	D	141	GLN
1	D	149	ASN
1	D	150	PRO
1	D	152	ASP
1	D	158	LEU
1	D	161	LEU
1	D	167	ASN
1	D	200	LEU
1	D	221	ARG
1	D	230	LEU
1	D	237	ASP
1	D	283	VAL
1	D	294	GLU
1	D	295	THR
1	D	297	SER
1	D	309	TRP
1	D	313	SER
1	D	322	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	107	ASN
1	A	132	ASN

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Mol	Chain	Res	Type
1	A	147	HIS
1	A	198	ASN
1	A	214	ASN
1	A	281	HIS
1	A	310	HIS
1	A	315	GLN
1	A	318	GLN
1	B	37	ASN
1	B	46	ASN
1	B	75	ASN
1	B	93	GLN
1	B	104	HIS
1	B	107	ASN
1	B	108	GLN
1	B	141	GLN
1	B	147	HIS
1	B	149	ASN
1	B	205	GLN
1	B	288	GLN
1	B	310	HIS
1	C	37	ASN
1	C	46	ASN
1	C	107	ASN
1	C	147	HIS
1	C	167	ASN
1	C	205	GLN
1	C	208	ASN
1	C	281	HIS
1	C	310	HIS
1	C	315	GLN
1	C	318	GLN
1	C	331	GLN
1	D	75	ASN
1	D	149	ASN
1	D	208	ASN
1	D	214	ASN
1	D	281	HIS
1	D	293	ASN
1	D	310	HIS
1	D	315	GLN
1	D	331	GLN

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	283/354 (79%)	-0.42	0 100 100	13, 26, 47, 55	0
1	B	278/354 (78%)	-0.33	4 (1%) 73 70	15, 27, 51, 64	0
1	C	283/354 (79%)	-0.28	5 (1%) 67 64	17, 28, 50, 66	0
1	D	281/354 (79%)	-0.35	5 (1%) 67 64	14, 26, 49, 65	0
All	All	1125/1416 (79%)	-0.34	14 (1%) 76 74	13, 27, 49, 66	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	ILE	4.5
1	C	50	ILE	3.9
1	B	208	ASN	3.2
1	D	342	TYR	3.2
1	D	207	GLY	2.8
1	B	38	ALA	2.7
1	C	38	ALA	2.6
1	B	178	PRO	2.6
1	C	71	LEU	2.5
1	C	51	ARG	2.3
1	C	76	PRO	2.3
1	D	185	THR	2.2
1	D	39	ASN	2.0
1	B	177	TYR	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	B	1002	1/1	0.99	0.08	26,26,26,26	0
2	FE	D	1004	1/1	0.99	0.05	31,31,31,31	0
2	FE	C	1003	1/1	1.00	0.05	31,31,31,31	0
2	FE	A	1001	1/1	1.00	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.