



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:25 AM UTC

PDB ID : 5FSW / pdb_00005fsw
Title : RNA dependent RNA polymerase QDE-1 from Thielavia terrestris
Authors : Qian, X.; Hamid, F.M.; El Sahili, A.; Darwis, D.A.; Wong, Y.H.; Bhushan, S.;
Makeyev, E.V.; Lescar, J.
Deposited on : 2016-01-08
Resolution : 3.19 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

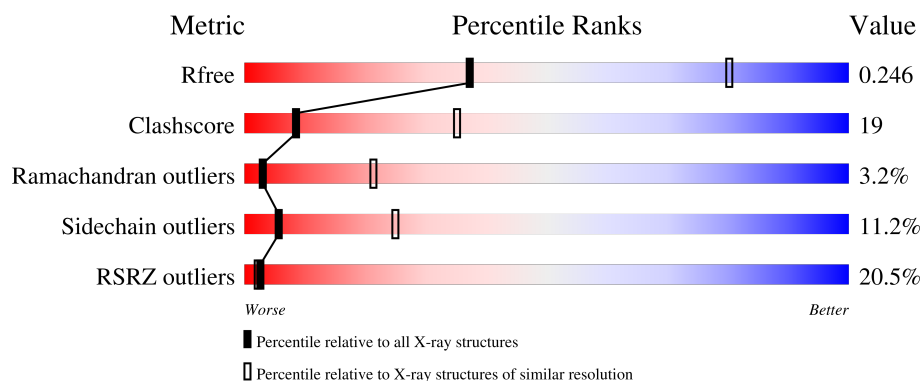
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	1034	6% 45% 34% 9% 11%
1	B	1034	13% 55% 29% 5% 11%
1	C	1034	25% 61% 23% 5% 11%
1	D	1034	29% 58% 26% 5% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28130 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 RNA DEPENDENT RNA POLYMERASE QDE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	0	0
			7358	4679	1307	1335	37			
1	B	922	Total	C	N	O	S	0	0	0
			6924	4462	1186	1244	32			
1	C	922	Total	C	N	O	S	0	0	0
			6924	4462	1186	1244	32			
1	D	922	Total	C	N	O	S	0	0	0
			6924	4462	1186	1244	32			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP G2R911
A	2	GLY	-	expression tag	UNP G2R911
A	3	HIS	-	expression tag	UNP G2R911
A	4	HIS	-	expression tag	UNP G2R911
A	5	HIS	-	expression tag	UNP G2R911
A	6	HIS	-	expression tag	UNP G2R911
A	7	HIS	-	expression tag	UNP G2R911
A	8	HIS	-	expression tag	UNP G2R911
A	9	SER	-	expression tag	UNP G2R911
A	10	SER	-	expression tag	UNP G2R911
A	11	GLY	-	expression tag	UNP G2R911
A	12	VAL	-	expression tag	UNP G2R911
A	13	ASP	-	expression tag	UNP G2R911
A	14	LEU	-	expression tag	UNP G2R911
A	15	GLY	-	expression tag	UNP G2R911
A	16	THR	-	expression tag	UNP G2R911
A	17	GLU	-	expression tag	UNP G2R911
A	18	ASN	-	expression tag	UNP G2R911
A	19	LEU	-	expression tag	UNP G2R911
A	20	TYR	-	expression tag	UNP G2R911
A	21	PHE	-	expression tag	UNP G2R911

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLN	-	expression tag	UNP G2R911
A	23	SER	-	expression tag	UNP G2R911
A	24	MET	-	expression tag	UNP G2R911
B	1	MET	-	expression tag	UNP G2R911
B	2	GLY	-	expression tag	UNP G2R911
B	3	HIS	-	expression tag	UNP G2R911
B	4	HIS	-	expression tag	UNP G2R911
B	5	HIS	-	expression tag	UNP G2R911
B	6	HIS	-	expression tag	UNP G2R911
B	7	HIS	-	expression tag	UNP G2R911
B	8	HIS	-	expression tag	UNP G2R911
B	9	SER	-	expression tag	UNP G2R911
B	10	SER	-	expression tag	UNP G2R911
B	11	GLY	-	expression tag	UNP G2R911
B	12	VAL	-	expression tag	UNP G2R911
B	13	ASP	-	expression tag	UNP G2R911
B	14	LEU	-	expression tag	UNP G2R911
B	15	GLY	-	expression tag	UNP G2R911
B	16	THR	-	expression tag	UNP G2R911
B	17	GLU	-	expression tag	UNP G2R911
B	18	ASN	-	expression tag	UNP G2R911
B	19	LEU	-	expression tag	UNP G2R911
B	20	TYR	-	expression tag	UNP G2R911
B	21	PHE	-	expression tag	UNP G2R911
B	22	GLN	-	expression tag	UNP G2R911
B	23	SER	-	expression tag	UNP G2R911
B	24	MET	-	expression tag	UNP G2R911
C	1	MET	-	expression tag	UNP G2R911
C	2	GLY	-	expression tag	UNP G2R911
C	3	HIS	-	expression tag	UNP G2R911
C	4	HIS	-	expression tag	UNP G2R911
C	5	HIS	-	expression tag	UNP G2R911
C	6	HIS	-	expression tag	UNP G2R911
C	7	HIS	-	expression tag	UNP G2R911
C	8	HIS	-	expression tag	UNP G2R911
C	9	SER	-	expression tag	UNP G2R911
C	10	SER	-	expression tag	UNP G2R911
C	11	GLY	-	expression tag	UNP G2R911
C	12	VAL	-	expression tag	UNP G2R911
C	13	ASP	-	expression tag	UNP G2R911
C	14	LEU	-	expression tag	UNP G2R911
C	15	GLY	-	expression tag	UNP G2R911

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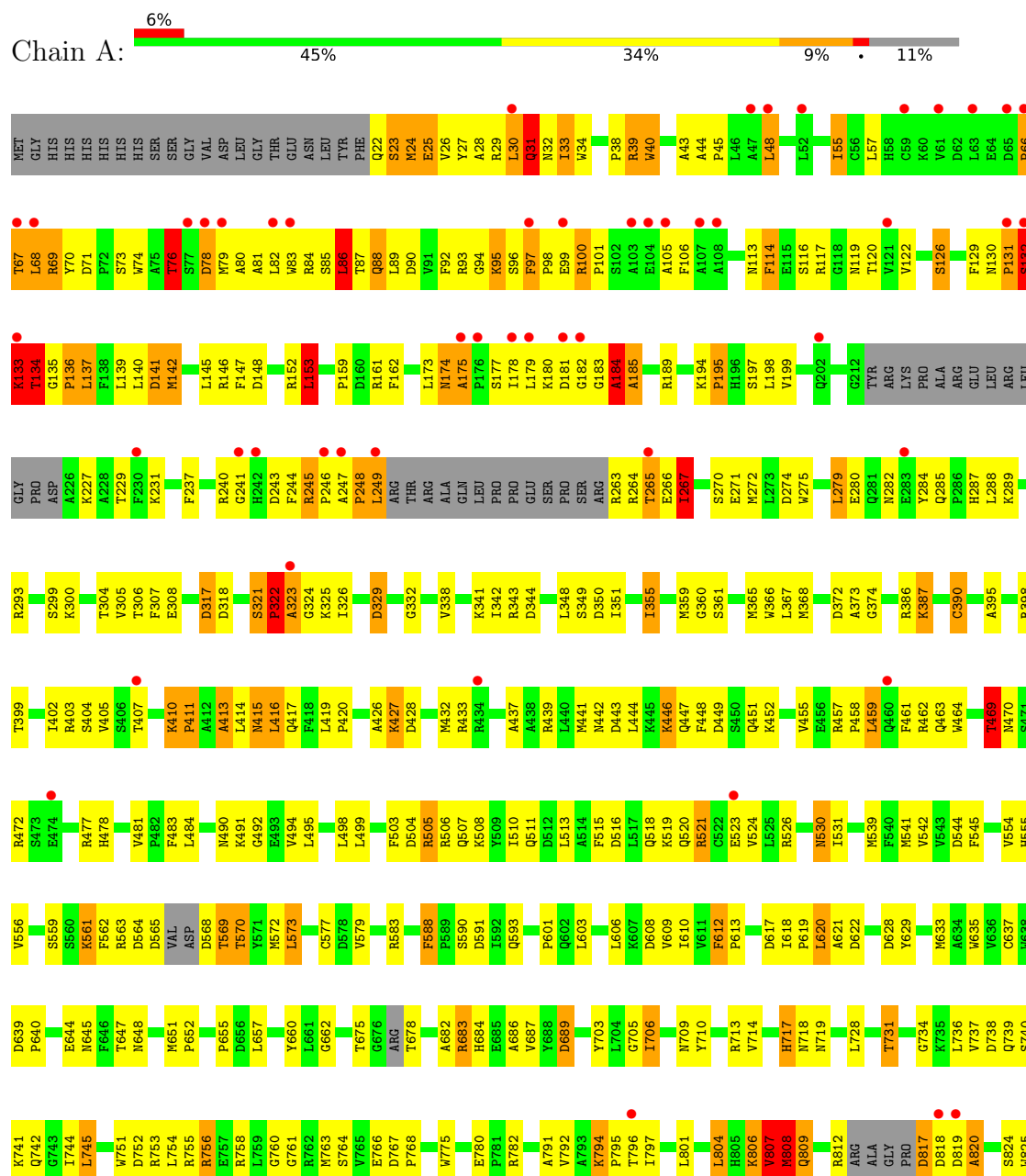
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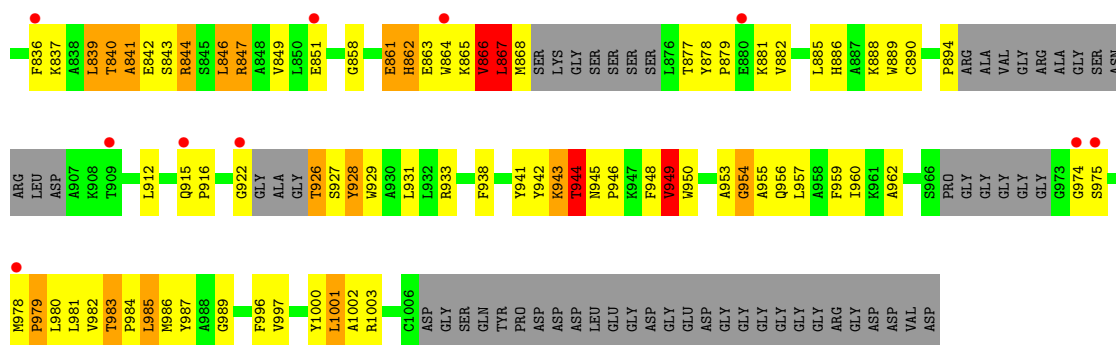
Chain	Residue	Modelled	Actual	Comment	Reference
C	16	THR	-	expression tag	UNP G2R911
C	17	GLU	-	expression tag	UNP G2R911
C	18	ASN	-	expression tag	UNP G2R911
C	19	LEU	-	expression tag	UNP G2R911
C	20	TYR	-	expression tag	UNP G2R911
C	21	PHE	-	expression tag	UNP G2R911
C	22	GLN	-	expression tag	UNP G2R911
C	23	SER	-	expression tag	UNP G2R911
C	24	MET	-	expression tag	UNP G2R911
D	1	MET	-	expression tag	UNP G2R911
D	2	GLY	-	expression tag	UNP G2R911
D	3	HIS	-	expression tag	UNP G2R911
D	4	HIS	-	expression tag	UNP G2R911
D	5	HIS	-	expression tag	UNP G2R911
D	6	HIS	-	expression tag	UNP G2R911
D	7	HIS	-	expression tag	UNP G2R911
D	8	HIS	-	expression tag	UNP G2R911
D	9	SER	-	expression tag	UNP G2R911
D	10	SER	-	expression tag	UNP G2R911
D	11	GLY	-	expression tag	UNP G2R911
D	12	VAL	-	expression tag	UNP G2R911
D	13	ASP	-	expression tag	UNP G2R911
D	14	LEU	-	expression tag	UNP G2R911
D	15	GLY	-	expression tag	UNP G2R911
D	16	THR	-	expression tag	UNP G2R911
D	17	GLU	-	expression tag	UNP G2R911
D	18	ASN	-	expression tag	UNP G2R911
D	19	LEU	-	expression tag	UNP G2R911
D	20	TYR	-	expression tag	UNP G2R911
D	21	PHE	-	expression tag	UNP G2R911
D	22	GLN	-	expression tag	UNP G2R911
D	23	SER	-	expression tag	UNP G2R911
D	24	MET	-	expression tag	UNP G2R911

3 Residue-property plots

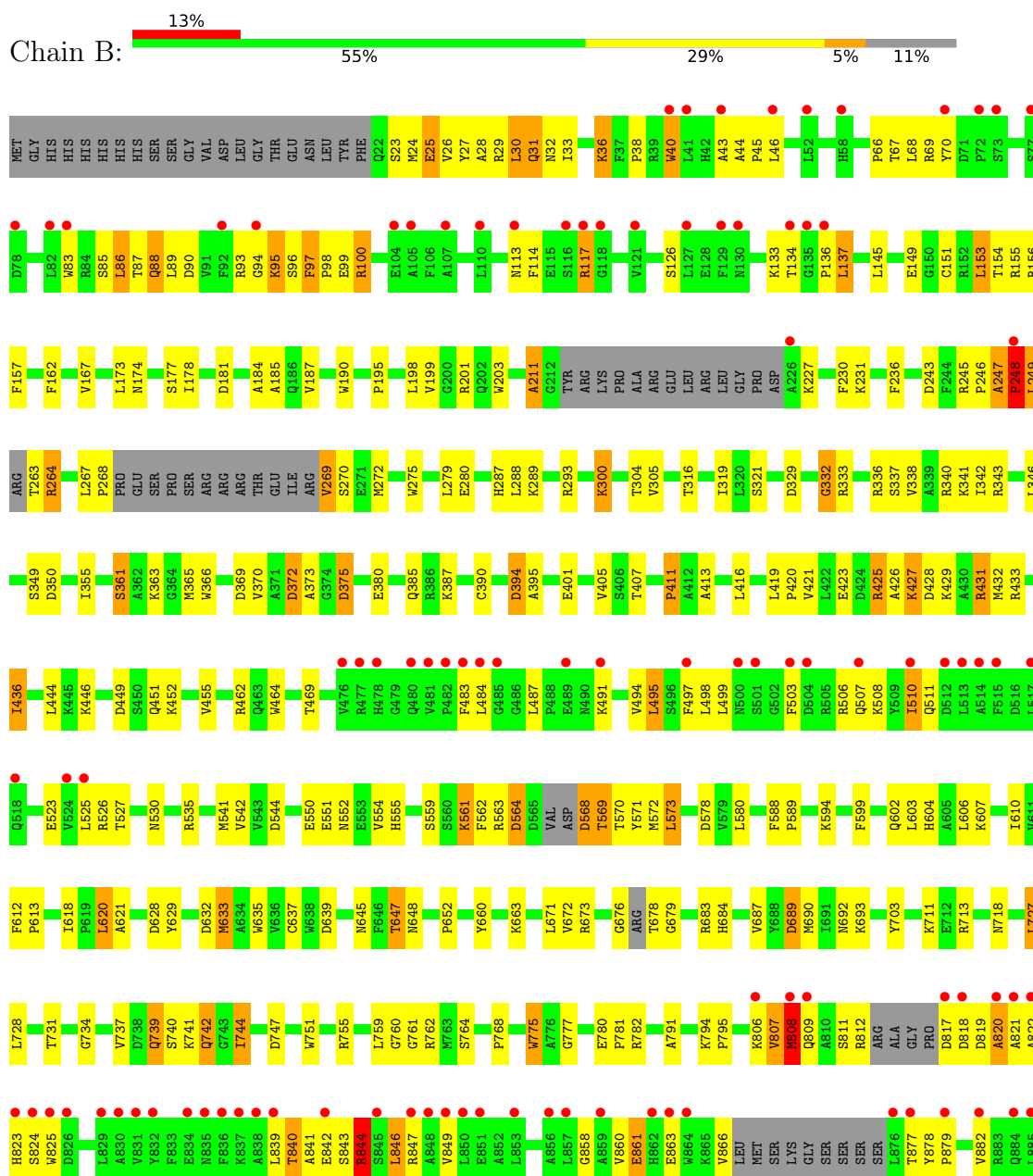
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

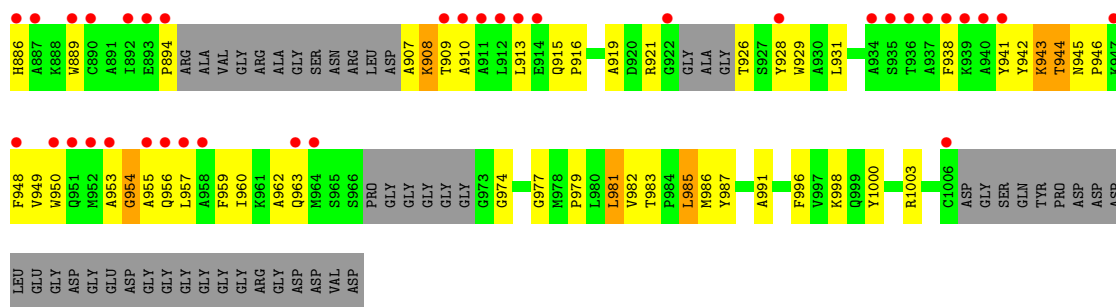
• Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1



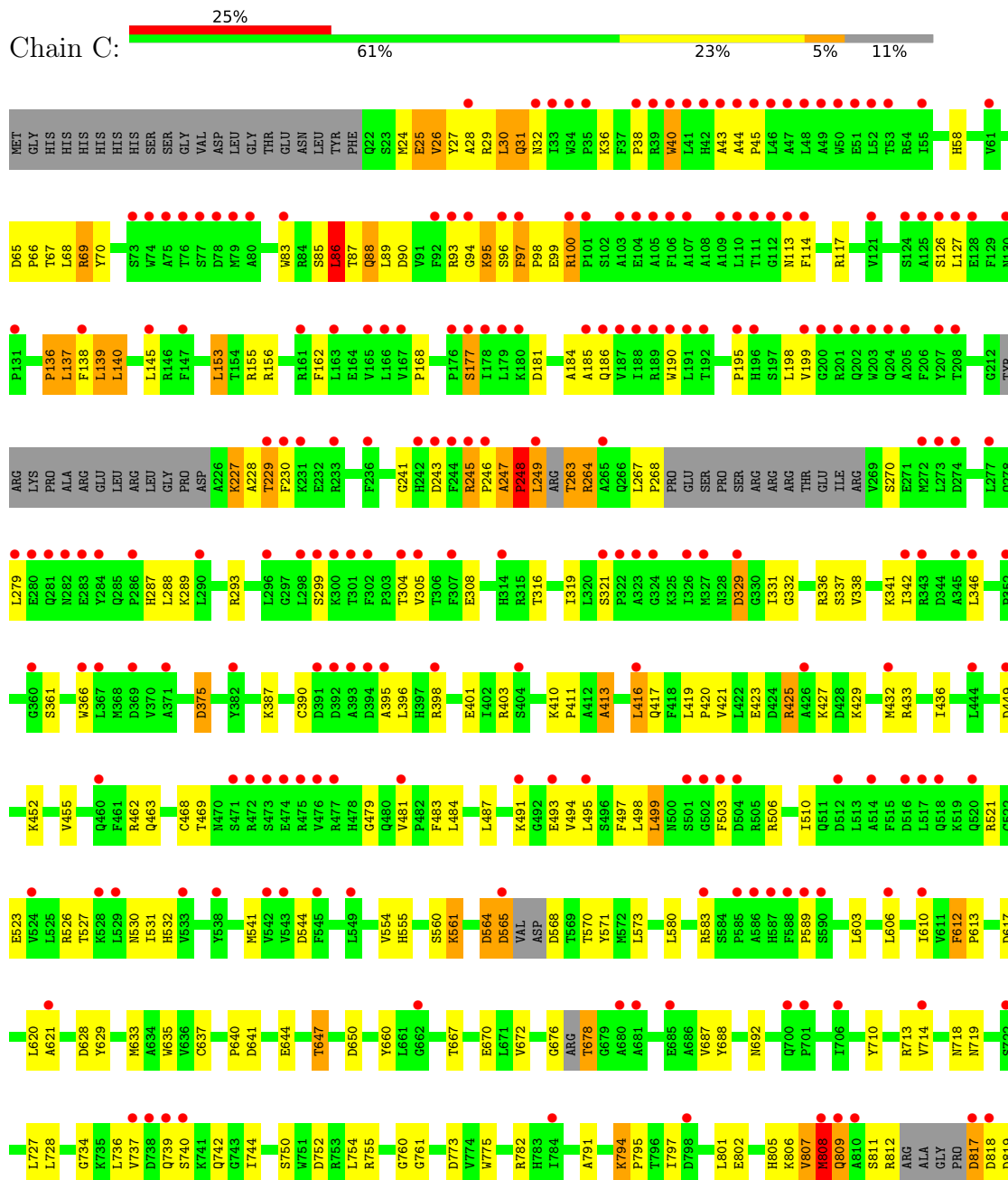


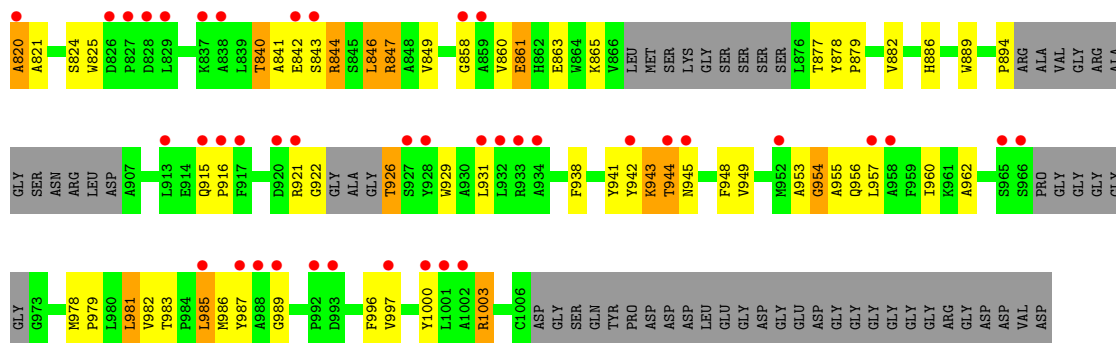
- Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1



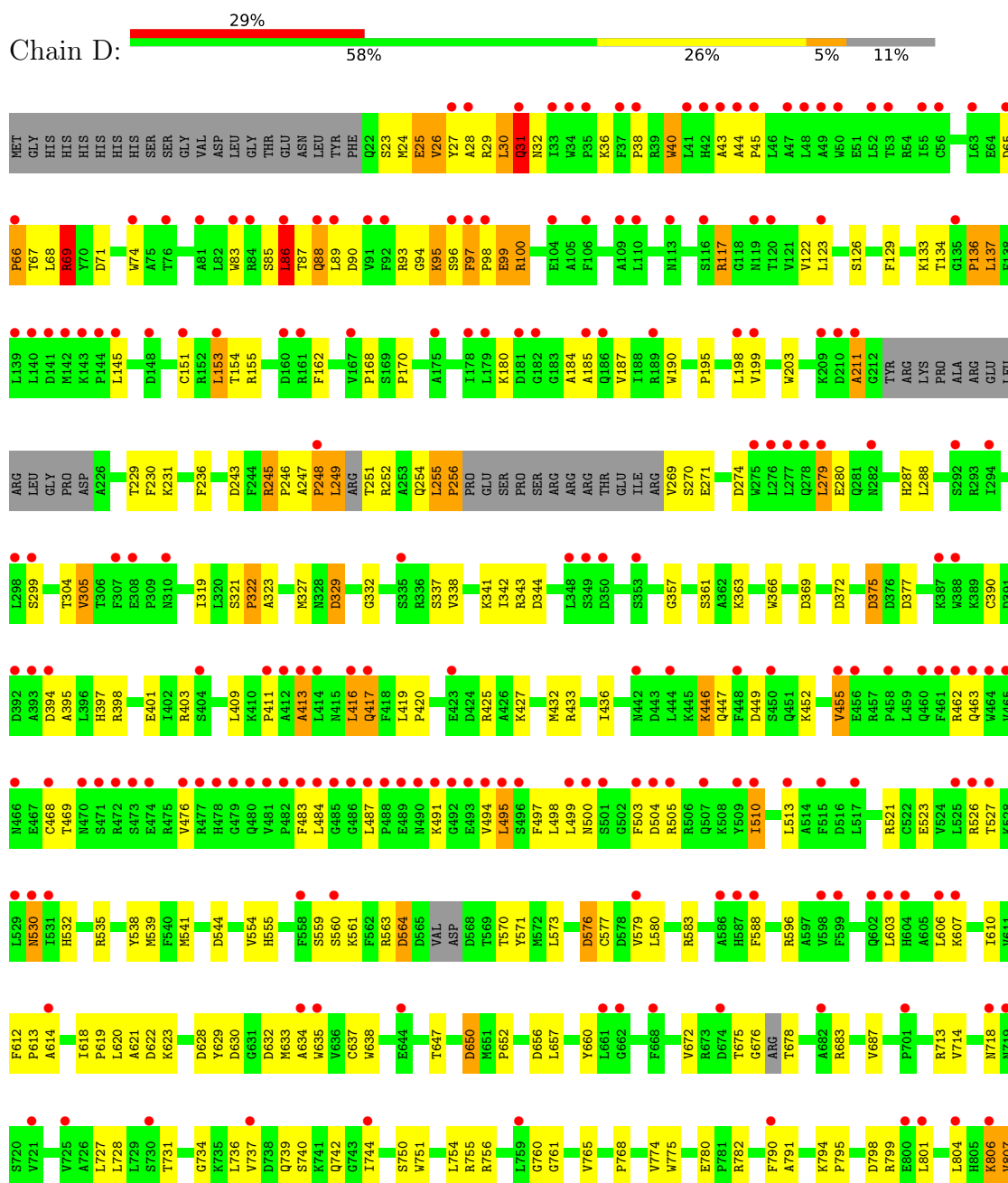


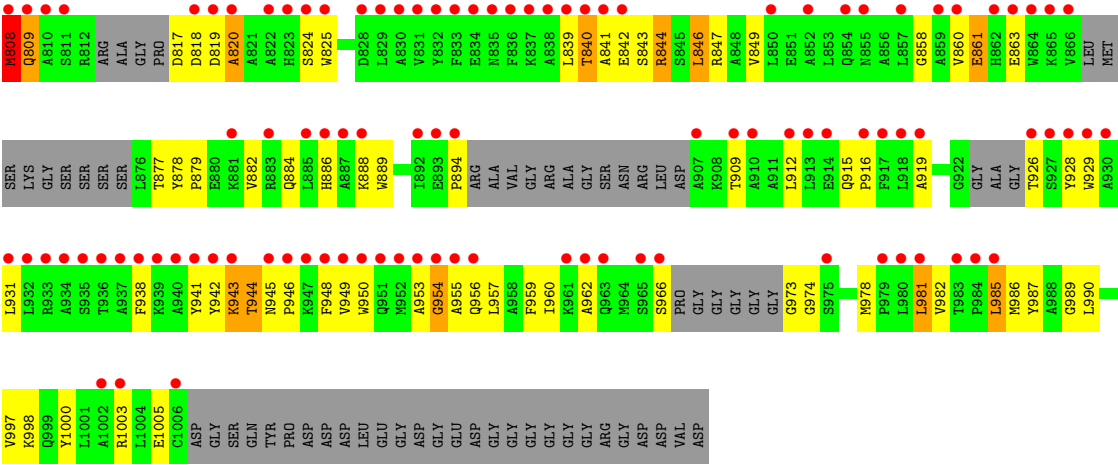
● Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1





• Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.23Å 165.95Å 173.89Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	48.91 – 3.19 48.91 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-3.19) 99.7 (48.91-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	22.98 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.213 , 0.251 0.209 , 0.246	Depositor DCC
R_{free} test set	3829 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k 0.009 for -h,-l,-k 0.052 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	28130	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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	1.21	28/7528 (0.4%)	1.34	64/10177 (0.6%)
1	B	1.11	11/7063 (0.2%)	1.25	46/9494 (0.5%)
1	C	0.79	1/7063 (0.0%)	1.16	35/9494 (0.4%)
1	D	0.77	0/7062	1.13	37/9491 (0.4%)
All	All	0.99	40/28716 (0.1%)	1.22	182/38656 (0.5%)

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	8
1	B	0	1
1	D	0	1
All	All	0	10

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	866	VAL	C-O	-8.61	1.14	1.24
1	A	504	ASP	CA-C	8.01	1.61	1.53
1	A	505	ARG	N-CA	7.66	1.56	1.46
1	A	321	SER	CA-C	-7.16	1.45	1.53
1	A	279	LEU	CA-C	7.11	1.62	1.52
1	A	68	LEU	N-CA	6.71	1.54	1.45
1	A	411	PRO	CA-C	-6.56	1.44	1.52
1	A	619	PRO	N-CA	-6.53	1.39	1.47
1	A	570	THR	CA-C	6.51	1.60	1.52
1	B	332	GLY	C-O	-6.46	1.16	1.24
1	A	601	PRO	C-O	-6.39	1.16	1.24
1	B	594	LYS	CA-C	6.32	1.61	1.52
1	C	410	LYS	C-O	6.23	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	ALA	CA-C	6.16	1.65	1.52
1	A	428	ASP	N-CA	6.11	1.53	1.46
1	A	365	MET	CA-C	-5.96	1.45	1.52
1	B	361	SER	CA-C	-5.88	1.44	1.52
1	A	414	LEU	N-CA	-5.86	1.39	1.46
1	A	132	SER	N-CA	5.79	1.53	1.46
1	A	153	LEU	CA-C	-5.73	1.45	1.52
1	B	684	HIS	N-CA	5.61	1.53	1.46
1	A	390	CYS	CA-C	-5.58	1.46	1.52
1	B	739	GLN	N-CA	5.51	1.52	1.46
1	A	329	ASP	CA-C	5.50	1.60	1.52
1	A	133	LYS	N-CA	5.48	1.56	1.46
1	A	731	THR	C-O	-5.45	1.17	1.24
1	A	324	GLY	N-CA	5.39	1.53	1.45
1	B	542	VAL	N-CA	-5.37	1.39	1.46
1	A	131	PRO	CA-C	5.34	1.59	1.52
1	B	552	ASN	N-CA	5.30	1.52	1.46
1	A	612	PHE	N-CA	5.26	1.53	1.45
1	A	579	VAL	C-O	-5.26	1.18	1.24
1	B	542	VAL	CA-C	-5.18	1.46	1.52
1	B	563	ARG	CA-C	-5.17	1.46	1.52
1	A	570	THR	CA-CB	5.15	1.63	1.53
1	A	593	GLN	C-O	-5.07	1.18	1.24
1	A	323	ALA	N-CA	5.05	1.55	1.46
1	B	604	HIS	CA-CB	5.05	1.61	1.53
1	A	556	VAL	C-O	-5.03	1.18	1.24
1	B	618	ILE	CA-CB	5.00	1.60	1.54

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	SER	CA-C-N	-19.83	95.06	119.84
1	A	321	SER	C-N-CA	-19.83	95.06	119.84
1	C	410	LYS	CA-C-N	14.13	135.04	119.93
1	C	410	LYS	C-N-CA	14.13	135.04	119.93
1	D	255	LEU	CA-C-N	12.71	135.73	119.84
1	D	255	LEU	C-N-CA	12.71	135.73	119.84
1	A	410	LYS	CA-C-N	9.95	130.01	119.76
1	A	410	LYS	C-N-CA	9.95	130.01	119.76
1	C	247	ALA	CA-C-N	9.76	132.04	119.84
1	C	247	ALA	C-N-CA	9.76	132.04	119.84
1	C	65	ASP	CA-C-N	9.03	131.13	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	ASP	C-N-CA	9.03	131.13	119.84
1	B	915	GLN	CA-C-N	8.98	131.06	119.84
1	B	915	GLN	C-N-CA	8.98	131.06	119.84
1	B	247	ALA	CA-C-N	8.82	130.86	119.84
1	B	247	ALA	C-N-CA	8.82	130.86	119.84
1	D	279	LEU	N-CA-C	8.79	122.01	111.82
1	C	331	ILE	CB-CA-C	-8.63	97.54	110.82
1	D	65	ASP	CA-C-N	8.42	130.36	119.84
1	D	65	ASP	C-N-CA	8.42	130.36	119.84
1	D	245	ARG	CA-C-N	8.40	128.84	120.52
1	D	245	ARG	C-N-CA	8.40	128.84	120.52
1	C	915	GLN	CA-C-N	8.26	130.16	119.84
1	C	915	GLN	C-N-CA	8.26	130.16	119.84
1	C	229	THR	N-CA-C	-7.94	98.57	110.24
1	B	744	ILE	CB-CA-C	-7.83	100.22	111.34
1	D	915	GLN	CA-C-N	7.77	129.55	119.84
1	D	915	GLN	C-N-CA	7.77	129.55	119.84
1	A	943	LYS	CA-C-N	7.71	135.57	121.70
1	A	943	LYS	C-N-CA	7.71	135.57	121.70
1	A	506	ARG	N-CA-C	-7.62	104.22	113.97
1	A	279	LEU	N-CA-C	7.61	121.81	112.23
1	C	612	PHE	CA-C-N	-7.49	112.61	120.03
1	C	612	PHE	C-N-CA	-7.49	112.61	120.03
1	A	386	ARG	N-CA-C	7.23	119.88	108.67
1	B	718	ASN	N-CA-C	7.20	121.16	112.38
1	B	300	LYS	CA-CB-CG	7.05	128.20	114.10
1	B	375	ASP	N-CA-C	-7.02	103.28	112.41
1	A	846	LEU	N-CA-C	7.00	124.54	114.39
1	A	531	ILE	CB-CA-C	-6.76	104.64	111.80
1	A	569	THR	N-CA-C	6.74	120.49	109.85
1	B	569	THR	N-CA-C	6.72	120.11	108.76
1	A	25	GLU	CA-C-N	6.66	133.69	121.70
1	A	25	GLU	C-N-CA	6.66	133.69	121.70
1	A	806	LYS	CA-C-N	6.62	133.61	121.70
1	A	806	LYS	C-N-CA	6.62	133.61	121.70
1	C	279	LEU	N-CA-C	6.60	120.55	112.23
1	A	322	PRO	CA-C-N	6.59	133.57	121.70
1	A	322	PRO	C-N-CA	6.59	133.57	121.70
1	A	504	ASP	N-CA-C	6.53	117.08	108.07
1	C	25	GLU	CA-C-N	6.51	133.42	121.70
1	C	25	GLU	C-N-CA	6.51	133.42	121.70
1	A	55	ILE	CB-CA-C	-6.51	103.64	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	LYS	N-CA-C	6.51	121.22	113.28
1	B	762	ARG	N-CA-C	-6.32	104.30	111.07
1	B	321	SER	N-CA-C	6.29	118.75	109.50
1	B	921	ARG	N-CA-C	6.28	118.92	111.33
1	B	602	GLN	N-CA-C	6.24	119.74	111.75
1	A	928	TYR	N-CA-C	6.20	119.31	111.69
1	A	469	THR	N-CA-C	6.18	116.24	108.45
1	B	578	ASP	N-CA-C	6.13	119.12	110.23
1	B	33	ILE	N-CA-C	-6.12	106.55	111.81
1	A	184	ALA	CA-C-N	6.11	132.69	121.70
1	A	184	ALA	C-N-CA	6.11	132.69	121.70
1	B	280	GLU	N-CA-C	-6.11	104.55	111.14
1	C	177	SER	CB-CA-C	-6.10	100.67	110.79
1	D	943	LYS	CA-C-N	6.09	132.66	121.70
1	D	943	LYS	C-N-CA	6.09	132.66	121.70
1	D	1005	GLU	N-CA-C	6.09	120.55	113.18
1	B	167	VAL	N-CA-C	6.05	114.81	107.61
1	B	943	LYS	CA-C-N	6.04	132.58	121.70
1	B	943	LYS	C-N-CA	6.04	132.58	121.70
1	B	672	VAL	N-CA-C	-6.04	104.85	110.53
1	D	305	VAL	N-CA-C	6.03	116.80	108.12
1	A	132	SER	CA-C-N	6.03	132.54	121.70
1	A	132	SER	C-N-CA	6.03	132.54	121.70
1	C	846	LEU	N-CA-C	5.99	123.38	114.09
1	A	618	ILE	CB-CA-C	-5.98	104.33	110.13
1	C	943	LYS	CA-C-N	5.98	132.46	121.70
1	C	943	LYS	C-N-CA	5.98	132.46	121.70
1	D	25	GLU	CA-C-N	5.96	132.44	121.70
1	D	25	GLU	C-N-CA	5.96	132.44	121.70
1	A	846	LEU	CA-C-N	5.96	132.43	121.70
1	A	846	LEU	C-N-CA	5.96	132.43	121.70
1	B	919	ALA	N-CA-C	5.95	117.57	111.14
1	B	372	ASP	N-CA-C	-5.92	99.15	108.63
1	B	571	TYR	CA-CB-CG	5.90	124.51	113.90
1	B	542	VAL	N-CA-C	-5.89	99.80	108.99
1	A	648	ASN	N-CA-C	5.83	118.47	110.24
1	B	679	GLY	N-CA-C	5.83	118.84	111.85
1	A	33	ILE	N-CA-C	-5.81	107.19	111.90
1	A	689	ASP	CB-CA-C	-5.79	101.72	110.92
1	A	775	TRP	N-CA-C	5.78	118.96	109.76
1	D	808	MET	CA-C-N	5.77	132.09	121.70
1	D	808	MET	C-N-CA	5.77	132.09	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	959	PHE	N-CA-C	-5.76	103.99	111.02
1	B	808	MET	CA-C-N	5.75	132.05	121.70
1	B	808	MET	C-N-CA	5.75	132.05	121.70
1	B	373	ALA	N-CA-C	-5.73	105.01	112.23
1	A	979	PRO	CB-CA-C	-5.72	107.06	111.87
1	A	683	ARG	N-CA-C	5.71	117.50	111.28
1	B	370	VAL	N-CA-C	-5.70	104.32	112.35
1	C	808	MET	CA-C-N	5.69	131.95	121.70
1	C	808	MET	C-N-CA	5.69	131.95	121.70
1	A	808	MET	CA-C-N	5.69	131.95	121.70
1	A	808	MET	C-N-CA	5.69	131.95	121.70
1	B	991	ALA	CA-C-N	5.69	125.62	119.76
1	B	991	ALA	C-N-CA	5.69	125.62	119.76
1	B	93	ARG	N-CA-C	5.67	117.97	107.60
1	C	531	ILE	CB-CA-C	-5.62	105.84	111.80
1	D	229	THR	N-CA-C	5.62	118.12	109.07
1	C	25	GLU	N-CA-C	5.62	121.00	114.04
1	A	231	LYS	N-CA-C	5.61	118.21	109.52
1	B	711	LYS	N-CA-C	5.60	117.46	111.36
1	A	949	VAL	CB-CA-C	-5.58	104.51	112.22
1	A	308	GLU	N-CA-C	-5.57	102.61	110.29
1	D	271	GLU	CB-CG-CD	5.56	122.05	112.60
1	C	773	ASP	CB-CA-C	5.55	120.25	110.37
1	C	241	GLY	N-CA-C	5.54	118.83	110.75
1	B	846	LEU	N-CA-C	5.49	122.57	113.89
1	D	357	GLY	N-CA-C	5.47	117.97	110.69
1	A	244	PHE	N-CA-C	5.46	118.62	109.95
1	A	839	LEU	CA-C-N	5.44	131.50	121.70
1	A	839	LEU	C-N-CA	5.44	131.50	121.70
1	D	919	ALA	N-CA-C	5.42	116.99	111.14
1	A	76	THR	N-CA-C	5.40	121.27	114.31
1	B	25	GLU	N-CA-C	5.38	121.39	114.56
1	C	487	LEU	CA-C-N	5.35	125.35	119.89
1	C	487	LEU	C-N-CA	5.35	125.35	119.89
1	D	978	MET	N-CA-C	5.35	116.41	109.72
1	B	561	LYS	N-CA-C	5.34	122.17	110.80
1	A	265	THR	CB-CA-C	-5.33	100.51	109.83
1	A	153	LEU	N-CA-C	-5.31	104.92	111.40
1	D	614	ALA	N-CA-C	-5.28	106.61	113.16
1	A	355	ILE	CG1-CB-CG2	-5.28	94.86	110.70
1	D	846	LEU	N-CA-C	5.28	122.23	113.89
1	A	944	THR	N-CA-CB	5.26	120.44	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	GLU	CA-C-N	5.25	131.15	121.70
1	B	25	GLU	C-N-CA	5.25	131.15	121.70
1	C	227	LYS	N-CA-C	-5.25	102.52	110.28
1	D	99	GLU	CB-CG-CD	5.22	121.48	112.60
1	A	959	PHE	CB-CA-C	-5.22	102.62	110.92
1	B	632	ASP	CB-CG-OD2	-5.20	106.44	118.40
1	C	263	THR	CA-C-N	5.20	131.06	121.70
1	C	263	THR	C-N-CA	5.20	131.06	121.70
1	A	31	GLN	CA-C-N	5.20	131.05	121.70
1	A	31	GLN	C-N-CA	5.20	131.05	121.70
1	B	436	ILE	CB-CA-C	-5.19	105.05	112.22
1	A	132	SER	N-CA-C	5.19	121.86	110.80
1	A	944	THR	OG1-CB-CG2	-5.19	98.91	109.30
1	B	370	VAL	CB-CA-C	5.17	118.94	111.65
1	D	375	ASP	N-CA-C	-5.16	106.30	112.59
1	A	841	ALA	CA-C-N	5.16	130.98	121.70
1	A	841	ALA	C-N-CA	5.16	130.98	121.70
1	A	351	ILE	CB-CA-C	-5.16	105.32	110.89
1	B	279	LEU	N-CA-C	5.14	119.55	113.28
1	D	839	LEU	N-CA-C	5.14	119.30	112.72
1	D	86	LEU	CA-C-N	5.13	130.94	121.70
1	D	86	LEU	C-N-CA	5.13	130.94	121.70
1	A	86	LEU	CA-C-N	5.13	130.94	121.70
1	A	86	LEU	C-N-CA	5.13	130.94	121.70
1	B	385	GLN	CB-CA-C	-5.12	101.34	110.70
1	A	613	PRO	CB-CA-C	-5.11	103.55	110.60
1	A	588	PHE	CA-CB-CG	5.10	118.90	113.80
1	D	487	LEU	CA-C-N	5.10	125.09	119.89
1	D	487	LEU	C-N-CA	5.10	125.09	119.89
1	B	648	ASN	N-CA-C	5.08	116.85	110.24
1	D	25	GLU	N-CA-C	5.08	121.61	110.80
1	D	806	LYS	CA-C-N	5.07	130.83	121.70
1	D	806	LYS	C-N-CA	5.07	130.83	121.70
1	B	839	LEU	N-CA-C	5.05	119.18	112.72
1	C	713	ARG	CG-CD-NE	5.05	123.11	112.00
1	D	31	GLN	CA-C-N	5.05	130.79	121.70
1	D	31	GLN	C-N-CA	5.05	130.79	121.70
1	D	650	ASP	N-CA-C	5.04	116.34	109.18
1	C	805	HIS	N-CA-C	-5.04	100.08	110.80
1	C	86	LEU	CA-C-N	5.03	130.76	121.70
1	C	86	LEU	C-N-CA	5.03	130.76	121.70
1	C	140	LEU	N-CA-C	5.02	116.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	983	THR	CA-C-N	5.01	125.03	119.32
1	A	983	THR	C-N-CA	5.01	125.03	119.32
1	B	279	LEU	CB-CA-C	-5.00	100.11	109.72

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	SER	Peptide
1	A	174	ASN	Peptide
1	A	322	PRO	Peptide
1	A	373	ALA	Peptide
1	A	426	ALA	Peptide
1	A	68	LEU	Peptide
1	A	76	THR	Peptide
1	A	867	LEU	Peptide
1	B	568	ASP	Peptide
1	D	69	ARG	Peptide

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	7358	0	7279	462	0
1	B	6924	0	6423	230	0
1	C	6924	0	6423	193	0
1	D	6924	0	6422	214	0
All	All	28130	0	26547	1038	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1038) 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:A:321:SER:O	1:A:323:ALA:HA	1.24	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:LYS:HB2	1:A:944:THR:OG1	1.16	1.25
1:A:321:SER:O	1:A:323:ALA:CA	1.86	1.23
1:A:133:LYS:CA	1:A:135:GLY:H	1.56	1.17
1:A:355:ILE:CD1	1:A:405:VAL:HG12	1.75	1.16
1:A:86:LEU:HB3	1:A:87:THR:OG1	1.47	1.15
1:A:133:LYS:HA	1:A:135:GLY:N	1.63	1.13
1:A:80:ALA:O	1:A:84:ARG:HG3	1.50	1.09
1:C:986:MET:HE2	1:D:499:LEU:O	1.51	1.09
1:A:87:THR:HG22	1:A:92:PHE:HB3	1.13	1.07
1:A:280:GLU:OE2	1:A:683:ARG:HD3	1.54	1.06
1:B:511:GLN:NE2	1:B:808:MET:O	1.89	1.06
1:A:462:ARG:HD3	1:B:986:MET:HE1	1.36	1.05
1:A:819:ASP:HA	1:A:820:ALA:O	1.56	1.03
1:A:943:LYS:CB	1:A:944:THR:OG1	2.07	1.02
1:A:355:ILE:HD13	1:A:405:VAL:HG12	1.39	1.01
1:D:819:ASP:HA	1:D:820:ALA:O	1.62	1.00
1:B:943:LYS:HB2	1:B:944:THR:CB	1.92	0.99
1:A:280:GLU:OE2	1:A:683:ARG:CD	2.08	0.99
1:D:943:LYS:HB2	1:D:944:THR:CB	1.93	0.98
1:A:441:MET:HE2	1:A:792:VAL:HG13	1.46	0.97
1:B:819:ASP:HA	1:B:820:ALA:O	1.62	0.97
1:D:279:LEU:HB2	1:D:683:ARG:CZ	1.95	0.97
1:A:133:LYS:HA	1:A:135:GLY:H	0.80	0.97
1:C:943:LYS:HB2	1:C:944:THR:CB	1.93	0.96
1:A:321:SER:C	1:A:323:ALA:HA	1.90	0.95
1:C:819:ASP:HA	1:C:820:ALA:O	1.66	0.94
1:A:173:LEU:HD11	1:A:180:LYS:HG2	1.47	0.94
1:A:87:THR:HG22	1:A:92:PHE:CB	1.97	0.93
1:B:23:SER:CB	1:B:24:MET:HA	1.98	0.93
1:A:31:GLN:HB3	1:A:32:ASN:HB3	1.52	0.91
1:C:806:LYS:HB3	1:C:807:VAL:CB	2.02	0.89
1:B:87:THR:HA	1:B:88:GLN:O	1.73	0.89
1:D:846:LEU:H	1:D:847:ARG:CB	1.85	0.89
1:A:745:LEU:HD23	1:A:745:LEU:O	1.73	0.88
1:A:839:LEU:H	1:A:840:THR:HG22	1.35	0.88
1:A:843:SER:OG	1:A:847:ARG:HB2	1.72	0.88
1:C:846:LEU:H	1:C:847:ARG:CB	1.86	0.87
1:A:23:SER:OG	1:A:26:VAL:O	1.91	0.87
1:A:943:LYS:HB2	1:A:944:THR:CB	2.04	0.87
1:D:87:THR:HA	1:D:88:GLN:O	1.76	0.86
1:B:846:LEU:H	1:B:847:ARG:CB	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:SER:HB3	1:A:323:ALA:C	2.01	0.85
1:A:462:ARG:HD3	1:B:986:MET:CE	2.07	0.85
1:A:804:LEU:C	1:A:807:VAL:HG11	2.02	0.84
1:A:804:LEU:HA	1:A:807:VAL:HG11	1.60	0.84
1:C:87:THR:HA	1:C:88:GLN:O	1.78	0.83
1:A:804:LEU:CA	1:A:807:VAL:HG11	2.08	0.83
1:A:922:GLY:C	1:A:926:THR:N	2.37	0.82
1:D:23:SER:CB	1:D:24:MET:HA	2.10	0.82
1:A:979:PRO:O	1:B:959:PHE:CE1	2.33	0.82
1:A:703:TYR:HA	1:A:706:ILE:CG2	2.09	0.82
1:D:846:LEU:N	1:D:847:ARG:CB	2.41	0.82
1:B:31:GLN:HB3	1:B:32:ASN:HB3	1.61	0.82
1:A:129:PHE:CZ	1:A:179:LEU:CD1	2.63	0.82
1:A:263:ARG:HB2	1:A:264:ARG:HA	1.62	0.81
1:A:87:THR:HA	1:A:88:GLN:O	1.79	0.81
1:A:367:LEU:HD21	1:A:545:PHE:CE1	2.16	0.81
1:A:87:THR:CG2	1:A:92:PHE:HB3	2.05	0.81
1:C:95:LYS:H	1:C:96:SER:HA	1.46	0.80
1:B:846:LEU:N	1:B:847:ARG:CB	2.44	0.80
1:C:846:LEU:N	1:C:847:ARG:CB	2.44	0.80
1:A:705:GLY:O	1:A:709:ASN:ND2	2.15	0.80
1:C:184:ALA:HA	1:C:185:ALA:C	2.07	0.80
1:A:710:TYR:O	1:A:714:VAL:HG23	1.81	0.79
1:A:979:PRO:HB3	1:B:981:LEU:HD22	1.64	0.79
1:A:181:ASP:OD1	1:A:182:GLY:N	2.16	0.79
1:A:539:MET:CE	1:A:609:VAL:C	2.55	0.79
1:C:1000:TYR:CE2	1:D:985:LEU:HD23	2.17	0.79
1:A:33:ILE:HG22	1:A:140:LEU:HD11	1.65	0.79
1:A:280:GLU:OE2	1:A:683:ARG:NE	2.16	0.79
1:A:299:SER:OG	1:A:403:ARG:NH1	2.15	0.79
1:A:321:SER:C	1:A:323:ALA:N	2.40	0.78
1:A:912:LEU:O	1:A:915:GLN:CG	2.30	0.78
1:A:662:GLY:O	1:A:745:LEU:HB3	1.82	0.78
1:B:95:LYS:H	1:B:96:SER:HA	1.46	0.78
1:D:97:PHE:HB3	1:D:98:PRO:HA	1.64	0.78
1:B:433:ARG:NH2	1:B:782:ARG:O	2.16	0.78
1:D:31:GLN:HB3	1:D:32:ASN:HB3	1.65	0.78
1:A:807:VAL:HG13	1:A:807:VAL:O	1.85	0.78
1:C:811:SER:O	1:C:817:ASP:N	2.17	0.77
1:C:299:SER:OG	1:C:403:ARG:NH1	2.17	0.77
1:D:299:SER:OG	1:D:403:ARG:NH1	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:PHE:HB3	1:C:98:PRO:HA	1.66	0.77
1:A:97:PHE:HB3	1:A:98:PRO:HA	1.64	0.77
1:A:734:GLY:O	1:A:737:VAL:HG22	1.84	0.77
1:B:97:PHE:HB3	1:B:98:PRO:HA	1.64	0.77
1:B:734:GLY:O	1:B:737:VAL:HG22	1.84	0.77
1:D:256:PRO:C	1:D:269:VAL:N	2.43	0.76
1:A:31:GLN:CB	1:A:32:ASN:HB3	2.15	0.76
1:A:819:ASP:CA	1:A:820:ALA:O	2.33	0.76
1:C:31:GLN:HB3	1:C:32:ASN:HB3	1.66	0.76
1:A:355:ILE:HD11	1:A:405:VAL:HG12	1.63	0.76
1:A:120:THR:OG1	1:A:159:PRO:HB3	1.86	0.76
1:A:717:HIS:NE2	1:A:766:GLU:OE1	2.18	0.76
1:A:246:PRO:CB	1:A:247:ALA:HB2	2.16	0.76
1:C:734:GLY:O	1:C:737:VAL:HG22	1.86	0.76
1:A:116:SER:HB3	1:A:119:ASN:OD1	1.85	0.75
1:A:194:LYS:HE3	1:A:195:PRO:HD2	1.67	0.75
1:D:734:GLY:O	1:D:737:VAL:HG22	1.85	0.75
1:D:884:GLN:O	1:D:888:LYS:HD2	1.87	0.75
1:A:912:LEU:O	1:A:915:GLN:HG2	1.87	0.75
1:B:31:GLN:CB	1:B:32:ASN:HB3	2.16	0.75
1:B:246:PRO:CB	1:B:247:ALA:HB2	2.16	0.75
1:A:184:ALA:HA	1:A:185:ALA:CB	2.16	0.75
1:A:703:TYR:HA	1:A:706:ILE:HG22	1.66	0.75
1:A:79:MET:HG3	1:A:83:TRP:CD1	2.21	0.75
1:C:561:LYS:HG2	1:C:570:THR:OG1	1.87	0.74
1:A:79:MET:SD	1:A:106:PHE:CE2	2.80	0.74
1:A:858:GLY:HA2	1:A:941:TYR:OH	1.86	0.74
1:D:31:GLN:CB	1:D:32:ASN:HB3	2.17	0.74
1:D:246:PRO:CB	1:D:247:ALA:HB2	2.17	0.74
1:D:858:GLY:HA2	1:D:941:TYR:OH	1.87	0.74
1:C:31:GLN:CB	1:C:32:ASN:HB3	2.17	0.74
1:C:263:THR:N	1:C:264:ARG:HB2	2.01	0.74
1:B:338:VAL:O	1:B:342:ILE:HG13	1.88	0.74
1:B:426:ALA:HA	1:B:645:ASN:O	1.88	0.74
1:A:355:ILE:HD12	1:A:405:VAL:HA	1.70	0.74
1:A:983:THR:HB	1:A:984:PRO:HD2	1.68	0.74
1:C:433:ARG:NH2	1:C:782:ARG:O	2.21	0.74
1:B:541:MET:HG2	1:B:612:PHE:CE2	2.23	0.73
1:A:415:ASN:OD1	1:A:417:GLN:HB3	1.87	0.73
1:A:439:ARG:NH1	1:A:639:ASP:OD2	2.20	0.73
1:C:565:ASP:C	1:C:568:ASP:N	2.46	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:LEU:HG	1:A:1002:ALA:N	2.03	0.73
1:D:619:PRO:HG2	1:D:622:ASP:HB2	1.68	0.73
1:C:1000:TYR:CZ	1:D:985:LEU:HD23	2.24	0.73
1:A:74:TRP:CD1	1:A:82:LEU:HG	2.23	0.72
1:C:246:PRO:CB	1:C:247:ALA:HB2	2.18	0.72
1:A:321:SER:O	1:A:323:ALA:N	2.21	0.72
1:A:745:LEU:O	1:A:745:LEU:CD2	2.37	0.72
1:A:27:TYR:HB3	1:A:28:ALA:HA	1.71	0.72
1:A:184:ALA:HA	1:A:185:ALA:HB3	1.70	0.72
1:A:839:LEU:HB3	1:A:840:THR:HB	1.69	0.72
1:C:858:GLY:HA2	1:C:941:TYR:OH	1.88	0.72
1:A:516:ASP:O	1:A:520:GLN:HG3	1.88	0.72
1:B:332:GLY:O	1:B:366:TRP:HA	1.89	0.71
1:B:858:GLY:HA2	1:B:941:TYR:OH	1.89	0.71
1:A:305:VAL:HG13	1:A:307:PHE:CE1	2.26	0.71
1:A:355:ILE:CD1	1:A:405:VAL:CG1	2.63	0.71
1:A:745:LEU:HD23	1:A:745:LEU:C	2.15	0.71
1:A:129:PHE:CZ	1:A:179:LEU:HD11	2.24	0.71
1:D:184:ALA:HA	1:D:185:ALA:C	2.16	0.71
1:A:433:ARG:NH2	1:A:782:ARG:O	2.22	0.70
1:A:912:LEU:O	1:A:915:GLN:HG3	1.92	0.70
1:B:943:LYS:CB	1:B:944:THR:CB	2.70	0.70
1:C:30:LEU:HD22	1:C:190:TRP:CE3	2.26	0.70
1:A:807:VAL:O	1:A:807:VAL:CG1	2.40	0.69
1:B:23:SER:CB	1:B:24:MET:CA	2.70	0.69
1:C:95:LYS:N	1:C:96:SER:HA	2.07	0.69
1:A:806:LYS:HB3	1:A:807:VAL:HB	1.74	0.69
1:C:156:ARG:HD3	1:C:396:LEU:HD13	1.74	0.69
1:A:867:LEU:HD13	1:A:885:LEU:HD23	1.75	0.69
1:C:338:VAL:O	1:C:342:ILE:HG13	1.91	0.69
1:A:318:ASP:HB3	1:A:326:ILE:HG23	1.75	0.69
1:A:561:LYS:HG2	1:A:561:LYS:O	1.92	0.69
1:C:304:THR:HG21	1:C:342:ILE:HG12	1.75	0.69
1:A:87:THR:OG1	1:A:87:THR:O	2.04	0.69
1:A:174:ASN:OD1	1:A:175:ALA:HB3	1.92	0.69
1:B:184:ALA:HA	1:B:185:ALA:C	2.16	0.69
1:A:113:ASN:O	1:A:114:PHE:HB2	1.92	0.69
1:A:413:ALA:O	1:A:635:TRP:NE1	2.26	0.69
1:A:505:ARG:HG3	1:A:505:ARG:O	1.93	0.69
1:A:989:GLY:HA2	1:B:996:PHE:CD2	2.29	0.68
1:A:338:VAL:O	1:A:342:ILE:HG13	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:HA	1:A:446:LYS:HD3	1.75	0.68
1:B:263:THR:N	1:B:264:ARG:HB2	2.09	0.68
1:A:978:MET:HB3	1:B:959:PHE:HZ	1.59	0.68
1:A:469:THR:HG22	1:A:470:ASN:H	1.59	0.67
1:A:866:VAL:O	1:A:867:LEU:HG	1.94	0.67
1:C:806:LYS:CB	1:C:807:VAL:CB	2.72	0.67
1:D:338:VAL:O	1:D:342:ILE:HG13	1.93	0.67
1:D:943:LYS:CB	1:D:944:THR:CB	2.70	0.67
1:A:511:GLN:CD	1:A:808:MET:HG2	2.20	0.67
1:D:806:LYS:HB3	1:D:807:VAL:CB	2.25	0.67
1:A:142:MET:SD	1:A:142:MET:N	2.67	0.67
1:A:441:MET:CE	1:A:792:VAL:HG13	2.24	0.67
1:C:922:GLY:HA3	1:D:974:GLY:O	1.94	0.67
1:B:573:LEU:HG	1:B:599:PHE:CD1	2.29	0.67
1:D:170:PRO:O	1:D:180:LYS:HB3	1.95	0.67
1:A:846:LEU:H	1:A:847:ARG:HB3	1.59	0.66
1:B:95:LYS:N	1:B:96:SER:HA	2.08	0.66
1:D:251:THR:N	1:D:252:ARG:HB2	2.10	0.66
1:A:797:ILE:O	1:A:801:LEU:HG	1.95	0.66
1:C:943:LYS:CB	1:C:944:THR:CB	2.70	0.66
1:D:95:LYS:N	1:D:96:SER:HA	2.10	0.66
1:D:343:ARG:NH1	1:D:344:ASP:OD1	2.28	0.66
1:C:985:LEU:HD23	1:D:1000:TYR:CZ	2.31	0.66
1:A:539:MET:HE2	1:A:610:ILE:N	2.11	0.66
1:A:812:ARG:C	1:A:817:ASP:N	2.54	0.66
1:A:79:MET:HG3	1:A:83:TRP:NE1	2.10	0.66
1:B:812:ARG:O	1:B:823:HIS:CE1	2.49	0.66
1:A:140:LEU:HD23	1:A:142:MET:HE1	1.78	0.66
1:C:922:GLY:CA	1:D:974:GLY:O	2.43	0.66
1:A:572:MET:HG3	1:A:573:LEU:HD13	1.77	0.66
1:C:462:ARG:HH12	1:D:990:LEU:HG	1.61	0.66
1:C:797:ILE:O	1:C:801:LEU:HG	1.96	0.66
1:C:979:PRO:HA	1:D:981:LEU:HD13	1.76	0.65
1:D:795:PRO:O	1:D:799:ARG:HB2	1.97	0.65
1:A:806:LYS:N	1:A:807:VAL:HB	2.12	0.65
1:B:304:THR:HG21	1:B:342:ILE:HG12	1.78	0.65
1:D:304:THR:HG21	1:D:342:ILE:HG12	1.78	0.65
1:B:541:MET:HE2	1:B:633:MET:C	2.22	0.65
1:D:819:ASP:CA	1:D:820:ALA:O	2.42	0.65
1:A:840:THR:O	1:A:840:THR:HG23	1.96	0.65
1:C:228:ALA:O	1:C:229:THR:C	2.39	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:LEU:C	1:A:807:VAL:CG1	2.68	0.65
1:A:174:ASN:CG	1:A:175:ALA:N	2.55	0.65
1:A:321:SER:C	1:A:323:ALA:CA	2.56	0.65
1:B:156:ARG:HG2	1:B:275:TRP:CZ2	2.31	0.65
1:A:95:LYS:N	1:A:96:SER:HA	2.12	0.65
1:A:439:ARG:HH22	1:A:639:ASP:CG	2.04	0.65
1:A:863:GLU:O	1:A:866:VAL:O	2.15	0.64
1:A:73:SER:O	1:A:76:THR:OG1	2.14	0.64
1:A:129:PHE:CE1	1:A:179:LEU:HD12	2.33	0.64
1:A:304:THR:HG21	1:A:342:ILE:HG12	1.80	0.64
1:D:25:GLU:H	1:D:26:VAL:C	2.06	0.64
1:A:33:ILE:CG2	1:A:140:LEU:HD11	2.27	0.64
1:A:304:THR:OG1	1:A:402:ILE:HG12	1.98	0.64
1:B:907:ALA:HA	1:B:908:LYS:HG3	1.80	0.64
1:D:541:MET:HG2	1:D:612:PHE:CE2	2.33	0.64
1:A:126:SER:HB3	1:A:141:ASP:OD2	1.98	0.64
1:A:367:LEU:HD21	1:A:545:PHE:HE1	1.59	0.64
1:B:449:ASP:HA	1:B:452:LYS:HE3	1.79	0.64
1:C:30:LEU:HD13	1:C:190:TRP:CB	2.28	0.64
1:C:982:VAL:HG22	1:D:500:ASN:O	1.98	0.63
1:B:369:ASP:HB3	1:B:372:ASP:HB2	1.80	0.63
1:B:812:ARG:O	1:B:823:HIS:NE2	2.32	0.63
1:C:986:MET:HE2	1:D:499:LEU:C	2.23	0.63
1:A:441:MET:HG2	1:A:796:THR:OG1	1.98	0.63
1:A:477:ARG:HD3	1:A:478:HIS:CE1	2.34	0.63
1:D:332:GLY:O	1:D:366:TRP:HA	1.99	0.63
1:D:982:VAL:HG21	1:D:990:LEU:HD12	1.79	0.63
1:C:983:THR:HG22	1:D:966:SER:HB2	1.81	0.63
1:D:433:ARG:NH2	1:D:782:ARG:O	2.32	0.63
1:C:541:MET:HG2	1:C:612:PHE:CE2	2.34	0.63
1:C:979:PRO:HA	1:D:981:LEU:HD22	1.81	0.63
1:D:369:ASP:HB3	1:D:372:ASP:HB2	1.80	0.63
1:C:425:ARG:CZ	1:C:425:ARG:HA	2.29	0.62
1:C:1003:ARG:NE	1:D:476:VAL:O	2.29	0.62
1:B:29:ARG:NH1	1:B:178:ILE:HG21	2.14	0.62
1:C:981:LEU:O	1:D:962:ALA:HB1	2.00	0.62
1:A:282:ASN:HA	1:A:284:TYR:CE1	2.33	0.62
1:A:321:SER:HB3	1:A:323:ALA:CA	2.29	0.62
1:A:129:PHE:CZ	1:A:179:LEU:HD12	2.35	0.62
1:A:240:ARG:HG2	1:A:241:GLY:H	1.64	0.62
1:A:130:ASN:OD1	1:A:139:LEU:HD21	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:CD1	1:A:180:LYS:HG2	2.26	0.62
1:A:451:GLN:HG3	1:A:464:TRP:CZ2	2.35	0.62
1:B:157:PHE:CE2	1:B:272:MET:HG3	2.34	0.62
1:A:449:ASP:HA	1:A:452:LYS:HE3	1.81	0.62
1:D:449:ASP:HA	1:D:452:LYS:HE3	1.81	0.62
1:D:495:LEU:HD23	1:D:510:ILE:HD13	1.82	0.62
1:B:635:TRP:CH2	1:B:637:CYS:HB2	2.35	0.62
1:A:979:PRO:HA	1:B:981:LEU:HD13	1.81	0.62
1:C:25:GLU:H	1:C:26:VAL:C	2.08	0.61
1:A:866:VAL:O	1:A:867:LEU:CB	2.45	0.61
1:B:819:ASP:CA	1:B:820:ALA:O	2.42	0.61
1:A:922:GLY:C	1:B:974:GLY:HA3	2.24	0.61
1:D:24:MET:SD	1:D:24:MET:N	2.73	0.61
1:A:505:ARG:O	1:A:505:ARG:CG	2.49	0.61
1:A:66:PRO:O	1:A:67:THR:OG1	2.14	0.61
1:A:559:SER:HB3	1:A:608:ASP:OD2	2.00	0.61
1:A:175:ALA:CB	1:A:179:LEU:HD13	2.30	0.61
1:A:133:LYS:CA	1:A:135:GLY:N	2.41	0.60
1:C:1000:TYR:CE2	1:D:985:LEU:CD2	2.83	0.60
1:A:836:PHE:O	1:A:840:THR:HG21	2.01	0.60
1:C:996:PHE:CD1	1:D:989:GLY:HA2	2.37	0.60
1:B:27:TYR:CB	1:B:28:ALA:HA	2.30	0.60
1:B:32:ASN:OD1	1:B:36:LYS:NZ	2.25	0.60
1:A:359:MET:HE1	1:A:398:ARG:O	2.02	0.60
1:A:945:ASN:HB3	1:A:948:PHE:HB3	1.83	0.60
1:C:660:TYR:CE1	1:C:754:LEU:HA	2.36	0.60
1:C:945:ASN:HB3	1:C:948:PHE:HB3	1.83	0.60
1:A:568:ASP:O	1:B:343:ARG:NH2	2.34	0.60
1:C:978:MET:O	1:D:981:LEU:HD13	2.02	0.60
1:A:841:ALA:HB3	1:A:842:GLU:HB2	1.82	0.60
1:B:361:SER:HB3	1:B:390:CYS:HB2	1.84	0.60
1:D:555:HIS:CE1	1:D:603:LEU:HB2	2.37	0.60
1:B:945:ASN:HB3	1:B:948:PHE:HB3	1.82	0.59
1:D:619:PRO:HG2	1:D:622:ASP:CB	2.31	0.59
1:D:656:ASP:OD1	1:D:657:LEU:N	2.35	0.59
1:A:470:ASN:OD1	1:A:472:ARG:CB	2.50	0.59
1:A:981:LEU:HD23	1:B:962:ALA:HB1	1.84	0.59
1:B:97:PHE:HB3	1:B:98:PRO:CA	2.32	0.59
1:A:355:ILE:HD11	1:A:405:VAL:CG1	2.32	0.59
1:A:657:LEU:HD12	1:A:731:THR:HG22	1.84	0.59
1:A:846:LEU:N	1:A:847:ARG:HB3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:LYS:HB3	1:B:807:VAL:CB	2.32	0.59
1:A:739:GLN:HA	1:A:744:ILE:HD12	1.83	0.59
1:A:86:LEU:HB3	1:A:87:THR:CB	2.32	0.59
1:A:738:ASP:OD1	1:A:741:LYS:HE3	2.03	0.59
1:A:806:LYS:H	1:A:807:VAL:HB	1.67	0.59
1:B:841:ALA:HB3	1:B:842:GLU:HB2	1.85	0.59
1:B:428:ASP:OD2	1:B:431:ARG:HB2	2.03	0.58
1:C:739:GLN:HA	1:C:744:ILE:HD12	1.85	0.58
1:A:980:LEU:HD23	1:B:497:PHE:CD1	2.38	0.58
1:A:100:ARG:NH1	1:A:101:PRO:O	2.36	0.58
1:A:367:LEU:C	1:A:367:LEU:HD12	2.28	0.58
1:A:539:MET:HE3	1:A:609:VAL:C	2.28	0.58
1:D:95:LYS:H	1:D:96:SER:HA	1.68	0.58
1:D:409:LEU:HD11	1:D:539:MET:SD	2.43	0.58
1:A:299:SER:HG	1:A:403:ARG:HH11	1.50	0.58
1:A:808:MET:CB	1:A:809:GLN:HB2	2.33	0.58
1:C:819:ASP:CA	1:C:820:ALA:O	2.45	0.58
1:C:841:ALA:HB3	1:C:842:GLU:HB2	1.84	0.58
1:D:841:ALA:HB3	1:D:842:GLU:HB2	1.84	0.58
1:A:861:GLU:OE1	1:A:945:ASN:OD1	2.22	0.58
1:A:982:VAL:HG23	1:A:982:VAL:O	2.03	0.58
1:A:132:SER:HA	1:A:133:LYS:HB3	1.85	0.58
1:C:44:ALA:HB1	1:C:45:PRO:HA	1.85	0.58
1:C:361:SER:HB3	1:C:390:CYS:HB2	1.85	0.58
1:C:97:PHE:HB3	1:C:98:PRO:CA	2.33	0.58
1:A:44:ALA:HB1	1:A:45:PRO:HA	1.86	0.58
1:C:449:ASP:HA	1:C:452:LYS:HE3	1.85	0.58
1:A:119:ASN:OD1	1:A:147:PHE:CE1	2.57	0.57
1:A:240:ARG:HG3	1:A:266:GLU:HG2	1.85	0.57
1:A:29:ARG:NE	1:A:133:LYS:HB2	2.18	0.57
1:A:31:GLN:HB3	1:A:32:ASN:CB	2.31	0.57
1:A:78:ASP:O	1:A:81:ALA:N	2.36	0.57
1:B:495:LEU:HD23	1:B:510:ILE:HD13	1.87	0.57
1:B:559:SER:HA	1:B:607:LYS:HD2	1.87	0.57
1:A:177:SER:O	1:A:181:ASP:HB3	2.05	0.57
1:A:539:MET:CE	1:A:610:ILE:N	2.68	0.57
1:A:439:ARG:NH2	1:A:639:ASP:OD1	2.33	0.57
1:B:25:GLU:H	1:B:26:VAL:C	2.11	0.57
1:D:361:SER:HB3	1:D:390:CYS:HB2	1.86	0.57
1:A:441:MET:HE2	1:A:792:VAL:CG1	2.30	0.57
1:C:462:ARG:NH1	1:D:990:LEU:HG	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ALA:HB1	1:D:45:PRO:HA	1.87	0.57
1:A:25:GLU:H	1:A:26:VAL:C	2.13	0.57
1:B:44:ALA:HB1	1:B:45:PRO:HA	1.87	0.57
1:A:470:ASN:OD1	1:A:472:ARG:HB2	2.05	0.57
1:A:80:ALA:O	1:A:84:ARG:CG	2.40	0.57
1:A:683:ARG:HH11	1:A:683:ARG:HG2	1.69	0.57
1:C:416:LEU:HD12	1:C:417:GLN:N	2.20	0.57
1:A:915:GLN:N	1:A:916:PRO:HD3	2.20	0.56
1:A:928:TYR:HA	1:A:931:LEU:HD23	1.86	0.56
1:D:945:ASN:HB3	1:D:948:PHE:HB3	1.86	0.56
1:A:588:PHE:CD1	1:A:652:PRO:HG3	2.40	0.56
1:C:986:MET:CE	1:D:499:LEU:O	2.41	0.56
1:A:95:LYS:H	1:A:96:SER:HA	1.70	0.56
1:B:304:THR:HG22	1:B:305:VAL:N	2.20	0.56
1:D:83:TRP:HA	1:D:86:LEU:HD22	1.87	0.56
1:D:576:ASP:HB3	1:D:596:ARG:HH21	1.71	0.56
1:A:83:TRP:HA	1:A:86:LEU:HD22	1.86	0.56
1:C:921:ARG:O	1:C:926:THR:N	2.38	0.56
1:B:36:LYS:H	1:B:36:LYS:HD2	1.69	0.56
1:B:806:LYS:H	1:B:807:VAL:CB	2.18	0.56
1:C:860:VAL:O	1:C:863:GLU:HB2	2.06	0.56
1:A:979:PRO:CB	1:B:981:LEU:HD22	2.35	0.56
1:A:752:ASP:OD1	1:A:755:ARG:NH2	2.38	0.56
1:A:806:LYS:CA	1:A:807:VAL:HB	2.36	0.56
1:A:836:PHE:O	1:A:840:THR:CG2	2.54	0.56
1:A:886:HIS:NE2	1:A:890:CYS:SG	2.79	0.56
1:B:43:ALA:O	1:B:44:ALA:HB3	2.06	0.56
1:D:504:ASP:OD1	1:D:505:ARG:HB2	2.06	0.56
1:A:321:SER:CA	1:A:323:ALA:HA	2.35	0.56
1:A:29:ARG:CZ	1:A:133:LYS:HB2	2.36	0.55
1:B:85:SER:HB2	1:B:86:LEU:HB2	1.88	0.55
1:B:444:LEU:HD13	1:B:525:LEU:CD2	2.36	0.55
1:C:894:PRO:HB3	1:C:929:TRP:CZ3	2.41	0.55
1:D:394:ASP:OD1	1:D:397:HIS:CG	2.59	0.55
1:A:962:ALA:HB1	1:B:981:LEU:HG	1.88	0.55
1:C:156:ARG:HD3	1:C:396:LEU:CD1	2.36	0.55
1:D:85:SER:HB2	1:D:86:LEU:HB2	1.88	0.55
1:A:886:HIS:O	1:A:889:TRP:HB3	2.07	0.55
1:C:83:TRP:HA	1:C:86:LEU:HD22	1.87	0.55
1:A:862:HIS:O	1:A:865:LYS:HB2	2.06	0.55
1:C:43:ALA:O	1:C:44:ALA:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HD2	1:A:133:LYS:HB2	1.88	0.55
1:A:806:LYS:H	1:A:807:VAL:CB	2.19	0.55
1:B:83:TRP:HA	1:B:86:LEU:HD22	1.88	0.55
1:A:43:ALA:O	1:A:44:ALA:HB3	2.07	0.55
1:A:861:GLU:HG2	1:A:941:TYR:CZ	2.42	0.55
1:D:43:ALA:O	1:D:44:ALA:HB3	2.06	0.55
1:D:739:GLN:HA	1:D:744:ILE:HD12	1.88	0.55
1:A:459:LEU:HD11	1:B:985:LEU:HD11	1.88	0.55
1:A:603:LEU:HB3	1:A:606:LEU:HD12	1.89	0.55
1:B:953:ALA:O	1:B:955:ALA:N	2.40	0.55
1:C:85:SER:HB2	1:C:86:LEU:HB2	1.89	0.55
1:D:246:PRO:HB2	1:D:247:ALA:HB2	1.89	0.55
1:B:588:PHE:CD2	1:B:652:PRO:HG3	2.42	0.55
1:A:246:PRO:HB2	1:A:247:ALA:HB2	1.89	0.54
1:C:555:HIS:CE1	1:C:603:LEU:HB2	2.42	0.54
1:A:85:SER:HB2	1:A:86:LEU:HB2	1.87	0.54
1:A:980:LEU:N	1:B:981:LEU:HD13	2.22	0.54
1:B:739:GLN:HA	1:B:744:ILE:HD12	1.90	0.54
1:B:775:TRP:NE1	1:B:781:PRO:HD3	2.23	0.54
1:D:23:SER:CB	1:D:24:MET:CA	2.83	0.54
1:A:119:ASN:OD1	1:A:119:ASN:O	2.24	0.54
1:A:140:LEU:N	1:A:140:LEU:HD12	2.22	0.54
1:B:268:PRO:O	1:B:270:SER:N	2.40	0.54
1:C:861:GLU:O	1:C:865:LYS:N	2.31	0.54
1:A:439:ARG:NH2	1:A:639:ASP:CG	2.65	0.54
1:A:962:ALA:HB1	1:B:981:LEU:HD23	1.89	0.54
1:A:979:PRO:O	1:B:959:PHE:HE1	1.86	0.54
1:B:860:VAL:O	1:B:863:GLU:HB2	2.08	0.54
1:C:27:TYR:CB	1:C:28:ALA:HA	2.38	0.54
1:A:736:LEU:HD22	1:A:739:GLN:OE1	2.07	0.54
1:A:953:ALA:O	1:A:955:ALA:N	2.41	0.54
1:B:68:LEU:CA	1:B:69:ARG:HB2	2.38	0.54
1:B:29:ARG:HH11	1:B:178:ILE:HG21	1.72	0.54
1:B:246:PRO:HB2	1:B:247:ALA:HB2	1.88	0.54
1:A:24:MET:SD	1:A:24:MET:N	2.74	0.53
1:A:361:SER:HB3	1:A:390:CYS:HB2	1.89	0.53
1:A:867:LEU:HA	1:A:881:LYS:HD2	1.89	0.53
1:D:538:TYR:CE1	1:D:635:TRP:HB2	2.43	0.53
1:A:621:ALA:HB2	1:A:629:TYR:CE2	2.44	0.53
1:C:31:GLN:HB2	1:C:32:ASN:HB3	1.91	0.53
1:C:808:MET:CB	1:C:809:GLN:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:MET:HG2	1:A:612:PHE:CE2	2.43	0.53
1:A:837:LYS:C	1:A:840:THR:HG22	2.33	0.53
1:A:841:ALA:HB3	1:A:842:GLU:CB	2.38	0.53
1:B:660:TYR:CD1	1:B:660:TYR:N	2.76	0.53
1:D:794:LYS:HD3	1:D:798:ASP:OD2	2.07	0.53
1:A:321:SER:O	1:A:323:ALA:CB	2.55	0.53
1:C:332:GLY:O	1:C:366:TRP:HA	2.08	0.53
1:A:31:GLN:NE2	1:A:134:THR:OG1	2.42	0.53
1:A:78:ASP:O	1:A:79:MET:C	2.51	0.53
1:A:367:LEU:HD22	1:A:542:VAL:CG1	2.38	0.53
1:D:363:LYS:NZ	1:D:630:ASP:OD2	2.42	0.53
1:D:495:LEU:HD23	1:D:510:ILE:CD1	2.39	0.53
1:A:29:ARG:CD	1:A:133:LYS:HB2	2.39	0.53
1:A:843:SER:O	1:A:844:ARG:HB2	2.09	0.53
1:C:978:MET:O	1:D:981:LEU:CD1	2.57	0.53
1:A:588:PHE:HD2	1:A:591:ASP:OD1	1.91	0.53
1:D:136:PRO:O	1:D:137:LEU:CB	2.57	0.53
1:D:808:MET:CB	1:D:809:GLN:HB2	2.39	0.53
1:B:419:LEU:HB2	1:B:420:PRO:HD3	1.91	0.53
1:D:321:SER:O	1:D:323:ALA:N	2.42	0.53
1:D:794:LYS:HB3	1:D:795:PRO:HD3	1.90	0.53
1:C:136:PRO:O	1:C:137:LEU:CB	2.57	0.53
1:C:841:ALA:HB3	1:C:842:GLU:CB	2.39	0.53
1:A:982:VAL:HG21	1:A:987:TYR:HD2	1.74	0.52
1:C:714:VAL:O	1:C:718:ASN:HB2	2.09	0.52
1:D:860:VAL:O	1:D:863:GLU:HB2	2.09	0.52
1:C:621:ALA:HB2	1:C:629:TYR:CE1	2.44	0.52
1:C:979:PRO:O	1:D:959:PHE:CD1	2.62	0.52
1:A:97:PHE:HB3	1:A:98:PRO:CA	2.35	0.52
1:C:603:LEU:HB3	1:C:606:LEU:HD12	1.90	0.52
1:D:841:ALA:HB3	1:D:842:GLU:CB	2.40	0.52
1:A:490:ASN:C	1:A:490:ASN:OD1	2.51	0.52
1:B:673:ARG:HA	1:B:676:GLY:C	2.34	0.52
1:A:180:LYS:HD2	1:A:183:GLY:CA	2.39	0.52
1:A:267:ILE:O	1:A:267:ILE:CG2	2.54	0.52
1:B:811:SER:CB	1:B:822:ALA:H	2.22	0.52
1:A:270:SER:CB	1:A:684:HIS:HD2	2.22	0.52
1:A:640:PRO:O	1:A:644:GLU:HG2	2.10	0.52
1:A:806:LYS:CB	1:A:807:VAL:HB	2.39	0.52
1:C:425:ARG:NH1	1:C:647:THR:O	2.42	0.52
1:D:953:ALA:O	1:D:956:GLN:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:O	1:A:137:LEU:HB3	2.10	0.52
1:A:675:THR:HG21	1:A:682:ALA:HA	1.90	0.52
1:D:304:THR:HG22	1:D:305:VAL:HG22	1.91	0.52
1:D:498:LEU:O	1:D:503:PHE:HB2	2.10	0.52
1:A:136:PRO:O	1:A:137:LEU:CB	2.57	0.52
1:A:878:TYR:HB3	1:A:879:PRO:HD3	1.92	0.52
1:D:603:LEU:HB3	1:D:606:LEU:HD12	1.91	0.52
1:D:621:ALA:HB2	1:D:629:TYR:CE2	2.45	0.52
1:A:572:MET:HG3	1:A:573:LEU:CD1	2.40	0.52
1:A:55:ILE:HD11	1:A:83:TRP:NE1	2.24	0.51
1:A:305:VAL:HG13	1:A:307:PHE:HE1	1.70	0.51
1:A:843:SER:HG	1:A:847:ARG:HB2	1.75	0.51
1:B:423:GLU:O	1:B:429:LYS:HG2	2.09	0.51
1:C:136:PRO:O	1:C:137:LEU:HB3	2.10	0.51
1:C:308:GLU:OE1	1:C:308:GLU:HA	2.10	0.51
1:A:83:TRP:O	1:A:87:THR:OG1	2.26	0.51
1:A:133:LYS:HD2	1:A:134:THR:HA	1.93	0.51
1:A:847:ARG:NH1	1:A:851:GLU:OE2	2.43	0.51
1:D:953:ALA:O	1:D:955:ALA:N	2.42	0.51
1:A:105:ALA:HA	1:A:147:PHE:CE2	2.45	0.51
1:A:332:GLY:O	1:A:366:TRP:HA	2.10	0.51
1:A:444:LEU:HD23	1:A:796:THR:CG2	2.40	0.51
1:B:136:PRO:O	1:B:137:LEU:CB	2.58	0.51
1:B:203:TRP:HB3	1:B:236:PHE:HB3	1.93	0.51
1:B:635:TRP:CZ2	1:B:637:CYS:HB2	2.46	0.51
1:A:367:LEU:HD21	1:A:545:PHE:CD1	2.46	0.51
1:A:846:LEU:HA	1:A:849:VAL:HG23	1.93	0.51
1:A:980:LEU:HD22	1:B:987:TYR:CD1	2.45	0.51
1:B:808:MET:CB	1:B:809:GLN:HB2	2.40	0.51
1:A:120:THR:OG1	1:A:159:PRO:CB	2.56	0.51
1:A:864:TRP:O	1:A:867:LEU:O	2.28	0.51
1:B:498:LEU:O	1:B:503:PHE:HB2	2.10	0.51
1:A:683:ARG:HG2	1:A:683:ARG:NH1	2.26	0.51
1:B:841:ALA:HB3	1:B:842:GLU:CB	2.40	0.51
1:D:97:PHE:HB3	1:D:98:PRO:CA	2.35	0.51
1:D:199:VAL:HG12	1:D:199:VAL:O	2.11	0.51
1:B:806:LYS:N	1:B:807:VAL:CB	2.74	0.51
1:D:136:PRO:O	1:D:137:LEU:HB3	2.10	0.51
1:A:194:LYS:HE3	1:A:195:PRO:CD	2.37	0.51
1:A:248:PRO:HG3	1:A:271:GLU:OE2	2.10	0.51
1:D:981:LEU:HD12	1:D:982:VAL:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HD13	1:C:190:TRP:CG	2.46	0.50
1:D:713:ARG:HG2	1:D:768:PRO:HD3	1.93	0.50
1:A:621:ALA:HB2	1:A:629:TYR:CZ	2.46	0.50
1:A:686:ALA:O	1:A:689:ASP:HB2	2.12	0.50
1:B:287:HIS:ND1	1:B:671:LEU:HD11	2.26	0.50
1:C:246:PRO:HB2	1:C:247:ALA:HB2	1.90	0.50
1:D:279:LEU:CB	1:D:683:ARG:CZ	2.80	0.50
1:A:539:MET:CE	1:A:610:ILE:HB	2.41	0.50
1:A:824:SER:O	1:A:938:PHE:HZ	1.94	0.50
1:C:996:PHE:CD1	1:C:996:PHE:C	2.89	0.50
1:D:894:PRO:HB3	1:D:929:TRP:CZ3	2.47	0.50
1:A:79:MET:CG	1:A:83:TRP:NE1	2.74	0.50
1:A:957:LEU:HA	1:A:960:ILE:HD12	1.92	0.50
1:D:31:GLN:HB2	1:D:32:ASN:HB3	1.92	0.50
1:A:555:HIS:CE1	1:A:603:LEU:HB2	2.46	0.50
1:B:98:PRO:O	1:B:100:ARG:N	2.45	0.50
1:B:268:PRO:O	1:B:269:VAL:C	2.55	0.50
1:B:432:MET:HE2	1:B:436:ILE:HG13	1.94	0.50
1:B:555:HIS:CE1	1:B:599:PHE:CD1	2.99	0.50
1:B:621:ALA:HB2	1:B:629:TYR:CE1	2.46	0.50
1:C:419:LEU:HB2	1:C:420:PRO:HD3	1.93	0.50
1:B:981:LEU:HD12	1:B:982:VAL:N	2.27	0.50
1:D:878:TYR:HB3	1:D:879:PRO:HD3	1.92	0.50
1:A:355:ILE:HD11	1:A:402:ILE:HG23	1.94	0.50
1:A:432:MET:SD	1:A:432:MET:C	2.95	0.50
1:A:962:ALA:HB1	1:B:981:LEU:CG	2.41	0.50
1:D:419:LEU:HB2	1:D:420:PRO:HD3	1.93	0.50
1:A:985:LEU:HD13	1:A:986:MET:N	2.27	0.50
1:C:498:LEU:O	1:C:503:PHE:HB2	2.12	0.50
1:D:246:PRO:HB3	1:D:247:ALA:HB2	1.93	0.50
1:A:38:PRO:HB2	1:A:40:TRP:CE3	2.47	0.49
1:A:179:LEU:HD23	1:A:180:LYS:HB3	1.93	0.49
1:A:411:PRO:HD3	1:A:562:PHE:CE1	2.48	0.49
1:A:498:LEU:O	1:A:503:PHE:HB2	2.11	0.49
1:C:861:GLU:HG2	1:C:941:TYR:CZ	2.47	0.49
1:D:256:PRO:O	1:D:269:VAL:N	2.46	0.49
1:A:416:LEU:HD12	1:A:417:GLN:N	2.27	0.49
1:C:878:TYR:HB3	1:C:879:PRO:HD3	1.94	0.49
1:C:985:LEU:HD23	1:D:1000:TYR:CE2	2.47	0.49
1:D:886:HIS:O	1:D:889:TRP:HB3	2.12	0.49
1:A:953:ALA:O	1:A:956:GLN:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:LEU:HD12	1:B:960:ILE:HG13	1.94	0.49
1:C:30:LEU:HB3	1:C:190:TRP:CE2	2.48	0.49
1:B:673:ARG:C	1:B:676:GLY:H	2.21	0.49
1:C:886:HIS:O	1:C:889:TRP:HB3	2.13	0.49
1:A:717:HIS:HE2	1:A:766:GLU:CD	2.19	0.49
1:B:775:TRP:HE1	1:B:781:PRO:HD3	1.78	0.49
1:C:957:LEU:HA	1:C:960:ILE:HD12	1.95	0.49
1:D:909:THR:O	1:D:912:LEU:HB2	2.12	0.49
1:D:931:LEU:HD12	1:D:960:ILE:HG13	1.95	0.49
1:A:93:ARG:N	1:A:94:GLY:HA3	2.27	0.49
1:A:175:ALA:HB1	1:A:179:LEU:HD13	1.93	0.49
1:A:996:PHE:CD1	1:A:996:PHE:C	2.90	0.49
1:B:136:PRO:O	1:B:137:LEU:HB3	2.13	0.49
1:B:27:TYR:CB	1:B:28:ALA:CA	2.91	0.49
1:B:246:PRO:HB3	1:B:247:ALA:HB2	1.92	0.49
1:B:878:TYR:HB3	1:B:879:PRO:HD3	1.93	0.49
1:D:93:ARG:N	1:D:94:GLY:HA3	2.28	0.49
1:D:843:SER:O	1:D:844:ARG:HB2	2.13	0.49
1:B:425:ARG:NH1	1:B:647:THR:O	2.44	0.49
1:C:98:PRO:O	1:C:100:ARG:N	2.46	0.49
1:A:825:TRP:HB2	1:A:942:TYR:CE2	2.48	0.49
1:A:866:VAL:O	1:A:867:LEU:CG	2.60	0.49
1:C:818:ASP:HB2	1:C:820:ALA:HB3	1.95	0.49
1:A:180:LYS:HD2	1:A:183:GLY:HA3	1.94	0.48
1:A:321:SER:CB	1:A:323:ALA:CA	2.91	0.48
1:A:444:LEU:HD23	1:A:796:THR:HG22	1.94	0.48
1:A:980:LEU:H	1:B:981:LEU:HD13	1.78	0.48
1:B:394:ASP:OD1	1:B:395:ALA:N	2.46	0.48
1:B:953:ALA:O	1:B:954:GLY:C	2.55	0.48
1:B:957:LEU:HA	1:B:960:ILE:HD12	1.94	0.48
1:C:68:LEU:CA	1:C:69:ARG:CB	2.90	0.48
1:D:982:VAL:HG21	1:D:990:LEU:CD1	2.43	0.48
1:A:655:PRO:HD2	1:A:731:THR:OG1	2.13	0.48
1:D:530:ASN:OD1	1:D:530:ASN:N	2.45	0.48
1:D:588:PHE:CD2	1:D:652:PRO:HG3	2.48	0.48
1:A:953:ALA:O	1:A:954:GLY:C	2.55	0.48
1:C:953:ALA:O	1:C:955:ALA:N	2.45	0.48
1:B:46:LEU:HD12	1:B:201:ARG:CZ	2.42	0.48
1:A:48:LEU:HD12	1:A:48:LEU:C	2.38	0.48
1:A:840:THR:O	1:A:840:THR:CG2	2.60	0.48
1:A:541:MET:HE2	1:A:633:MET:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:ALA:HB1	1:B:981:LEU:CD2	2.44	0.48
1:C:127:LEU:HD21	1:C:140:LEU:CG	2.44	0.48
1:C:931:LEU:HD12	1:C:960:ILE:HG13	1.95	0.48
1:C:843:SER:O	1:C:844:ARG:HB2	2.14	0.48
1:A:839:LEU:N	1:A:840:THR:HG22	2.16	0.48
1:A:79:MET:CG	1:A:83:TRP:CE2	2.96	0.48
1:B:451:GLN:HG3	1:B:464:TRP:CZ2	2.49	0.48
1:B:894:PRO:HB3	1:B:929:TRP:CZ3	2.49	0.48
1:A:34:TRP:CE3	1:A:140:LEU:HD21	2.49	0.48
1:A:410:LYS:HG2	1:A:411:PRO:N	2.29	0.48
1:B:149:GLU:HB3	1:B:300:LYS:HD3	1.96	0.48
1:C:413:ALA:O	1:C:635:TRP:NE1	2.47	0.48
1:D:69:ARG:CZ	1:D:74:TRP:CZ2	2.96	0.48
1:A:660:TYR:OH	1:A:758:ARG:NE	2.47	0.47
1:C:953:ALA:O	1:C:956:GLN:N	2.39	0.47
1:A:270:SER:OG	1:A:684:HIS:CD2	2.67	0.47
1:A:938:PHE:O	1:A:942:TYR:HB3	2.14	0.47
1:B:153:LEU:HB3	1:B:162:PHE:CZ	2.49	0.47
1:C:541:MET:HE2	1:C:633:MET:C	2.39	0.47
1:D:736:LEU:HD22	1:D:739:GLN:OE1	2.14	0.47
1:A:931:LEU:HD12	1:A:960:ILE:HG13	1.96	0.47
1:B:38:PRO:HB2	1:B:40:TRP:CE3	2.49	0.47
1:B:87:THR:HA	1:B:88:GLN:C	2.38	0.47
1:B:861:GLU:HG2	1:B:941:TYR:CZ	2.49	0.47
1:C:94:GLY:HA2	1:C:95:LYS:HB2	1.97	0.47
1:C:375:ASP:OD1	1:C:375:ASP:N	2.47	0.47
1:C:479:GLY:O	1:D:1000:TYR:HE2	1.97	0.47
1:D:38:PRO:HB2	1:D:40:TRP:CE3	2.49	0.47
1:A:98:PRO:O	1:A:100:ARG:N	2.47	0.47
1:B:24:MET:SD	1:B:24:MET:N	2.74	0.47
1:B:843:SER:O	1:B:844:ARG:HB2	2.13	0.47
1:C:58:HIS:CD2	1:C:98:PRO:HB3	2.50	0.47
1:D:953:ALA:O	1:D:954:GLY:C	2.57	0.47
1:A:79:MET:HE3	1:A:82:LEU:HD22	1.95	0.47
1:D:538:TYR:HA	1:D:634:ALA:O	2.14	0.47
1:A:246:PRO:HB3	1:A:247:ALA:HB2	1.93	0.47
1:A:317:ASP:OD1	1:A:317:ASP:N	2.48	0.47
1:B:425:ARG:HD2	1:B:589:PRO:O	2.15	0.47
1:A:86:LEU:HD23	1:A:87:THR:CG2	2.45	0.47
1:A:132:SER:CA	1:A:133:LYS:HB3	2.44	0.47
1:A:321:SER:O	1:A:322:PRO:C	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:CD2	1:A:545:PHE:HE1	2.26	0.47
1:A:588:PHE:CE1	1:A:652:PRO:HG3	2.50	0.47
1:B:886:HIS:O	1:B:889:TRP:HB3	2.14	0.47
1:C:635:TRP:CH2	1:C:637:CYS:HB2	2.50	0.47
1:C:736:LEU:HD22	1:C:739:GLN:OE1	2.14	0.47
1:C:812:ARG:C	1:C:817:ASP:N	2.72	0.47
1:C:820:ALA:HB1	1:C:821:ALA:CA	2.45	0.47
1:D:87:THR:HA	1:D:88:GLN:C	2.40	0.47
1:A:837:LYS:C	1:A:840:THR:CG2	2.88	0.47
1:B:31:GLN:HB2	1:B:32:ASN:HB3	1.93	0.47
1:B:808:MET:H	1:B:809:GLN:HB3	1.79	0.47
1:B:996:PHE:CE1	1:B:1000:TYR:HB2	2.50	0.47
1:D:957:LEU:HA	1:D:960:ILE:HD12	1.95	0.47
1:A:199:VAL:HG12	1:A:199:VAL:O	2.15	0.47
1:A:635:TRP:CH2	1:A:637:CYS:HB2	2.50	0.47
1:A:751:TRP:CZ2	1:A:755:ARG:HD3	2.50	0.47
1:A:974:GLY:O	1:A:975:SER:CB	2.62	0.47
1:B:495:LEU:HD23	1:B:510:ILE:CD1	2.43	0.47
1:C:38:PRO:HB2	1:C:40:TRP:CE3	2.50	0.47
1:C:321:SER:OG	1:C:617:ASP:HA	2.14	0.47
1:D:68:LEU:CA	1:D:69:ARG:HB2	2.45	0.47
1:D:246:PRO:HA	1:D:254:GLN:HB2	1.97	0.47
1:D:329:ASP:HB3	1:D:628:ASP:HB2	1.96	0.47
1:A:132:SER:HA	1:A:133:LYS:CB	2.44	0.47
1:A:446:LYS:NZ	1:A:447:GLN:HB3	2.30	0.47
1:A:304:THR:HG22	1:A:305:VAL:HG12	1.97	0.46
1:D:535:ARG:NH1	1:D:564:ASP:OD2	2.48	0.46
1:D:713:ARG:HD2	1:D:765:VAL:CB	2.45	0.46
1:B:199:VAL:HG12	1:B:199:VAL:O	2.14	0.46
1:B:248:PRO:HA	1:B:249:LEU:HA	1.61	0.46
1:B:603:LEU:HB3	1:B:606:LEU:HD12	1.96	0.46
1:B:953:ALA:O	1:B:956:GLN:N	2.38	0.46
1:C:432:MET:HE2	1:C:436:ILE:HG13	1.97	0.46
1:A:86:LEU:N	1:A:87:THR:C	2.74	0.46
1:A:511:GLN:OE1	1:A:808:MET:HG2	2.15	0.46
1:B:484:LEU:HG	1:B:882:VAL:HG11	1.97	0.46
1:B:491:LYS:O	1:B:494:VAL:HB	2.15	0.46
1:B:573:LEU:HG	1:B:599:PHE:CE1	2.50	0.46
1:B:663:LYS:HZ1	1:B:742:GLN:HG3	1.80	0.46
1:D:203:TRP:HB3	1:D:236:PHE:HB3	1.97	0.46
1:D:541:MET:HE2	1:D:633:MET:C	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:SER:HA	1:D:607:LYS:HD2	1.97	0.46
1:B:497:PHE:HA	1:B:987:TYR:OH	2.16	0.46
1:B:555:HIS:HE1	1:B:599:PHE:CE1	2.33	0.46
1:B:713:ARG:HG2	1:B:768:PRO:HD3	1.98	0.46
1:C:153:LEU:HB3	1:C:162:PHE:CZ	2.50	0.46
1:A:515:PHE:CE1	1:A:519:LYS:HE3	2.51	0.46
1:B:86:LEU:N	1:B:87:THR:C	2.74	0.46
1:B:363:LYS:HE3	1:B:387:LYS:HE3	1.96	0.46
1:B:428:ASP:CG	1:B:431:ARG:HB2	2.41	0.46
1:A:837:LYS:HA	1:A:840:THR:HG21	1.96	0.46
1:B:94:GLY:HA2	1:B:95:LYS:HB2	1.98	0.46
1:B:982:VAL:O	1:B:983:THR:C	2.58	0.46
1:C:177:SER:O	1:C:181:ASP:HB2	2.16	0.46
1:C:199:VAL:HG12	1:C:199:VAL:O	2.15	0.46
1:C:289:LYS:O	1:C:293:ARG:HG2	2.16	0.46
1:D:98:PRO:O	1:D:100:ARG:N	2.49	0.46
1:A:173:LEU:HA	1:A:174:ASN:HA	1.55	0.46
1:A:267:ILE:O	1:A:267:ILE:HG22	2.15	0.46
1:A:794:LYS:CB	1:A:795:PRO:HD3	2.46	0.46
1:A:819:ASP:N	1:A:820:ALA:O	2.49	0.46
1:B:411:PRO:CG	1:B:562:PHE:CZ	2.98	0.46
1:C:329:ASP:HB3	1:C:628:ASP:HB2	1.98	0.46
1:A:419:LEU:HB2	1:A:420:PRO:HD3	1.97	0.46
1:A:507:GLN:OE1	1:A:508:LYS:N	2.49	0.46
1:B:928:TYR:HA	1:B:931:LEU:HD23	1.98	0.46
1:C:497:PHE:HA	1:C:987:TYR:OH	2.16	0.46
1:C:506:ARG:HA	1:C:821:ALA:O	2.15	0.46
1:D:806:LYS:CB	1:D:807:VAL:CB	2.93	0.46
1:A:55:ILE:HD11	1:A:83:TRP:CD1	2.51	0.46
1:A:343:ARG:HH22	1:B:568:ASP:HB2	1.81	0.46
1:B:177:SER:O	1:B:181:ASP:HB2	2.16	0.46
1:B:791:ALA:O	1:B:795:PRO:HG2	2.16	0.46
1:D:416:LEU:HD12	1:D:417:GLN:N	2.31	0.46
1:D:824:SER:O	1:D:938:PHE:HZ	1.98	0.46
1:A:766:GLU:CD	1:A:766:GLU:H	2.23	0.46
1:B:329:ASP:HB3	1:B:628:ASP:HB2	1.98	0.46
1:C:25:GLU:N	1:C:26:VAL:C	2.74	0.46
1:C:985:LEU:CD2	1:D:1000:TYR:CZ	2.97	0.46
1:A:29:ARG:O	1:A:30:LEU:HB2	2.15	0.45
1:A:248:PRO:HA	1:A:249:LEU:HA	1.71	0.45
1:A:756:ARG:NH2	1:D:775:TRP:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:THR:H	1:A:843:SER:HA	1.80	0.45
1:C:794:LYS:HB3	1:C:795:PRO:HD3	1.99	0.45
1:D:938:PHE:O	1:D:942:TYR:HB3	2.16	0.45
1:A:152:ARG:HH22	1:A:360:GLY:CA	2.30	0.45
1:B:671:LEU:HD21	1:B:693:LYS:HE2	1.98	0.45
1:D:497:PHE:HA	1:D:987:TYR:OH	2.16	0.45
1:D:676:GLY:HA3	1:D:678:THR:N	2.32	0.45
1:A:245:ARG:HD2	1:A:265:THR:HG22	1.98	0.45
1:D:541:MET:HE1	1:D:632:ASP:HB3	1.99	0.45
1:A:555:HIS:C	1:A:555:HIS:CD2	2.94	0.45
1:C:985:LEU:HD13	1:C:986:MET:N	2.32	0.45
1:D:541:MET:HE1	1:D:583:ARG:HD3	1.99	0.45
1:A:451:GLN:HG3	1:A:464:TRP:CH2	2.52	0.45
1:C:139:LEU:HD22	1:C:139:LEU:HA	1.87	0.45
1:C:564:ASP:O	1:C:568:ASP:N	2.50	0.45
1:A:79:MET:HG3	1:A:83:TRP:CE2	2.51	0.45
1:A:539:MET:CE	1:A:609:VAL:O	2.64	0.45
1:A:620:LEU:O	1:A:621:ALA:C	2.57	0.45
1:A:866:VAL:O	1:A:867:LEU:HB2	2.15	0.45
1:B:824:SER:O	1:B:938:PHE:HZ	2.00	0.45
1:D:523:GLU:HA	1:D:526:ARG:HG2	1.99	0.45
1:D:861:GLU:HG2	1:D:941:TYR:CZ	2.52	0.45
1:A:305:VAL:CG1	1:A:307:PHE:CE1	2.98	0.45
1:C:484:LEU:HG	1:C:882:VAL:HG11	1.99	0.45
1:C:962:ALA:HB1	1:D:981:LEU:HD23	1.99	0.45
1:A:162:PHE:CE2	1:A:237:PHE:HD1	2.34	0.45
1:B:69:ARG:HG3	1:B:70:TYR:N	2.31	0.45
1:B:421:VAL:HG13	1:B:589:PRO:HA	1.99	0.45
1:B:946:PRO:O	1:B:950:TRP:HD1	2.00	0.45
1:C:953:ALA:O	1:C:954:GLY:C	2.60	0.45
1:D:946:PRO:O	1:D:950:TRP:HD1	1.99	0.45
1:A:94:GLY:HA2	1:A:95:LYS:CB	2.47	0.45
1:A:133:LYS:N	1:A:135:GLY:HA3	2.32	0.45
1:B:811:SER:O	1:B:812:ARG:C	2.60	0.45
1:C:24:MET:SD	1:C:24:MET:N	2.75	0.45
1:C:248:PRO:HA	1:C:249:LEU:HA	1.72	0.45
1:A:289:LYS:O	1:A:293:ARG:HG2	2.17	0.45
1:A:372:ASP:OD1	1:A:374:GLY:N	2.39	0.45
1:A:427:LYS:N	1:A:645:ASN:O	2.47	0.45
1:A:523:GLU:HA	1:A:526:ARG:HG2	1.99	0.45
1:D:714:VAL:O	1:D:718:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:985:LEU:HD13	1:D:986:MET:N	2.32	0.45
1:A:565:ASP:OD2	1:A:568:ASP:N	2.50	0.44
1:A:980:LEU:N	1:A:980:LEU:HD12	2.32	0.44
1:B:977:GLY:C	1:B:979:PRO:HD3	2.42	0.44
1:C:938:PHE:O	1:C:942:TYR:HB3	2.17	0.44
1:A:272:MET:O	1:A:275:TRP:HB3	2.18	0.44
1:A:1000:TYR:CD1	1:A:1000:TYR:C	2.95	0.44
1:B:432:MET:HE2	1:B:436:ILE:CG1	2.47	0.44
1:B:806:LYS:CB	1:B:807:VAL:CB	2.95	0.44
1:D:818:ASP:HB2	1:D:820:ALA:HB3	1.99	0.44
1:A:29:ARG:O	1:A:30:LEU:CB	2.65	0.44
1:A:79:MET:HE2	1:A:83:TRP:NE1	2.33	0.44
1:A:184:ALA:HA	1:A:185:ALA:HB2	1.98	0.44
1:C:30:LEU:HD22	1:C:190:TRP:CD2	2.51	0.44
1:C:718:ASN:O	1:C:719:ASN:C	2.60	0.44
1:D:248:PRO:HA	1:D:249:LEU:HA	1.71	0.44
1:D:928:TYR:HA	1:D:931:LEU:HD23	1.99	0.44
1:A:189:ARG:NH1	1:A:189:ARG:HB2	2.32	0.44
1:B:86:LEU:H	1:B:87:THR:C	2.26	0.44
1:B:751:TRP:CZ2	1:B:755:ARG:HD3	2.52	0.44
1:C:523:GLU:HA	1:C:526:ARG:HG2	1.98	0.44
1:C:806:LYS:CA	1:C:807:VAL:CB	2.95	0.44
1:C:996:PHE:CE1	1:D:989:GLY:HA2	2.51	0.44
1:D:327:MET:HE1	1:D:619:PRO:HA	2.00	0.44
1:A:511:GLN:HG2	1:A:808:MET:HE2	2.00	0.44
1:A:979:PRO:HD2	1:B:959:PHE:CZ	2.52	0.44
1:A:986:MET:HE2	1:B:499:LEU:O	2.17	0.44
1:B:977:GLY:O	1:B:979:PRO:HD3	2.17	0.44
1:C:499:LEU:O	1:D:986:MET:HE2	2.17	0.44
1:A:325:LYS:HE3	1:A:622:ASP:OD2	2.17	0.44
1:A:343:ARG:O	1:A:344:ASP:C	2.61	0.44
1:A:355:ILE:HD11	1:A:402:ILE:CG2	2.47	0.44
1:A:745:LEU:CD2	1:A:745:LEU:C	2.83	0.44
1:B:94:GLY:HA2	1:B:95:LYS:CB	2.48	0.44
1:B:894:PRO:HB2	1:B:910:ALA:HA	2.00	0.44
1:C:491:LYS:O	1:C:494:VAL:HB	2.17	0.44
1:C:824:SER:O	1:C:938:PHE:HZ	2.01	0.44
1:A:470:ASN:OD1	1:A:472:ARG:NH1	2.51	0.44
1:A:477:ARG:CD	1:A:478:HIS:CE1	2.99	0.44
1:A:713:ARG:HG2	1:A:768:PRO:HD3	2.00	0.44
1:A:808:MET:H	1:A:809:GLN:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LYS:O	1:B:293:ARG:HG2	2.18	0.44
1:B:775:TRP:C	1:B:777:GLY:H	2.25	0.44
1:C:93:ARG:HA	1:C:94:GLY:C	2.43	0.44
1:D:86:LEU:N	1:D:87:THR:C	2.76	0.44
1:A:189:ARG:HB2	1:A:189:ARG:HH11	1.83	0.44
1:A:660:TYR:CE2	1:A:754:LEU:HA	2.52	0.44
1:A:791:ALA:O	1:A:795:PRO:HG2	2.18	0.44
1:B:28:ALA:HB3	1:B:134:THR:HG22	2.00	0.44
1:C:246:PRO:HB3	1:C:247:ALA:HB2	1.95	0.44
1:D:618:ILE:CG1	1:D:623:LYS:HG3	2.47	0.44
1:A:79:MET:HE2	1:A:83:TRP:HE1	1.83	0.44
1:A:194:LYS:CE	1:A:195:PRO:HD2	2.41	0.44
1:A:198:LEU:O	1:A:199:VAL:C	2.61	0.44
1:A:660:TYR:N	1:A:660:TYR:CD1	2.86	0.44
1:B:755:ARG:HA	1:B:759:LEU:HB2	1.99	0.44
1:C:29:ARG:O	1:C:30:LEU:HB2	2.17	0.44
1:C:263:THR:CB	1:C:264:ARG:HE	2.31	0.44
1:C:840:THR:HA	1:C:843:SER:CB	2.48	0.44
1:A:270:SER:HA	1:A:687:VAL:HG11	1.99	0.43
1:B:938:PHE:O	1:B:942:TYR:HB3	2.18	0.43
1:C:304:THR:HG22	1:C:305:VAL:N	2.32	0.43
1:A:714:VAL:O	1:A:718:ASN:HB2	2.18	0.43
1:A:949:VAL:CG2	1:A:950:TRP:N	2.80	0.43
1:C:87:THR:HA	1:C:88:GLN:C	2.41	0.43
1:C:541:MET:HE1	1:C:583:ARG:HD3	2.00	0.43
1:D:25:GLU:N	1:D:26:VAL:C	2.74	0.43
1:A:79:MET:O	1:A:83:TRP:N	2.36	0.43
1:A:753:ARG:CZ	1:D:774:VAL:HG21	2.49	0.43
1:B:211:ALA:HB2	1:B:231:LYS:O	2.17	0.43
1:D:791:ALA:O	1:D:795:PRO:HG2	2.18	0.43
1:A:395:ALA:HA	1:A:398:ARG:NH1	2.33	0.43
1:C:27:TYR:N	1:C:186:GLN:HG2	2.33	0.43
1:C:198:LEU:O	1:C:199:VAL:C	2.61	0.43
1:C:263:THR:CA	1:C:264:ARG:HB2	2.48	0.43
1:C:270:SER:HA	1:C:687:VAL:HG11	2.01	0.43
1:A:140:LEU:HD23	1:A:142:MET:CE	2.47	0.43
1:D:198:LEU:O	1:D:199:VAL:C	2.61	0.43
1:D:484:LEU:HG	1:D:882:VAL:HG11	2.00	0.43
1:A:794:LYS:HB3	1:A:795:PRO:HD3	2.00	0.43
1:B:287:HIS:HB2	1:B:690:MET:HG3	2.00	0.43
1:B:506:ARG:HA	1:B:821:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ARG:HB2	1:B:639:ASP:HB2	2.00	0.43
1:B:820:ALA:HB1	1:B:821:ALA:CA	2.47	0.43
1:A:245:ARG:HA	1:A:246:PRO:HD3	1.90	0.43
1:A:568:ASP:OD1	1:A:569:THR:N	2.52	0.43
1:A:760:GLY:HA3	1:A:761:GLY:HA3	1.66	0.43
1:A:986:MET:CE	1:B:462:ARG:HD3	2.48	0.43
1:B:133:LYS:HA	1:B:134:THR:HA	1.80	0.43
1:B:263:THR:CA	1:B:264:ARG:HB2	2.49	0.43
1:A:274:ASP:HA	1:A:279:LEU:HG	2.00	0.43
1:B:270:SER:HA	1:B:687:VAL:HG11	2.01	0.43
1:D:133:LYS:HA	1:D:134:THR:HA	1.78	0.43
1:A:140:LEU:N	1:A:140:LEU:CD1	2.81	0.43
1:A:321:SER:OG	1:A:617:ASP:HA	2.18	0.43
1:B:550:GLU:O	1:B:551:GLU:C	2.61	0.43
1:C:808:MET:HB3	1:C:809:GLN:HB2	2.01	0.43
1:C:989:GLY:C	1:D:462:ARG:HH22	2.27	0.43
1:D:395:ALA:HA	1:D:398:ARG:NH1	2.34	0.43
1:D:840:THR:HA	1:D:843:SER:CB	2.49	0.43
1:A:34:TRP:HB3	1:A:198:LEU:HD13	2.01	0.43
1:A:463:GLN:HE21	1:A:997:VAL:HG21	1.83	0.43
1:A:541:MET:HE1	1:A:583:ARG:HD3	2.01	0.43
1:C:29:ARG:O	1:C:30:LEU:CB	2.67	0.43
1:C:840:THR:H	1:C:843:SER:HA	1.84	0.43
1:D:245:ARG:HA	1:D:246:PRO:HD3	1.79	0.43
1:D:251:THR:CA	1:D:252:ARG:HB2	2.48	0.43
1:D:270:SER:HA	1:D:687:VAL:HG11	2.01	0.43
1:D:287:HIS:CD2	1:D:288:LEU:HD23	2.54	0.43
1:D:463:GLN:HE21	1:D:997:VAL:HG21	1.84	0.43
1:D:635:TRP:CH2	1:D:637:CYS:HB2	2.53	0.43
1:A:94:GLY:HA2	1:A:95:LYS:HB2	2.01	0.42
1:A:886:HIS:CD2	1:A:890:CYS:SG	3.11	0.42
1:B:198:LEU:O	1:B:199:VAL:C	2.61	0.42
1:C:421:VAL:HG13	1:C:589:PRO:HA	2.01	0.42
1:C:667:THR:OG1	1:C:670:GLU:CD	2.62	0.42
1:C:979:PRO:CA	1:D:981:LEU:HD22	2.48	0.42
1:B:29:ARG:O	1:B:30:LEU:HB2	2.20	0.42
1:C:423:GLU:O	1:C:429:LYS:HG2	2.19	0.42
1:C:554:VAL:HG21	1:C:610:ILE:HD11	2.02	0.42
1:C:676:GLY:HA3	1:C:678:THR:N	2.34	0.42
1:D:413:ALA:O	1:D:635:TRP:NE1	2.52	0.42
1:A:69:ARG:CG	1:A:70:TYR:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ASN:OD1	1:A:492:GLY:N	2.52	0.42
1:A:491:LYS:O	1:A:494:VAL:HB	2.19	0.42
1:A:974:GLY:O	1:A:975:SER:OG	2.24	0.42
1:B:825:TRP:HB2	1:B:942:TYR:CE2	2.55	0.42
1:B:913:LEU:HD13	1:B:929:TRP:HE3	1.84	0.42
1:C:94:GLY:HA2	1:C:95:LYS:CB	2.48	0.42
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.85	0.42
1:A:85:SER:N	1:A:86:LEU:HB2	2.35	0.42
1:A:561:LYS:HD3	1:A:563:ARG:NH1	2.34	0.42
1:A:590:SER:OG	1:A:651:MET:SD	2.75	0.42
1:A:718:ASN:O	1:A:719:ASN:C	2.63	0.42
1:B:620:LEU:O	1:B:621:ALA:C	2.62	0.42
1:C:752:ASP:HA	1:C:755:ARG:NH2	2.34	0.42
1:C:760:GLY:HA3	1:C:761:GLY:HA3	1.70	0.42
1:D:211:ALA:HB2	1:D:231:LYS:O	2.20	0.42
1:D:432:MET:HE2	1:D:436:ILE:HG13	2.01	0.42
1:A:410:LYS:HG2	1:A:411:PRO:O	2.20	0.42
1:A:554:VAL:HG21	1:A:610:ILE:HD11	2.00	0.42
1:A:660:TYR:HE2	1:A:754:LEU:HA	1.85	0.42
1:A:808:MET:HB3	1:A:809:GLN:HB2	1.99	0.42
1:B:113:ASN:O	1:B:114:PHE:HB2	2.19	0.42
1:B:760:GLY:HA3	1:B:761:GLY:HA3	1.75	0.42
1:C:86:LEU:N	1:C:87:THR:C	2.77	0.42
1:C:621:ALA:HB2	1:C:629:TYR:CZ	2.55	0.42
1:A:442:ASN:O	1:A:446:LYS:HB3	2.20	0.42
1:A:808:MET:N	1:A:809:GLN:HB3	2.34	0.42
1:A:886:HIS:O	1:A:890:CYS:N	2.42	0.42
1:A:928:TYR:OH	1:B:963:GLN:NE2	2.52	0.42
1:C:287:HIS:CD2	1:C:288:LEU:HD23	2.55	0.42
1:D:321:SER:C	1:D:323:ALA:N	2.78	0.42
1:D:538:TYR:CZ	1:D:635:TRP:HB2	2.54	0.42
1:A:86:LEU:H	1:A:87:THR:C	2.27	0.42
1:A:133:LYS:C	1:A:133:LYS:CD	2.91	0.42
1:A:455:VAL:CG2	1:A:461:PHE:CE1	3.02	0.42
1:A:470:ASN:OD1	1:A:472:ARG:HB3	2.20	0.42
1:A:510:ILE:HD13	1:A:510:ILE:HG21	1.52	0.42
1:A:843:SER:OG	1:A:847:ARG:CB	2.57	0.42
1:B:155:ARG:NH2	1:B:401:GLU:OE2	2.51	0.42
1:B:555:HIS:CE1	1:B:599:PHE:CE1	3.07	0.42
1:D:564:ASP:HB3	1:D:571:TYR:HE2	1.85	0.42
1:A:175:ALA:HB3	1:A:179:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:PHE:CE1	1:A:518:GLN:HG2	2.55	0.42
1:B:523:GLU:HA	1:B:526:ARG:HG2	2.02	0.42
1:C:25:GLU:CB	1:C:26:VAL:HG22	2.50	0.42
1:C:85:SER:N	1:C:86:LEU:HB2	2.35	0.42
1:D:155:ARG:NH2	1:D:401:GLU:OE2	2.53	0.42
1:A:25:GLU:CB	1:A:26:VAL:HG22	2.50	0.42
1:A:152:ARG:HH22	1:A:360:GLY:N	2.18	0.42
1:A:355:ILE:HD12	1:A:404:SER:O	2.19	0.42
1:C:155:ARG:NH2	1:C:401:GLU:OE2	2.53	0.42
1:C:710:TYR:C	1:C:710:TYR:CD1	2.97	0.42
1:D:29:ARG:O	1:D:30:LEU:CB	2.68	0.42
1:D:29:ARG:O	1:D:30:LEU:HB2	2.19	0.42
1:D:94:GLY:HA2	1:D:95:LYS:CB	2.50	0.42
1:D:760:GLY:HA3	1:D:761:GLY:HA3	1.74	0.42
1:D:825:TRP:HB2	1:D:942:TYR:CE2	2.55	0.42
1:B:25:GLU:CB	1:B:26:VAL:HG22	2.50	0.42
1:B:287:HIS:CD2	1:B:288:LEU:HD23	2.55	0.42
1:B:794:LYS:HB3	1:B:795:PRO:HD3	2.01	0.42
1:C:138:PHE:HE1	1:C:168:PRO:HG2	1.85	0.42
1:C:791:ALA:O	1:C:795:PRO:HG2	2.19	0.42
1:C:943:LYS:CA	1:C:944:THR:CB	2.98	0.42
1:D:943:LYS:CA	1:D:944:THR:CB	2.97	0.42
1:A:287:HIS:CD2	1:A:288:LEU:HD23	2.54	0.41
1:A:946:PRO:O	1:A:950:TRP:HD1	2.02	0.41
1:D:23:SER:CB	1:D:26:VAL:O	2.68	0.41
1:D:94:GLY:HA2	1:D:95:LYS:HB2	2.01	0.41
1:D:808:MET:H	1:D:809:GLN:HB3	1.84	0.41
1:D:966:SER:C	1:D:973:GLY:HA2	2.45	0.41
1:A:179:LEU:HD23	1:A:180:LYS:CB	2.50	0.41
1:A:284:TYR:CE2	1:A:285:GLN:HG2	2.54	0.41
1:A:306:THR:HA	1:A:399:THR:HA	2.02	0.41
1:A:524:VAL:HG12	1:A:530:ASN:HD21	1.85	0.41
1:B:151:CYS:SG	1:B:154:THR:HG23	2.60	0.41
1:B:187:VAL:O	1:B:190:TRP:HB3	2.20	0.41
1:C:808:MET:H	1:C:809:GLN:HB3	1.86	0.41
1:D:579:VAL:HG12	1:D:638:TRP:HB3	2.01	0.41
1:A:153:LEU:HB3	1:A:162:PHE:CZ	2.55	0.41
1:A:484:LEU:HG	1:A:882:VAL:HG11	2.02	0.41
1:A:523:GLU:O	1:A:524:VAL:C	2.61	0.41
1:A:818:ASP:CG	1:A:820:ALA:HB3	2.45	0.41
1:A:978:MET:O	1:A:980:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ASP:OD1	1:B:564:ASP:C	2.63	0.41
1:B:840:THR:HA	1:B:843:SER:CB	2.50	0.41
1:B:943:LYS:CA	1:B:944:THR:CB	2.98	0.41
1:D:247:ALA:O	1:D:248:PRO:C	2.64	0.41
1:D:635:TRP:CZ2	1:D:637:CYS:HB2	2.56	0.41
1:A:161:ARG:NH2	1:A:267:ILE:HG22	2.34	0.41
1:A:173:LEU:N	1:A:173:LEU:HD12	2.35	0.41
1:A:941:TYR:HD1	1:A:944:THR:HG21	1.85	0.41
1:B:487:LEU:HD21	1:B:954:GLY:HA3	2.02	0.41
1:D:455:VAL:O	1:D:505:ARG:CG	2.68	0.41
1:D:660:TYR:CD1	1:D:660:TYR:N	2.88	0.41
1:D:806:LYS:H	1:D:807:VAL:CB	2.33	0.41
1:A:572:MET:CE	1:B:572:MET:CG	2.98	0.41
1:B:355:ILE:CG1	1:B:405:VAL:HG12	2.50	0.41
1:D:86:LEU:H	1:D:87:THR:C	2.28	0.41
1:D:794:LYS:CB	1:D:795:PRO:HD3	2.50	0.41
1:A:437:ALA:HB1	1:A:441:MET:HE3	2.03	0.41
1:A:863:GLU:HG3	1:A:888:LYS:NZ	2.35	0.41
1:B:304:THR:HG22	1:B:305:VAL:HG22	2.03	0.41
1:B:365:MET:HG2	1:B:629:TYR:O	2.20	0.41
1:D:151:CYS:SG	1:D:154:THR:HG23	2.60	0.41
1:D:246:PRO:HB2	1:D:247:ALA:CB	2.51	0.41
1:D:274:ASP:HA	1:D:279:LEU:HG	2.03	0.41
1:D:790:PHE:O	1:D:795:PRO:HD3	2.20	0.41
1:B:268:PRO:HB2	1:B:270:SER:OG	2.20	0.41
1:B:349:SER:O	1:B:350:ASP:HB2	2.21	0.41
1:C:640:PRO:O	1:C:644:GLU:HG2	2.20	0.41
1:C:688:TYR:O	1:C:692:ASN:HB2	2.21	0.41
1:D:153:LEU:HB3	1:D:162:PHE:CZ	2.55	0.41
1:A:455:VAL:HG22	1:A:461:PHE:CE1	2.56	0.41
1:A:539:MET:HE1	1:A:610:ILE:HB	2.01	0.41
1:B:29:ARG:O	1:B:30:LEU:CB	2.69	0.41
1:B:806:LYS:CA	1:B:807:VAL:CB	2.98	0.41
1:D:85:SER:N	1:D:86:LEU:HB2	2.36	0.41
1:D:660:TYR:CE2	1:D:754:LEU:HA	2.55	0.41
1:A:329:ASP:HB3	1:A:628:ASP:HB2	2.03	0.41
1:A:343:ARG:NH2	1:B:568:ASP:O	2.54	0.41
1:A:457:ARG:O	1:A:458:PRO:C	2.64	0.41
1:A:573:LEU:C	1:A:573:LEU:HD22	2.46	0.41
1:A:943:LYS:CB	1:A:944:THR:CB	2.89	0.41
1:A:1000:TYR:CD1	1:A:1000:TYR:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLN:CB	1:B:32:ASN:CB	2.95	0.41
1:B:88:GLN:C	1:B:90:ASP:H	2.28	0.41
1:B:173:LEU:HA	1:B:174:ASN:HA	1.82	0.41
1:B:333:ARG:NE	1:B:380:GLU:OE2	2.40	0.41
1:B:727:LEU:O	1:B:731:THR:CB	2.68	0.41
1:C:113:ASN:O	1:C:114:PHE:HB2	2.21	0.41
1:C:981:LEU:HB2	1:D:962:ALA:HB1	2.02	0.41
1:D:129:PHE:CZ	1:D:168:PRO:HB2	2.56	0.41
1:D:491:LYS:O	1:D:494:VAL:HB	2.20	0.41
1:D:808:MET:HB3	1:D:809:GLN:HB2	2.03	0.41
1:C:69:ARG:HG3	1:C:70:TYR:N	2.35	0.41
1:C:245:ARG:HD2	1:C:245:ARG:O	2.21	0.41
1:C:463:GLN:HE21	1:C:997:VAL:HG21	1.86	0.41
1:D:187:VAL:O	1:D:190:TRP:HB3	2.20	0.41
1:D:554:VAL:HG21	1:D:610:ILE:HD11	2.03	0.41
1:A:367:LEU:H	1:A:367:LEU:HG	1.84	0.40
1:A:458:PRO:O	1:A:459:LEU:C	2.63	0.40
1:A:521:ARG:HE	1:A:521:ARG:HB3	1.61	0.40
1:A:989:GLY:C	1:B:462:ARG:HH22	2.29	0.40
1:C:68:LEU:CA	1:C:69:ARG:HB2	2.51	0.40
1:D:27:TYR:CB	1:D:28:ALA:HA	2.51	0.40
1:D:446:LYS:NZ	1:D:447:GLN:HB3	2.37	0.40
1:A:119:ASN:OD1	1:A:147:PHE:HE1	2.03	0.40
1:A:122:VAL:HG21	1:A:148:ASP:OD2	2.20	0.40
1:B:426:ALA:O	1:B:427:LYS:C	2.64	0.40
1:B:554:VAL:HG21	1:B:610:ILE:HD11	2.03	0.40
1:B:818:ASP:HB2	1:B:820:ALA:HB3	2.03	0.40
1:C:481:VAL:HG13	1:C:493:GLU:HG2	2.03	0.40
1:D:321:SER:O	1:D:322:PRO:C	2.63	0.40
1:A:348:LEU:C	1:A:350:ASP:H	2.30	0.40
1:A:491:LYS:HB2	1:A:491:LYS:HZ3	1.86	0.40
1:A:675:THR:CG2	1:A:682:ALA:HA	2.51	0.40
1:B:25:GLU:HB2	1:B:26:VAL:CG2	2.52	0.40
1:C:395:ALA:HA	1:C:398:ARG:NH1	2.37	0.40
1:C:825:TRP:HB2	1:C:942:TYR:CE2	2.57	0.40
1:D:751:TRP:CZ2	1:D:755:ARG:HD3	2.56	0.40
1:A:23:SER:HB2	1:A:25:GLU:OE1	2.21	0.40
1:A:405:VAL:HG23	1:A:407:THR:CG2	2.52	0.40
1:A:657:LEU:CD1	1:A:731:THR:HG22	2.50	0.40
1:B:154:THR:HA	1:B:162:PHE:CE1	2.57	0.40
1:B:507:GLN:OE1	1:B:508:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:GLU:N	1:D:683:ARG:CZ	2.85	0.40
1:A:25:GLU:N	1:A:26:VAL:C	2.79	0.40
1:A:247:ALA:HB1	1:A:248:PRO:HD2	2.04	0.40
1:A:573:LEU:C	1:A:573:LEU:CD2	2.95	0.40
1:A:894:PRO:HD3	1:A:929:TRP:CE2	2.57	0.40
1:B:86:LEU:HB3	1:B:87:THR:CB	2.51	0.40
1:B:555:HIS:CD2	1:B:555:HIS:C	2.99	0.40
1:B:689:ASP:O	1:B:692:ASN:HB3	2.20	0.40
1:B:703:TYR:HE2	1:B:747:ASP:HA	1.87	0.40
1:C:86:LEU:H	1:C:87:THR:C	2.30	0.40
1:C:794:LYS:CB	1:C:795:PRO:HD3	2.51	0.40
1:D:122:VAL:HG12	1:D:123:LEU:C	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	904/1034 (87%)	779 (86%)	90 (10%)	35 (4%)	2	18
1	B	888/1034 (86%)	779 (88%)	84 (10%)	25 (3%)	4	25
1	C	888/1034 (86%)	786 (88%)	75 (8%)	27 (3%)	3	23
1	D	886/1034 (86%)	787 (89%)	71 (8%)	28 (3%)	3	21
All	All	3566/4136 (86%)	3131 (88%)	320 (9%)	115 (3%)	3	21

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	A	88	GLN
1	A	133	LYS

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Mol	Chain	Res	Type
1	A	137	LEU
1	A	184	ALA
1	A	243	ASP
1	A	413	ALA
1	A	807	VAL
1	A	820	ALA
1	A	867	LEU
1	A	944	THR
1	A	954	GLY
1	B	88	GLN
1	B	137	LEU
1	B	243	ASP
1	B	248	PRO
1	B	413	ALA
1	B	820	ALA
1	B	944	THR
1	B	954	GLY
1	C	88	GLN
1	C	137	LEU
1	C	243	ASP
1	C	413	ALA
1	C	807	VAL
1	C	820	ALA
1	C	944	THR
1	C	954	GLY
1	D	88	GLN
1	D	117	ARG
1	D	137	LEU
1	D	243	ASP
1	D	576	ASP
1	D	807	VAL
1	D	820	ALA
1	D	944	THR
1	D	954	GLY
1	A	30	LEU
1	A	31	GLN
1	A	95	LYS
1	A	97	PHE
1	A	99	GLU
1	A	117	ARG
1	A	131	PRO
1	A	185	ALA

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Mol	Chain	Res	Type
1	A	844	ARG
1	B	95	LYS
1	B	99	GLU
1	B	117	ARG
1	B	211	ALA
1	B	807	VAL
1	C	30	LEU
1	C	69	ARG
1	C	95	LYS
1	C	99	GLU
1	C	117	ARG
1	D	95	LYS
1	D	97	PHE
1	D	99	GLU
1	D	211	ALA
1	D	329	ASP
1	D	413	ALA
1	A	86	LEU
1	A	114	PHE
1	A	134	THR
1	A	561	LYS
1	A	764	SER
1	B	30	LEU
1	B	86	LEU
1	B	97	PHE
1	B	269	VAL
1	B	561	LYS
1	B	844	ARG
1	C	31	GLN
1	C	86	LEU
1	C	97	PHE
1	C	248	PRO
1	C	264	ARG
1	C	329	ASP
1	C	561	LYS
1	C	844	ARG
1	D	30	LEU
1	D	31	GLN
1	D	86	LEU
1	D	844	ARG
1	A	89	LEU
1	B	89	LEU

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Mol	Chain	Res	Type
1	B	764	SER
1	C	89	LEU
1	D	69	ARG
1	D	89	LEU
1	D	561	LYS
1	A	481	VAL
1	A	847	ARG
1	B	31	GLN
1	B	264	ARG
1	C	809	GLN
1	C	847	ARG
1	D	322	PRO
1	A	248	PRO
1	A	809	GLN
1	B	908	LYS
1	C	100	ARG
1	D	100	ARG
1	D	809	GLN
1	A	100	ARG
1	A	267	ILE
1	B	100	ARG
1	A	175	ALA
1	A	136	PRO
1	C	26	VAL
1	C	136	PRO
1	D	66	PRO
1	D	26	VAL
1	D	136	PRO

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	775/856 (90%)	693 (89%)	82 (11%)	6	27
1	B	646/856 (76%)	572 (88%)	74 (12%)	5	24
1	C	650/856 (76%)	576 (89%)	74 (11%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	645/856 (75%)	570 (88%)	75 (12%)	5	24
All	All	2716/3424 (79%)	2411 (89%)	305 (11%)	6	25

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	23	SER
1	A	24	MET
1	A	39	ARG
1	A	40	TRP
1	A	48	LEU
1	A	57	LEU
1	A	67	THR
1	A	69	ARG
1	A	71	ASP
1	A	78	ASP
1	A	90	ASP
1	A	126	SER
1	A	133	LYS
1	A	134	THR
1	A	141	ASP
1	A	142	MET
1	A	145	LEU
1	A	146	ARG
1	A	153	LEU
1	A	178	ILE
1	A	195	PRO
1	A	197	SER
1	A	227	LYS
1	A	229	THR
1	A	245	ARG
1	A	249	LEU
1	A	267	ILE
1	A	300	LYS
1	A	317	ASP
1	A	341	LYS
1	A	349	SER
1	A	368	MET
1	A	387	LYS
1	A	415	ASN
1	A	416	LEU

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Mol	Chain	Res	Type
1	A	427	LYS
1	A	446	LYS
1	A	459	LEU
1	A	469	THR
1	A	483	PHE
1	A	495	LEU
1	A	499	LEU
1	A	513	LEU
1	A	521	ARG
1	A	530	ASN
1	A	544	ASP
1	A	564	ASP
1	A	570	THR
1	A	573	LEU
1	A	577	CYS
1	A	620	LEU
1	A	647	THR
1	A	678	THR
1	A	706	ILE
1	A	717	HIS
1	A	728	LEU
1	A	740	SER
1	A	742	GLN
1	A	745	LEU
1	A	756	ARG
1	A	763	MET
1	A	767	ASP
1	A	780	GLU
1	A	794	LYS
1	A	804	LEU
1	A	807	VAL
1	A	808	MET
1	A	817	ASP
1	A	840	THR
1	A	861	GLU
1	A	862	HIS
1	A	866	VAL
1	A	868	MET
1	A	877	THR
1	A	926	THR
1	A	927	SER
1	A	933	ARG

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Mol	Chain	Res	Type
1	A	949	VAL
1	A	985	LEU
1	A	1001	LEU
1	A	1003	ARG
1	B	36	LYS
1	B	40	TRP
1	B	66	PRO
1	B	67	THR
1	B	117	ARG
1	B	126	SER
1	B	145	LEU
1	B	153	LEU
1	B	195	PRO
1	B	227	LYS
1	B	230	PHE
1	B	245	ARG
1	B	248	PRO
1	B	249	LEU
1	B	267	LEU
1	B	316	THR
1	B	319	ILE
1	B	336	ARG
1	B	337	SER
1	B	340	ARG
1	B	341	LYS
1	B	346	LEU
1	B	375	ASP
1	B	394	ASP
1	B	407	THR
1	B	411	PRO
1	B	416	LEU
1	B	425	ARG
1	B	427	LYS
1	B	431	ARG
1	B	446	LYS
1	B	455	VAL
1	B	469	THR
1	B	483	PHE
1	B	495	LEU
1	B	510	ILE
1	B	527	THR
1	B	530	ASN

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Mol	Chain	Res	Type
1	B	544	ASP
1	B	564	ASP
1	B	569	THR
1	B	570	THR
1	B	573	LEU
1	B	580	LEU
1	B	613	PRO
1	B	620	LEU
1	B	633	MET
1	B	647	THR
1	B	678	THR
1	B	683	ARG
1	B	689	ASP
1	B	727	LEU
1	B	728	LEU
1	B	740	SER
1	B	741	LYS
1	B	742	GLN
1	B	775	TRP
1	B	780	GLU
1	B	808	MET
1	B	817	ASP
1	B	840	THR
1	B	844	ARG
1	B	849	VAL
1	B	861	GLU
1	B	866	VAL
1	B	877	THR
1	B	909	THR
1	B	916	PRO
1	B	926	THR
1	B	949	VAL
1	B	981	LEU
1	B	985	LEU
1	B	998	LYS
1	B	1003	ARG
1	C	36	LYS
1	C	40	TRP
1	C	66	PRO
1	C	67	THR
1	C	90	ASP
1	C	126	SER

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Mol	Chain	Res	Type
1	C	139	LEU
1	C	145	LEU
1	C	153	LEU
1	C	195	PRO
1	C	227	LYS
1	C	230	PHE
1	C	245	ARG
1	C	248	PRO
1	C	249	LEU
1	C	267	LEU
1	C	268	PRO
1	C	316	THR
1	C	319	ILE
1	C	336	ARG
1	C	337	SER
1	C	341	LYS
1	C	346	LEU
1	C	375	ASP
1	C	387	LYS
1	C	411	PRO
1	C	416	LEU
1	C	425	ARG
1	C	427	LYS
1	C	455	VAL
1	C	468	CYS
1	C	469	THR
1	C	483	PHE
1	C	495	LEU
1	C	499	LEU
1	C	510	ILE
1	C	521	ARG
1	C	527	THR
1	C	530	ASN
1	C	532	HIS
1	C	544	ASP
1	C	560	SER
1	C	564	ASP
1	C	565	ASP
1	C	571	TYR
1	C	573	LEU
1	C	580	LEU
1	C	613	PRO

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Mol	Chain	Res	Type
1	C	620	LEU
1	C	641	ASP
1	C	647	THR
1	C	650	ASP
1	C	672	VAL
1	C	678	THR
1	C	727	LEU
1	C	728	LEU
1	C	740	SER
1	C	742	GLN
1	C	750	SER
1	C	775	TRP
1	C	794	LYS
1	C	802	GLU
1	C	808	MET
1	C	817	ASP
1	C	840	THR
1	C	849	VAL
1	C	861	GLU
1	C	877	THR
1	C	916	PRO
1	C	926	THR
1	C	949	VAL
1	C	981	LEU
1	C	985	LEU
1	C	1003	ARG
1	D	36	LYS
1	D	40	TRP
1	D	66	PRO
1	D	67	THR
1	D	71	ASP
1	D	90	ASP
1	D	117	ARG
1	D	126	SER
1	D	145	LEU
1	D	153	LEU
1	D	195	PRO
1	D	230	PHE
1	D	248	PRO
1	D	249	LEU
1	D	255	LEU
1	D	256	PRO

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Mol	Chain	Res	Type
1	D	319	ILE
1	D	337	SER
1	D	341	LYS
1	D	375	ASP
1	D	377	ASP
1	D	411	PRO
1	D	416	LEU
1	D	417	GLN
1	D	425	ARG
1	D	427	LYS
1	D	446	LYS
1	D	455	VAL
1	D	468	CYS
1	D	469	THR
1	D	483	PHE
1	D	495	LEU
1	D	510	ILE
1	D	513	LEU
1	D	521	ARG
1	D	527	THR
1	D	530	ASN
1	D	532	HIS
1	D	544	ASP
1	D	560	SER
1	D	563	ARG
1	D	564	ASP
1	D	570	THR
1	D	573	LEU
1	D	577	CYS
1	D	580	LEU
1	D	613	PRO
1	D	620	LEU
1	D	647	THR
1	D	650	ASP
1	D	672	VAL
1	D	675	THR
1	D	727	LEU
1	D	728	LEU
1	D	731	THR
1	D	740	SER
1	D	742	GLN
1	D	750	SER

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Mol	Chain	Res	Type
1	D	756	ARG
1	D	780	GLU
1	D	801	LEU
1	D	804	LEU
1	D	808	MET
1	D	817	ASP
1	D	840	THR
1	D	849	VAL
1	D	861	GLU
1	D	877	THR
1	D	916	PRO
1	D	926	THR
1	D	949	VAL
1	D	981	LEU
1	D	985	LEU
1	D	998	LYS
1	D	1003	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	58	HIS
1	A	202	GLN
1	A	397	HIS
1	A	417	GLN
1	A	463	GLN
1	A	478	HIS
1	A	587	HIS
1	A	684	HIS
1	A	709	ASN
1	A	915	GLN
1	A	963	GLN
1	B	58	HIS
1	B	202	GLN
1	B	463	GLN
1	B	478	HIS
1	B	500	ASN
1	B	555	HIS
1	B	783	HIS
1	B	956	GLN
1	B	963	GLN

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Mol	Chain	Res	Type
1	C	58	HIS
1	C	202	GLN
1	C	295	GLN
1	C	417	GLN
1	C	463	GLN
1	C	478	HIS
1	C	823	HIS
1	C	963	GLN
1	D	417	GLN
1	D	447	GLN
1	D	463	GLN
1	D	478	HIS
1	D	823	HIS
1	D	963	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](#)

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	924/1034 (89%)	0.31	61 (6%) 24 15	11, 21, 94, 177	0
1	B	922/1034 (89%)	0.62	136 (14%) 5 4	9, 25, 146, 228	0
1	C	922/1034 (89%)	1.48	257 (27%) 1 1	25, 71, 152, 347	0
1	D	922/1034 (89%)	1.57	302 (32%) 1 1	24, 71, 221, 430	0
All	All	3690/4136 (89%)	0.99	756 (20%) 2 2	9, 53, 158, 430	0

All (756) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	LEU	11.2
1	B	484	LEU	9.4
1	B	934	ALA	8.1
1	B	951	GLN	8.1
1	B	836	PHE	8.1
1	B	894	PRO	8.0
1	D	43	ALA	7.6
1	D	936	THR	7.5
1	A	108	ALA	7.0
1	B	517	LEU	6.9
1	B	839	LEU	6.8
1	B	937	ALA	6.8
1	D	910	ALA	6.7
1	C	47	ALA	6.7
1	C	52	LEU	6.7
1	B	829	LEU	6.7
1	C	504	ASP	6.6
1	C	827	PRO	6.5
1	D	45	PRO	6.5
1	C	50	TRP	6.5
1	D	836	PHE	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	1002	ALA	6.4
1	C	988	ALA	6.3
1	B	955	ALA	6.3
1	D	277	LEU	6.2
1	D	413	ALA	6.2
1	B	507	GLN	6.1
1	D	966	SER	6.1
1	D	950	TRP	6.1
1	D	97	PHE	6.1
1	C	40	TRP	6.0
1	C	105	ALA	6.0
1	D	913	LEU	6.0
1	D	834	GLU	5.9
1	C	178	ILE	5.9
1	C	46	LEU	5.9
1	C	481	VAL	5.8
1	A	47	ALA	5.8
1	B	913	LEU	5.8
1	D	481	VAL	5.7
1	A	107	ALA	5.7
1	D	955	ALA	5.6
1	D	863	GLU	5.6
1	C	460	GLN	5.6
1	C	41	LEU	5.5
1	C	393	ALA	5.5
1	D	800	GLU	5.4
1	D	937	ALA	5.4
1	D	531	ILE	5.4
1	C	346	LEU	5.4
1	C	79	MET	5.3
1	D	804	LEU	5.3
1	C	76	THR	5.3
1	A	83	TRP	5.3
1	D	473	SER	5.3
1	D	44	ALA	5.3
1	A	175	ALA	5.3
1	D	820	ALA	5.2
1	B	938	PHE	5.2
1	D	210	ASP	5.2
1	D	894	PRO	5.2
1	B	909	THR	5.2
1	C	394	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	820	ALA	5.1
1	D	954	GLY	5.1
1	D	480	GLN	5.1
1	D	510	ILE	5.1
1	C	45	PRO	5.1
1	C	49	ALA	5.0
1	B	497	PHE	5.0
1	C	589	PRO	5.0
1	D	912	LEU	5.0
1	D	560	SER	5.0
1	B	847	ARG	4.9
1	D	417	GLN	4.9
1	D	182	GLY	4.9
1	C	520	GLN	4.9
1	D	479	GLY	4.8
1	C	93	ARG	4.8
1	C	818	ASP	4.8
1	C	301	THR	4.8
1	C	701	PRO	4.8
1	A	179	LEU	4.8
1	B	928	TYR	4.8
1	C	96	SER	4.8
1	D	92	PHE	4.8
1	D	951	GLN	4.7
1	A	818	ASP	4.7
1	B	877	THR	4.6
1	D	37	PHE	4.6
1	D	801	LEU	4.6
1	D	530	ASN	4.6
1	C	586	ALA	4.6
1	D	558	PHE	4.6
1	B	513	LEU	4.6
1	D	932	LEU	4.6
1	C	305	VAL	4.6
1	D	930	ALA	4.5
1	C	73	SER	4.5
1	D	835	ASN	4.5
1	B	514	ALA	4.5
1	D	526	ARG	4.5
1	D	949	VAL	4.5
1	C	304	THR	4.4
1	B	885	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	248	PRO	4.4
1	C	243	ASP	4.4
1	C	75	ALA	4.4
1	C	324	GLY	4.4
1	A	77	SER	4.4
1	D	492	GLY	4.3
1	D	943	LYS	4.3
1	B	911	ALA	4.3
1	B	41	LEU	4.3
1	C	474	GLU	4.3
1	C	97	PHE	4.3
1	D	819	ASP	4.3
1	D	963	GLN	4.3
1	D	916	PRO	4.3
1	D	948	PHE	4.3
1	D	495	LEU	4.3
1	B	809	GLN	4.3
1	D	476	VAL	4.3
1	A	52	LEU	4.2
1	D	139	LEU	4.2
1	B	838	ALA	4.2
1	A	79	MET	4.2
1	D	952	MET	4.2
1	D	460	GLN	4.2
1	D	833	PHE	4.2
1	D	468	CYS	4.2
1	C	205	ALA	4.1
1	B	950	TRP	4.1
1	B	922	GLY	4.1
1	D	662	GLY	4.1
1	D	31	GLN	4.1
1	D	38	PRO	4.1
1	B	824	SER	4.1
1	D	839	LEU	4.1
1	D	489	GLU	4.1
1	B	893	GLU	4.1
1	D	602	GLN	4.1
1	D	491	LYS	4.0
1	D	808	MET	4.0
1	C	78	ASP	4.0
1	C	987	TYR	4.0
1	B	882	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	819	ASP	4.0
1	C	828	ASP	4.0
1	D	938	PHE	4.0
1	C	35	PRO	4.0
1	C	300	LYS	4.0
1	D	866	VAL	4.0
1	D	76	THR	4.0
1	D	935	SER	4.0
1	C	472	ARG	3.9
1	C	817	ASP	3.9
1	A	82	LEU	3.9
1	D	276	LEU	3.9
1	B	845	SER	3.9
1	C	39	ARG	3.9
1	C	927	SER	3.9
1	B	952	MET	3.9
1	B	890	CYS	3.9
1	D	909	THR	3.9
1	C	38	PRO	3.9
1	C	307	PHE	3.9
1	B	83	TRP	3.9
1	B	864	TRP	3.9
1	C	74	TRP	3.9
1	C	529	LEU	3.9
1	D	810	ALA	3.9
1	C	138	PHE	3.8
1	A	78	ASP	3.8
1	C	279	LEU	3.8
1	C	53	THR	3.8
1	D	824	SER	3.8
1	D	634	ALA	3.8
1	C	542	VAL	3.8
1	D	598	VAL	3.8
1	C	188	ILE	3.8
1	D	474	GLU	3.8
1	D	928	TYR	3.8
1	C	476	VAL	3.8
1	C	966	SER	3.8
1	B	510	ILE	3.8
1	A	407	THR	3.7
1	C	404	SER	3.7
1	B	826	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	849	VAL	3.7
1	C	273	LEU	3.7
1	D	140	LEU	3.7
1	A	176	PRO	3.7
1	D	914	GLU	3.7
1	D	88	GLN	3.7
1	D	864	TRP	3.7
1	A	922	GLY	3.7
1	B	848	ALA	3.6
1	D	91	VAL	3.6
1	D	934	ALA	3.6
1	C	166	LEU	3.6
1	C	190	TRP	3.6
1	D	83	TRP	3.6
1	D	953	ALA	3.6
1	C	191	LEU	3.6
1	B	956	GLN	3.6
1	B	485	GLY	3.6
1	C	109	ALA	3.6
1	C	104	GLU	3.6
1	B	482	PRO	3.6
1	C	323	ALA	3.6
1	B	837	LYS	3.6
1	B	518	GLN	3.6
1	C	808	MET	3.6
1	C	829	LEU	3.6
1	C	280	GLU	3.5
1	C	503	PHE	3.5
1	C	917	PHE	3.5
1	C	34	TRP	3.5
1	D	493	GLU	3.5
1	C	281	GLN	3.5
1	C	55	ILE	3.5
1	A	836	PHE	3.5
1	B	939	LYS	3.5
1	D	926	THR	3.5
1	D	983	THR	3.5
1	D	49	ALA	3.5
1	D	931	LEU	3.5
1	D	392	ASP	3.5
1	B	476	VAL	3.4
1	A	67	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	820	ALA	3.4
1	D	28	ALA	3.4
1	C	501	SER	3.4
1	D	892	ILE	3.4
1	B	831	VAL	3.4
1	B	94	GLY	3.4
1	D	50	TRP	3.4
1	C	738	ASP	3.4
1	C	246	PRO	3.4
1	D	335	SER	3.4
1	B	52	LEU	3.4
1	C	997	VAL	3.4
1	D	933	ARG	3.4
1	B	118	GLY	3.4
1	C	44	ALA	3.4
1	C	502	GLY	3.4
1	C	204	GLN	3.4
1	C	473	SER	3.3
1	C	449	ASP	3.3
1	C	242	HIS	3.3
1	D	144	PRO	3.3
1	D	490	ASN	3.3
1	C	106	PHE	3.3
1	C	265	ALA	3.3
1	D	109	ALA	3.3
1	D	504	ASP	3.3
1	C	367	LEU	3.3
1	A	247	ALA	3.3
1	C	371	ALA	3.3
1	D	940	ALA	3.3
1	D	282	ASN	3.3
1	D	825	TRP	3.3
1	D	211	ALA	3.3
1	C	516	ASP	3.3
1	B	957	LEU	3.3
1	D	123	LEU	3.3
1	D	939	LYS	3.3
1	D	472	ARG	3.2
1	D	661	LEU	3.2
1	B	935	SER	3.2
1	C	416	LEU	3.2
1	D	394	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	936	THR	3.2
1	C	128	GLU	3.2
1	C	200	GLY	3.2
1	C	236	PHE	3.2
1	C	543	VAL	3.2
1	C	590	SER	3.2
1	D	199	VAL	3.2
1	D	831	VAL	3.2
1	C	809	GLN	3.2
1	B	892	ILE	3.2
1	B	117	ARG	3.2
1	C	28	ALA	3.2
1	D	175	ALA	3.2
1	D	945	ASN	3.2
1	B	136	PRO	3.2
1	D	485	GLY	3.2
1	C	51	GLU	3.2
1	D	41	LEU	3.2
1	C	147	PHE	3.2
1	C	207	TYR	3.2
1	B	503	PHE	3.1
1	D	941	TYR	3.1
1	C	77	SER	3.1
1	C	681	ALA	3.1
1	D	478	HIS	3.1
1	A	249	LEU	3.1
1	C	512	ASP	3.1
1	D	161	ARG	3.1
1	C	101	PRO	3.1
1	D	209	LYS	3.1
1	B	481	VAL	3.1
1	B	524	VAL	3.1
1	C	114	PHE	3.1
1	D	737	VAL	3.1
1	D	860	VAL	3.1
1	C	528	LYS	3.1
1	D	1006	CYS	3.1
1	D	470	ASN	3.1
1	A	97	PHE	3.1
1	C	244	PHE	3.1
1	C	545	PHE	3.1
1	D	893	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	466	ASN	3.0
1	D	985	LEU	3.0
1	D	721	VAL	3.0
1	D	828	ASP	3.0
1	D	832	TYR	3.0
1	C	127	LEU	3.0
1	C	945	ASN	3.0
1	C	700	GLN	3.0
1	B	40	TRP	3.0
1	B	914	GLU	3.0
1	C	932	LEU	3.0
1	D	606	LEU	3.0
1	C	107	ALA	3.0
1	B	512	ASP	3.0
1	C	826	ASP	3.0
1	C	186	GLN	3.0
1	A	66	PRO	3.0
1	A	131	PRO	3.0
1	C	110	LEU	3.0
1	D	275	TRP	3.0
1	C	322	PRO	3.0
1	D	484	LEU	3.0
1	D	822	ALA	3.0
1	C	92	PHE	3.0
1	D	120	THR	3.0
1	C	933	ARG	2.9
1	D	47	ALA	2.9
1	D	919	ALA	2.9
1	C	798	ASP	2.9
1	C	1001	LEU	2.9
1	D	829	LEU	2.9
1	C	916	PRO	2.9
1	D	837	LYS	2.9
1	B	958	ALA	2.9
1	C	859	ALA	2.9
1	D	852	ALA	2.9
1	C	299	SER	2.9
1	D	349	SER	2.9
1	D	142	MET	2.9
1	A	68	LEU	2.9
1	C	231	LYS	2.9
1	D	701	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	810	ALA	2.9
1	D	1002	ALA	2.9
1	C	187	VAL	2.9
1	B	515	PHE	2.9
1	D	927	SER	2.9
1	A	178	ILE	2.9
1	D	444	LEU	2.9
1	D	513	LEU	2.9
1	B	818	ASP	2.9
1	C	920	ASP	2.9
1	D	160	ASP	2.9
1	D	387	LYS	2.9
1	B	500	ASN	2.9
1	B	1006	CYS	2.9
1	C	934	ALA	2.9
1	D	308	GLU	2.9
1	D	393	ALA	2.9
1	D	887	ALA	2.9
1	B	110	LEU	2.9
1	D	517	LEU	2.9
1	B	134	THR	2.9
1	D	682	ALA	2.9
1	B	104	GLU	2.9
1	D	929	TRP	2.9
1	A	974	GLY	2.9
1	B	850	LEU	2.9
1	C	680	ALA	2.8
1	D	718	ASN	2.8
1	D	63	LEU	2.8
1	D	587	HIS	2.8
1	B	105	ALA	2.8
1	C	43	ALA	2.8
1	C	80	ALA	2.8
1	D	841	ALA	2.8
1	C	369	ASP	2.8
1	D	527	THR	2.8
1	D	668	PHE	2.8
1	C	928	TYR	2.8
1	B	886	HIS	2.8
1	D	604	HIS	2.8
1	D	353	SER	2.8
1	D	607	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	83	TRP	2.8
1	C	517	LEU	2.8
1	C	957	LEU	2.8
1	D	850	LEU	2.8
1	D	56	CYS	2.8
1	B	940	ALA	2.8
1	C	395	ALA	2.8
1	B	477	ARG	2.8
1	D	806	LYS	2.8
1	B	834	GLU	2.8
1	C	432	MET	2.8
1	B	830	ALA	2.8
1	B	887	ALA	2.8
1	C	233	ARG	2.8
1	D	494	VAL	2.8
1	A	48	LEU	2.8
1	D	179	LEU	2.8
1	A	851	GLU	2.8
1	A	181	ASP	2.7
1	B	70	TYR	2.7
1	D	1003	ARG	2.7
1	C	199	VAL	2.7
1	B	876	LEU	2.7
1	D	416	LEU	2.7
1	C	610	ILE	2.7
1	D	178	ILE	2.7
1	B	808	MET	2.7
1	B	964	MET	2.7
1	D	501	SER	2.7
1	B	835	ASN	2.7
1	C	958	ALA	2.7
1	D	412	ALA	2.7
1	B	480	GLN	2.7
1	C	195	PRO	2.7
1	C	706	ILE	2.7
1	D	588	PHE	2.7
1	D	744	ILE	2.7
1	C	274	ASP	2.7
1	D	455	VAL	2.7
1	D	946	PRO	2.7
1	B	504	ASP	2.7
1	C	993	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	249	LEU	2.7
1	C	314	HIS	2.7
1	D	113	ASN	2.7
1	C	992	PRO	2.7
1	D	463	GLN	2.7
1	A	283	GLU	2.7
1	D	53	THR	2.7
1	D	74	TRP	2.7
1	A	103	ALA	2.7
1	C	1000	TYR	2.7
1	D	725	VAL	2.7
1	B	78	ASP	2.7
1	B	953	ALA	2.6
1	C	471	SER	2.6
1	D	830	ALA	2.6
1	B	941	TYR	2.6
1	B	825	TRP	2.6
1	B	821	ALA	2.6
1	C	179	LEU	2.6
1	D	885	LEU	2.6
1	D	979	PRO	2.6
1	C	283	GLU	2.6
1	A	265	THR	2.6
1	C	145	LEU	2.6
1	D	918	LEU	2.6
1	D	27	TYR	2.6
1	D	33	ILE	2.6
1	A	242	HIS	2.6
1	B	823	HIS	2.6
1	D	404	SER	2.6
1	B	963	GLN	2.6
1	A	105	ALA	2.6
1	C	229	THR	2.6
1	C	837	LYS	2.6
1	D	635	TRP	2.6
1	C	784	ILE	2.6
1	B	478	HIS	2.6
1	B	884	GLN	2.6
1	D	956	GLN	2.6
1	C	94	GLY	2.6
1	D	442	ASN	2.6
1	D	500	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	889	TRP	2.5
1	D	34	TRP	2.5
1	C	230	PHE	2.5
1	D	509	TYR	2.5
1	D	975	SER	2.5
1	D	487	LEU	2.5
1	B	910	ALA	2.5
1	D	456	GLU	2.5
1	C	111	THR	2.5
1	C	302	PHE	2.5
1	D	862	HIS	2.5
1	A	241	GLY	2.5
1	B	857	LEU	2.5
1	C	606	LEU	2.5
1	D	292	SER	2.5
1	C	739	GLN	2.5
1	D	947	LYS	2.5
1	A	61	VAL	2.5
1	A	104	GLU	2.5
1	C	103	ALA	2.5
1	C	42	HIS	2.5
1	D	42	HIS	2.5
1	D	248	PRO	2.5
1	D	458	PRO	2.5
1	A	133	LYS	2.5
1	A	182	GLY	2.5
1	D	811	SER	2.5
1	C	33	ILE	2.5
1	C	327	MET	2.5
1	C	284	TYR	2.5
1	D	66	PRO	2.5
1	C	296	LEU	2.5
1	C	444	LEU	2.5
1	D	186	GLN	2.5
1	C	838	ALA	2.5
1	C	130	ASN	2.5
1	D	65	ASP	2.5
1	D	674	ASP	2.5
1	D	917	PHE	2.5
1	C	944	THR	2.5
1	D	840	THR	2.5
1	B	947	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	585	PRO	2.5
1	D	145	LEU	2.5
1	D	414	LEU	2.5
1	D	499	LEU	2.5
1	C	538	TYR	2.5
1	C	112	GLY	2.5
1	D	465	VAL	2.5
1	D	55	ILE	2.4
1	B	92	PHE	2.4
1	C	32	ASN	2.4
1	D	865	LYS	2.4
1	D	348	LEU	2.4
1	C	524	VAL	2.4
1	D	486	GLY	2.4
1	C	125	ALA	2.4
1	D	81	ALA	2.4
1	D	507	GLN	2.4
1	A	474	GLU	2.4
1	B	842	GLU	2.4
1	C	177	SER	2.4
1	D	299	SER	2.4
1	B	853	LEU	2.4
1	A	246	PRO	2.4
1	B	862	HIS	2.4
1	C	587	HIS	2.4
1	C	737	VAL	2.4
1	D	167	VAL	2.4
1	A	202	GLN	2.4
1	D	505	ARG	2.4
1	D	450	SER	2.4
1	B	82	LEU	2.4
1	D	110	LEU	2.4
1	D	984	PRO	2.4
1	D	350	ASP	2.4
1	D	818	ASP	2.4
1	C	942	TYR	2.4
1	D	886	HIS	2.4
1	B	43	ALA	2.4
1	B	806	LYS	2.4
1	C	475	ARG	2.4
1	B	489	GLU	2.4
1	D	857	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	981	LEU	2.4
1	D	471	SER	2.4
1	C	192	THR	2.4
1	D	962	ALA	2.4
1	D	106	PHE	2.4
1	D	52	LEU	2.4
1	B	58	HIS	2.3
1	C	113	ASN	2.3
1	D	719	ASN	2.3
1	D	141	ASP	2.3
1	D	942	TYR	2.3
1	C	952	MET	2.3
1	B	483	PHE	2.3
1	D	503	PHE	2.3
1	D	599	PHE	2.3
1	D	809	GLN	2.3
1	A	523	GLU	2.3
1	D	104	GLU	2.3
1	D	842	GLU	2.3
1	C	167	VAL	2.3
1	B	73	SER	2.3
1	C	286	PRO	2.3
1	C	366	TRP	2.3
1	C	100	ARG	2.3
1	D	838	ALA	2.3
1	B	912	LEU	2.3
1	D	89	LEU	2.3
1	C	493	GLU	2.3
1	A	121	VAL	2.3
1	C	131	PRO	2.3
1	A	132	SER	2.3
1	C	203	TRP	2.3
1	D	464	TRP	2.3
1	C	426	ALA	2.3
1	C	621	ALA	2.3
1	B	130	ASN	2.3
1	B	129	PHE	2.3
1	D	515	PHE	2.3
1	D	423	GLU	2.3
1	C	245	ARG	2.3
1	C	343	ARG	2.3
1	A	864	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	662	GLY	2.3
1	D	135	GLY	2.3
1	B	107	ALA	2.3
1	B	822	ALA	2.3
1	D	859	ALA	2.3
1	A	796	THR	2.3
1	D	96	SER	2.3
1	C	163	LEU	2.3
1	C	931	LEU	2.3
1	C	985	LEU	2.3
1	D	461	PHE	2.3
1	C	915	GLN	2.3
1	C	685	GLU	2.3
1	C	326	ILE	2.3
1	D	98	PRO	2.3
1	D	907	ALA	2.3
1	D	823	HIS	2.3
1	C	722	SER	2.3
1	B	832	TYR	2.3
1	A	915	GLN	2.3
1	C	180	LYS	2.3
1	C	165	VAL	2.3
1	C	329	ASP	2.3
1	C	565	ASP	2.3
1	A	99	GLU	2.2
1	C	185	ALA	2.2
1	D	614	ALA	2.2
1	D	153	LEU	2.2
1	D	198	LEU	2.2
1	D	980	LEU	2.2
1	D	483	PHE	2.2
1	B	116	SER	2.2
1	C	321	SER	2.2
1	C	382	TYR	2.2
1	C	921	ARG	2.2
1	C	518	GLN	2.2
1	C	714	VAL	2.2
1	D	854	GLN	2.2
1	D	148	ASP	2.2
1	C	342	ILE	2.2
1	C	858	GLY	2.2
1	C	989	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	411	PRO	2.2
1	A	230	PHE	2.2
1	D	888	LYS	2.2
1	C	189	ARG	2.2
1	D	477	ARG	2.2
1	C	126	SER	2.2
1	D	116	SER	2.2
1	D	278	GLN	2.2
1	D	181	ASP	2.2
1	B	879	PRO	2.2
1	C	360	GLY	2.2
1	D	482	PRO	2.2
1	D	525	LEU	2.2
1	C	161	ARG	2.2
1	D	84	ARG	2.2
1	A	30	LEU	2.2
1	B	863	GLU	2.2
1	C	282	ASN	2.2
1	D	48	LEU	2.2
1	D	279	LEU	2.2
1	D	603	LEU	2.2
1	B	72	PRO	2.2
1	B	226	ALA	2.2
1	C	345	ALA	2.2
1	D	151	CYS	2.2
1	C	392	ASP	2.2
1	C	491	LYS	2.2
1	D	448	PHE	2.2
1	A	460	GLN	2.2
1	C	495	LEU	2.2
1	D	310	ASN	2.2
1	B	135	GLY	2.2
1	D	488	PRO	2.2
1	B	817	ASP	2.2
1	A	909	THR	2.1
1	C	121	VAL	2.1
1	C	533	VAL	2.1
1	B	525	LEU	2.1
1	C	290	LEU	2.1
1	D	298	LEU	2.1
1	C	124	SER	2.1
1	C	272	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	740	SER	2.1
1	C	843	SER	2.1
1	D	496	SER	2.1
1	D	961	LYS	2.1
1	C	176	PRO	2.1
1	C	391	ASP	2.1
1	B	121	VAL	2.1
1	B	127	LEU	2.1
1	B	859	ALA	2.1
1	C	201	ARG	2.1
1	D	185	ALA	2.1
1	C	965	SER	2.1
1	B	948	PHE	2.1
1	D	579	VAL	2.1
1	C	208	THR	2.1
1	D	529	LEU	2.1
1	D	881	LYS	2.1
1	A	978	MET	2.1
1	A	975	SER	2.1
1	D	730	SER	2.1
1	D	790	PHE	2.1
1	D	965	SER	2.1
1	A	65	ASP	2.1
1	B	46	LEU	2.1
1	D	86	LEU	2.1
1	A	434	ARG	2.1
1	C	583	ARG	2.1
1	D	462	ARG	2.1
1	D	883	ARG	2.1
1	B	856	ALA	2.1
1	C	352	PRO	2.1
1	D	759	LEU	2.1
1	A	323	ALA	2.1
1	C	202	GLN	2.1
1	D	35	PRO	2.1
1	D	307	PHE	2.1
1	D	644	GLU	2.1
1	B	491	LYS	2.0
1	C	61	VAL	2.0
1	D	143	LYS	2.0
1	B	501	SER	2.0
1	A	63	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	113	ASN	2.0
1	C	277	LEU	2.0
1	C	298	LEU	2.0
1	C	549	LEU	2.0
1	D	119	ASN	2.0
1	D	855	ASN	2.0
1	C	196	HIS	2.0
1	D	388	TRP	2.0
1	A	59	CYS	2.0
1	D	586	ALA	2.0
1	C	588	PHE	2.0
1	C	842	GLU	2.0
1	C	398	ARG	2.0
1	B	77	SER	2.0
1	C	514	ALA	2.0
1	A	880	GLU	2.0
1	B	851	GLU	2.0
1	C	477	ARG	2.0
1	D	189	ARG	2.0
1	C	913	LEU	2.0
1	D	294	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.