



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:19 am BST

PDB ID : 5FSW
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

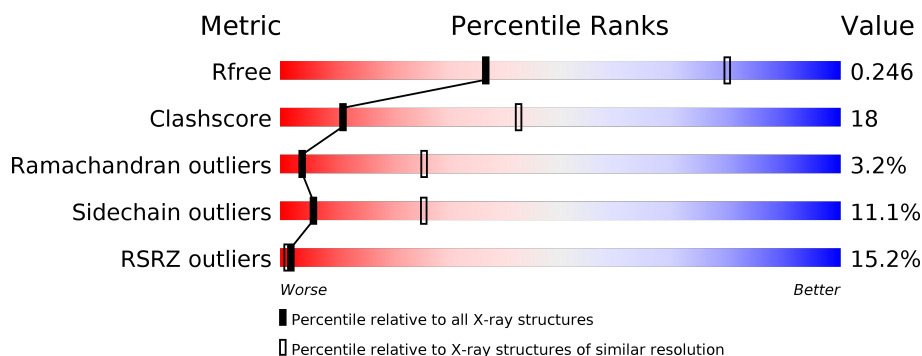
1 Overall quality at a glance ⓘ

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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	<div> <div>4%</div> <div>47%</div> <div>34%</div> <div>8%</div> <div>11%</div> </div>
1	B	1034	<div> <div>9%</div> <div>58%</div> <div>27%</div> <div>11%</div> </div>
1	C	1034	<div> <div>18%</div> <div>62%</div> <div>22%</div> <div>11%</div> </div>
1	D	1034	<div> <div>22%</div> <div>60%</div> <div>25%</div> <div>11%</div> </div>

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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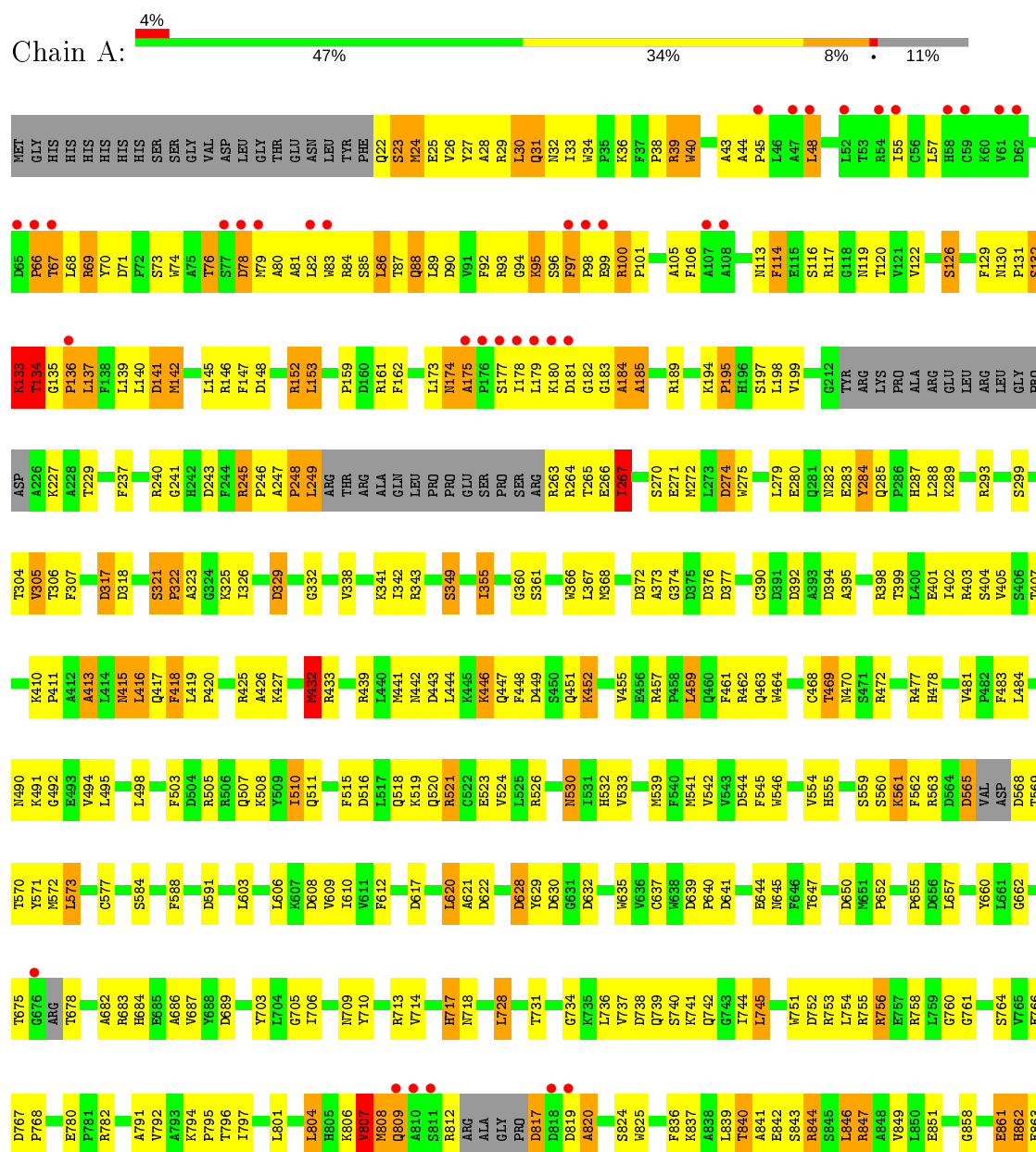
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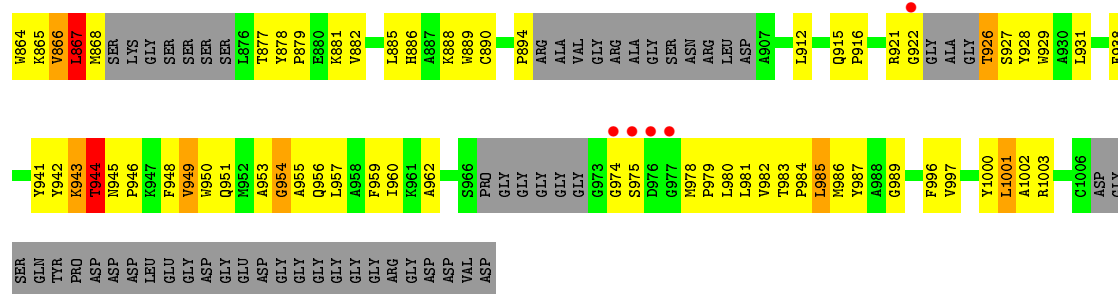
Chain	Residue	Modelled	Actual	Comment	Reference
C	16	THR	-	expression tag	UNP G2R911
C	17	GLU	-	expression tag	UNP G2R911
C	18	ASN	-	expression tag	UNP G2R911
C	19	LEU	-	expression tag	UNP G2R911
C	20	TYR	-	expression tag	UNP G2R911
C	21	PHE	-	expression tag	UNP G2R911
C	22	GLN	-	expression tag	UNP G2R911
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

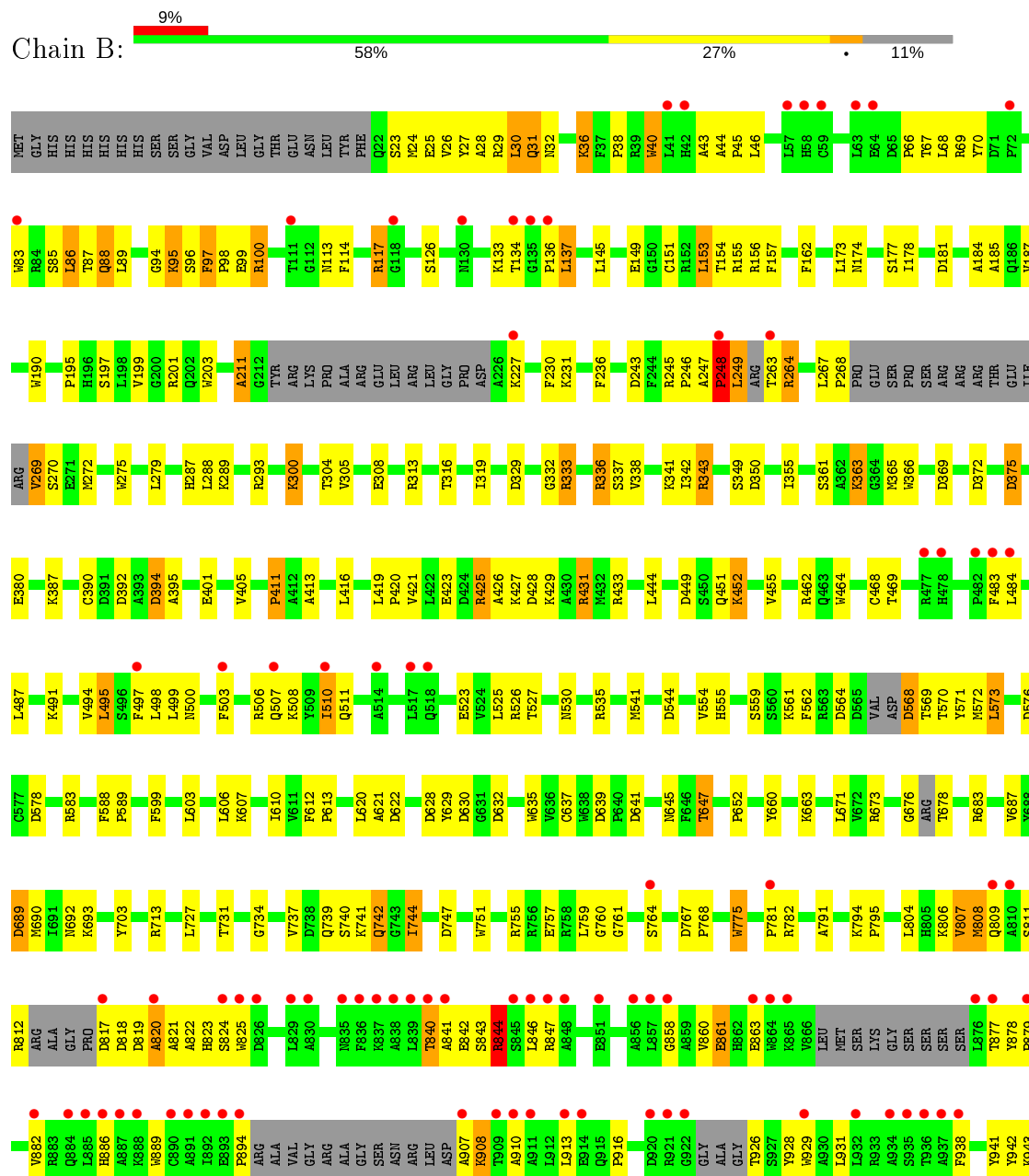
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

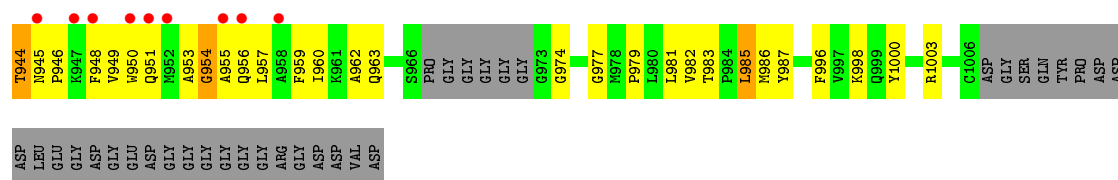
• Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1



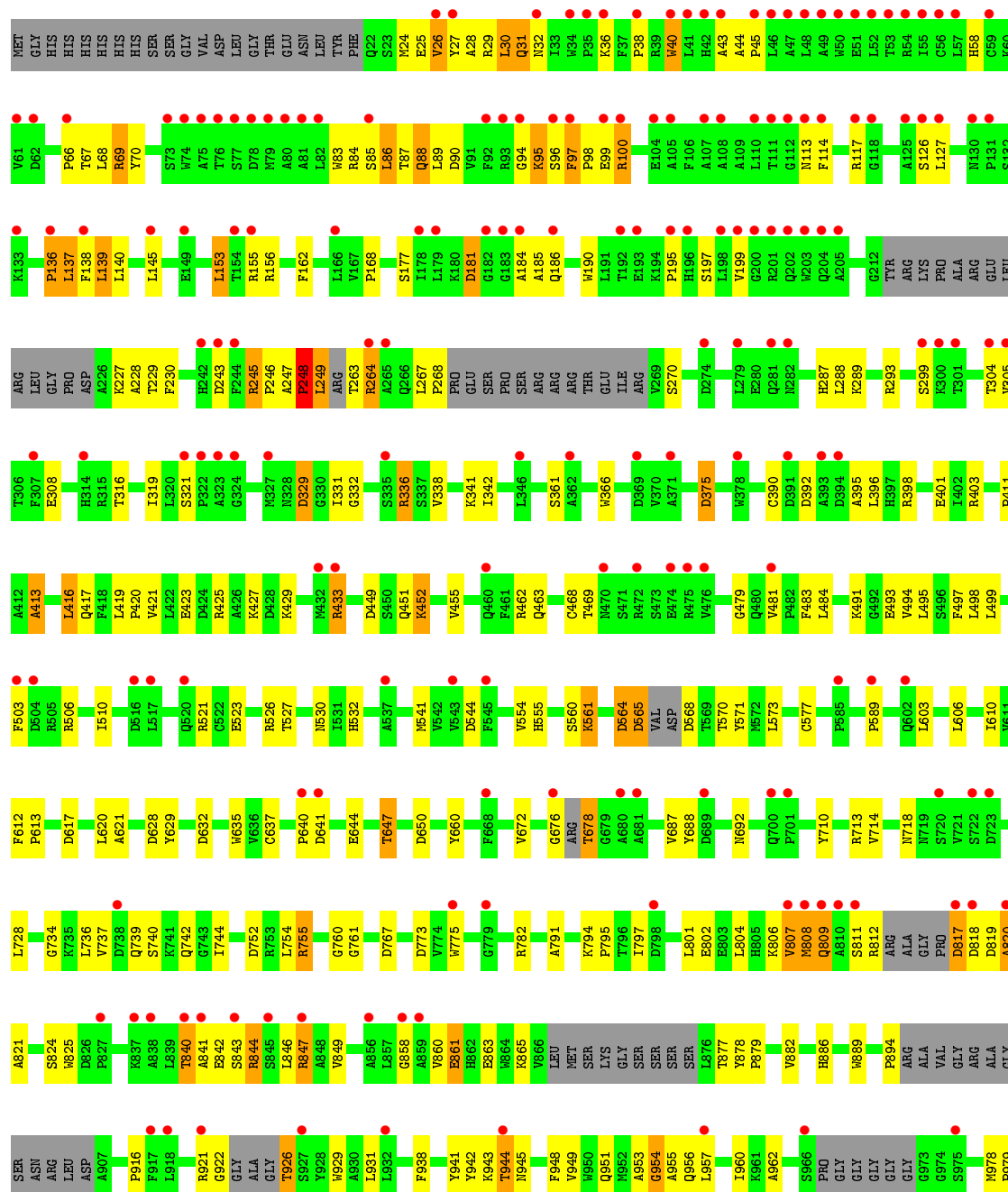


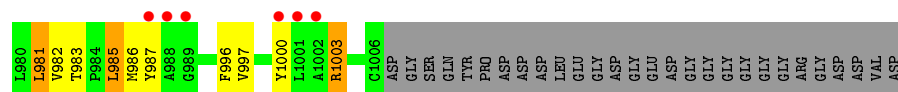
• Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1



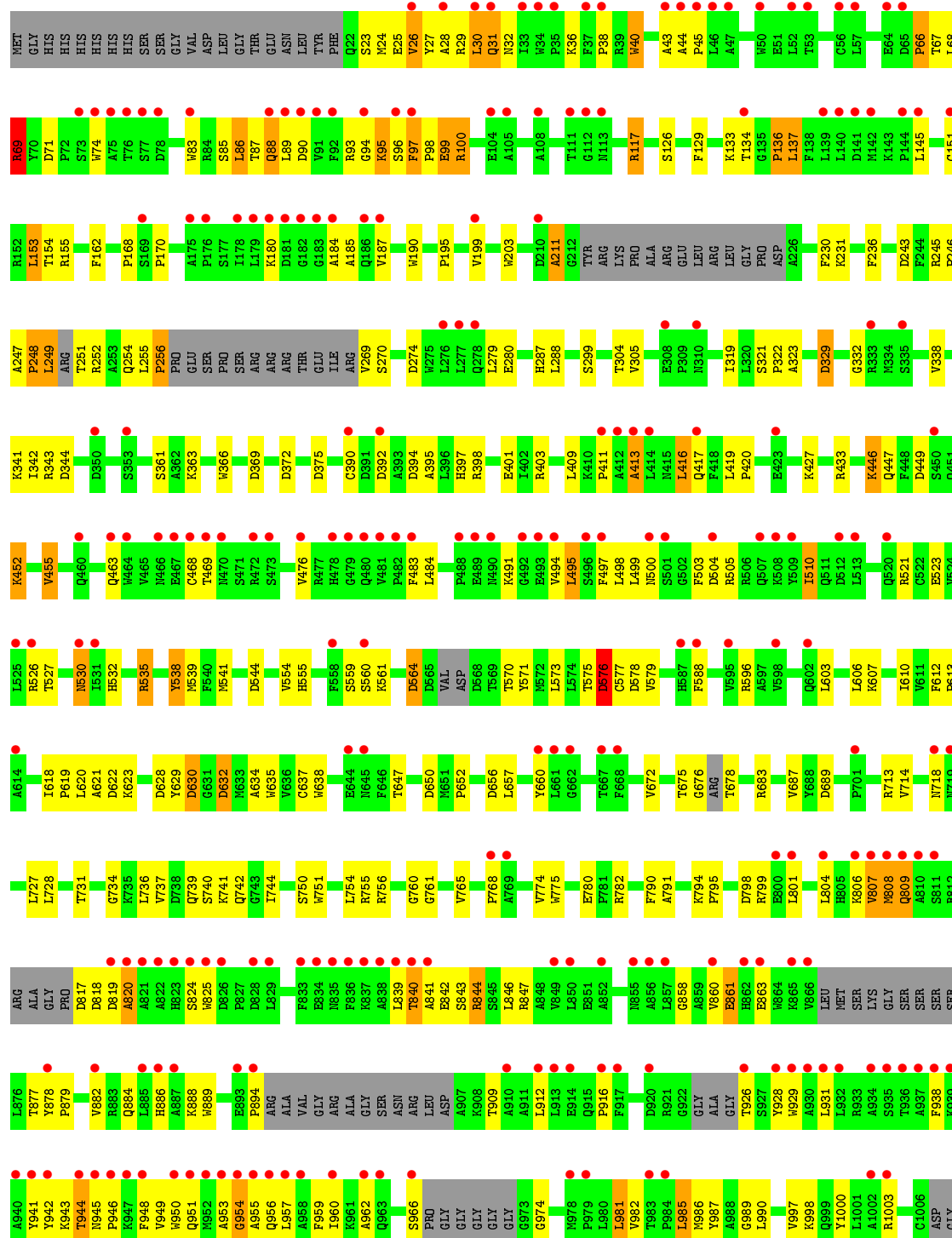


• Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1





● Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1



SER
GLN
TYR
PRO
ASP
ASP
ASP
LEU
GLY
GLY
ASP
GLY
GLU
ASP
GLY
GLY
GLY
GLY
GLY
ARG
GLY
ASP
ASP
VAL
ASP

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 , 78.1	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	0.85	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	0.92	8/7528 (0.1%)	1.07	25/10177 (0.2%)
1	B	0.82	6/7063 (0.1%)	0.97	20/9494 (0.2%)
1	C	0.56	0/7063	0.85	6/9494 (0.1%)
1	D	0.56	0/7062	0.82	5/9491 (0.1%)
All	All	0.74	14/28716 (0.0%)	0.93	56/38656 (0.1%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	GLU	CD-OE1	6.83	1.33	1.25
1	B	308	GLU	CG-CD	6.73	1.62	1.51
1	A	284	TYR	CD1-CE1	-6.49	1.29	1.39
1	A	401	GLU	CD-OE1	6.43	1.32	1.25
1	A	349	SER	CB-OG	6.19	1.50	1.42
1	A	546	TRP	CB-CG	6.06	1.61	1.50
1	B	308	GLU	CD-OE2	5.96	1.32	1.25
1	A	283	GLU	CD-OE2	5.92	1.32	1.25
1	B	632	ASP	CB-CG	5.78	1.63	1.51
1	A	571	TYR	CD1-CE1	-5.64	1.30	1.39
1	B	375	ASP	CB-CG	5.36	1.63	1.51
1	B	757	GLU	CD-OE1	-5.20	1.20	1.25
1	A	133	LYS	N-CA	5.15	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	PHE	CB-CG	-5.09	1.42	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	632	ASP	CB-CG-OD2	-13.18	106.44	118.30
1	A	425	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	B	632	ASP	CB-CG-OD1	11.51	128.66	118.30
1	B	333	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	A	650	ASP	CB-CG-OD1	8.67	126.10	118.30
1	B	583	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	630	ASP	CB-CG-OD1	7.92	125.42	118.30
1	B	583	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	376	ASP	CB-CG-OD1	-7.64	111.42	118.30
1	A	355	ILE	CG1-CB-CG2	-7.52	94.86	111.40
1	B	622	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	565	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C	331	ILE	CB-CA-C	-7.03	97.54	111.60
1	B	336	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	755	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	376	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	628	ASP	CB-CG-OD1	6.75	124.37	118.30
1	B	300	LYS	CA-CB-CG	6.73	128.20	113.40
1	A	571	TYR	CB-CG-CD1	-6.44	117.14	121.00
1	A	321	SER	C-N-CA	-6.42	95.06	122.00
1	C	336	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	425	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	535	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	152	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	921	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	D	535	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	578	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	B	576	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	B	571	TYR	CA-CB-CG	5.85	124.51	113.40
1	B	630	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	305	VAL	CG1-CB-CG2	-5.84	101.55	110.90
1	A	57	LEU	CA-CB-CG	5.72	128.47	115.30
1	A	377	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	744	ILE	CB-CA-C	-5.69	100.22	111.60
1	A	274	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	641	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	630	ASP	CB-CG-OD1	5.58	123.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	943	LYS	C-N-CA	5.55	135.57	121.70
1	A	432	MET	CG-SD-CE	-5.54	91.33	100.20
1	D	632	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	510	ILE	CG1-CB-CG2	-5.46	99.39	111.40
1	B	313	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	641	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	C	713	ARG	CG-CD-NE	5.39	123.11	111.80
1	B	343	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	571	TYR	CB-CA-C	-5.38	99.65	110.40
1	C	767	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	630	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	944	THR	N-CA-CB	5.34	120.44	110.30
1	B	279	LEU	CB-CA-C	-5.31	100.11	110.20
1	C	433	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	329	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	425	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	578	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	728	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	A	846	LEU	N-CA-C	5.01	124.54	111.00

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	444	0
1	B	6924	0	6423	216	0
1	C	6924	0	6423	181	0
1	D	6924	0	6422	199	0
All	All	28130	0	26547	981	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 18.

All (981) 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
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: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	1.34	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: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: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:A:321:SER:C	1:A:323:ALA:HA	1.90	0.90
1:C:806:LYS:HB3	1:C:807:VAL:CB	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:462:ARG:HD3	1:B:986:MET:CE	2.07	0.85
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: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:A:321:SER:HB3	1:A:323:ALA:C	2.01	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: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:804:LEU:C	1:A:807:VAL:HG11	2.02	0.79
1:C:1000:TYR:CE2	1:D:985:LEU:HD23	2.17	0.79
1:A:299:SER:OG	1:A:403:ARG:NH1	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:GLY:C	1:A:926:THR:N	2.37	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:O	1:A:807:VAL:HG13	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
1:C:97:PHE:HB3	1:C:98:PRO:HA	1.66	0.77
1:A:734:GLY:O	1:A:737:VAL:HG22	1.84	0.77
1:A:97:PHE:HB3	1:A:98:PRO:HA	1.64	0.77
1:B:734:GLY:O	1:B:737:VAL:HG22	1.84	0.77
1:B:97:PHE:HB3	1:B:98:PRO:HA	1.64	0.77
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:C:986:MET:HE2	1:D:499:LEU:O	1.84	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:C:184:ALA:HA	1:C:185:ALA:C	2.07	0.75
1:A:912:LEU:O	1:A:915:GLN:HG2	1.87	0.75
1:B:246:PRO:CB	1:B:247:ALA:HB2	2.16	0.75
1:B:31:GLN:CB	1:B:32:ASN:HB3	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:A:539:MET:CE	1:A:609:VAL:C	2.55	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:246:PRO:CB	1:D:247:ALA:HB2	2.17	0.74
1:D:31:GLN:CB	1:D:32:ASN:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:321:SER:C	1:A:323:ALA:N	2.40	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: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:184:ALA:HA	1:A:185:ALA:HB3	1.70	0.72
1:A:27:TYR:HB3	1:A:28:ALA:HA	1.71	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:D:256:PRO:C	1:D:269:VAL:N	2.43	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:129:PHE:CZ	1:A:179:LEU:HD11	2.24	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:87:THR:O	1:A:87:THR:OG1	2.04	0.70
1:A:807:VAL:CG1	1:A:807:VAL:O	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:O	1:A:561:LYS:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:THR:HG21	1:C:342:ILE:HG12	1.75	0.69
1:A:174:ASN:OD1	1:A:175:ALA:HB3	1.92	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
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:C:565:ASP:C	1:C:568:ASP:N	2.46	0.68
1:C:986:MET:CE	1:D:499:LEU:O	2.41	0.68
1:A:539:MET:HE2	1:A:610:ILE:N	2.08	0.68
1:A:441:MET:CE	1:A:792:VAL:HG13	2.24	0.67
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:23:SER:HG	1:A:24:MET:HA	1.59	0.67
1:D:806:LYS:HB3	1:D:807:VAL:CB	2.25	0.67
1:A:142:MET:N	1:A:142:MET:SD	2.67	0.67
1:C:922:GLY:HA3	1:D:974:GLY:O	1.94	0.67
1:A:745:LEU:C	1:A:745:LEU:HD23	2.15	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:184:ALA:HA	1:D:185:ALA:C	2.16	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:795:PRO:O	1:D:799:ARG:HB2	1.97	0.65
1:C:979:PRO:HA	1:D:981:LEU:HD13	1.76	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:D:819:ASP:CA	1:D:820:ALA:O	2.42	0.65
1:A:840:THR:HG23	1:A:840:THR:O	1.96	0.65
1:A:441:MET:HE2	1:A:792:VAL:HG13	1.78	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:863:GLU:O	1:A:866:VAL:O	2.15	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:A:73:SER:O	1:A:76:THR:OG1	2.14	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:B:184:ALA:HA	1:B:185:ALA:C	2.16	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:A:477:ARG:HD3	1:A:478:HIS:CE1	2.34	0.63
1:A:441:MET:HG2	1:A:796:THR:OG1	1.98	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:D:369:ASP:HB3	1:D:372:ASP:HB2	1.80	0.63
1:C:979:PRO:HA	1:D:981:LEU:HD22	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:GLN:CD	1:A:808:MET:HG2	2.20	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
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: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:812:ARG:C	1:A:817:ASP:N	2.54	0.61
1:D:24:MET:N	1:D:24:MET:SD	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:843:SER:HG	1:A:847:ARG:HB2	1.66	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:C:228:ALA:O	1:C:229:THR:C	2.39	0.60
1:A:174:ASN:CG	1:A:175:ALA:N	2.55	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:A:439:ARG:HH22	1:A:639:ASP:CG	2.04	0.60
1:A:804:LEU:C	1:A:807:VAL:CG1	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:GLU:H	1:D:26:VAL:C	2.06	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:541:MET:HE3	1:A:632:ASP:HB2	1.84	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
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:738:ASP:OD1	1:A:741:LYS:HE3	2.03	0.59
1:A:86:LEU:HB3	1:A:87:THR:CB	2.32	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:D:409:LEU:HD11	1:D:539:MET:SD	2.43	0.58
1:D:95:LYS:H	1:D:96:SER:HA	1.68	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:922:GLY:C	1:B:974:GLY:HA3	2.24	0.58
1:A:982:VAL:O	1:A:982:VAL:HG23	2.03	0.58
1:A:132:SER:HA	1:A:133:LYS:HB3	1.85	0.58
1:C:361:SER:HB3	1:C:390:CYS:HB2	1.85	0.58
1:C:44:ALA:HB1	1:C:45:PRO:HA	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:321:SER:C	1:A:323:ALA:CA	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:PHE:HZ	1:A:584:SER:HG	1.53	0.57
1:A:439:ARG:NH2	1:A:639:ASP:OD1	2.33	0.57
1:C:25:GLU:H	1:C:26:VAL:C	2.08	0.57
1:D:361:SER:HB3	1:D:390:CYS:HB2	1.86	0.57
1:C:462:ARG:NH1	1:D:990:LEU:HG	2.19	0.57
1:D:44:ALA:HB1	1:D:45:PRO:HA	1.87	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:683:ARG:HG2	1:A:683:ARG:HH11	1.69	0.57
1:A:80:ALA:O	1:A:84:ARG:CG	2.40	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:B:304:THR:HG22	1:B:305:VAL:N	2.20	0.56
1:D:576:ASP:HB3	1:D:596:ARG:HH21	1.71	0.56
1:D:83:TRP:HA	1:D:86:LEU:HD22	1.87	0.56
1:A:95:LYS:H	1:A:96:SER:HA	1.70	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:A:539:MET:CE	1:A:610:ILE:N	2.68	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:A:539:MET:HE3	1:A:609:VAL:C	2.26	0.55
1:B:444:LEU:HD13	1:B:525:LEU:CD2	2.36	0.55
1:B:85:SER:HB2	1:B:86:LEU:HB2	1.88	0.55
1:C:894:PRO:HB3	1:C:929:TRP:CZ3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:ASP:OD1	1:D:397:HIS:CG	2.59	0.55
1:A:267:ILE:CG2	1:A:267:ILE:O	2.54	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
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: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:A:980:LEU:N	1:B:981:LEU:HD13	2.22	0.54
1:D:23:SER:CB	1:D:24:MET:CA	2.83	0.54
1:A:119:ASN:O	1:A:119:ASN:OD1	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:B:860:VAL:O	1:B:863:GLU:HB2	2.08	0.54
1:A:979:PRO:O	1:B:959:PHE:HE1	1.86	0.54
1:A:962:ALA:HB1	1:B:981:LEU:HD23	1.89	0.54
1:C:27:TYR:CB	1:C:28:ALA:HA	2.38	0.54
1:B:25:GLU:H	1:B:26:VAL:C	2.11	0.54
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:541:MET:HG2	1:A:612:PHE:CE2	2.43	0.53
1:A:841:ALA:HB3	1:A:842:GLU:CB	2.38	0.53
1:B:660:TYR:N	1:B:660:TYR:CD1	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: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:C:541:MET:HE3	1:C:632:ASP:HB2	1.91	0.52
1:A:180:LYS:HD2	1:A:183:GLY:CA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:SER:CB	1:B:822:ALA:H	2.22	0.52
1:A:640:PRO:O	1:A:644:GLU:HG2	2.10	0.52
1:A:270:SER:CB	1:A:684:HIS:HD2	2.22	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
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:C:136:PRO:O	1:C:137:LEU:HB3	2.10	0.52
1:A:25:GLU:H	1:A:26:VAL:C	2.13	0.51
1:A:305:VAL:HG13	1:A:307:PHE:HE1	1.70	0.51
1:A:55:ILE:HD11	1:A:83:TRP:NE1	2.24	0.51
1:B:423:GLU:O	1:B:429:LYS:HG2	2.09	0.51
1:C:308:GLU:OE1	1:C:308:GLU:HA	2.10	0.51
1:A:133:LYS:HD2	1:A:134:THR:HA	1.93	0.51
1:A:83:TRP:O	1:A:87:THR:OG1	2.26	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:C:986:MET:HE2	1:D:500:ASN:HA	1.92	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:NH1	1:A:683:ARG:HG2	2.26	0.51
1:B:841:ALA:HB3	1:B:842:GLU:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:VAL:HG12	1:D:199:VAL:O	2.11	0.51
1:D:97:PHE:HB3	1:D:98:PRO:CA	2.35	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
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: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: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: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:179:LEU:HD23	1:A:180:LYS:HB3	1.93	0.49
1:A:38:PRO:HB2	1:A:40:TRP:CE3	2.47	0.49
1:A:498:LEU:O	1:A:503:PHE:HB2	2.11	0.49
1:A:411:PRO:HD3	1:A:562:PHE:CE1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:439:ARG:NH2	1:A:639:ASP:CG	2.65	0.49
1:C:886:HIS:O	1:C:889:TRP:HB3	2.13	0.49
1:B:775:TRP:HE1	1:B:781:PRO:HD3	1.78	0.49
1:A:837:LYS:C	1:A:840:THR:HG22	2.33	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:175:ALA:HB1	1:A:179:LEU:HD13	1.93	0.49
1:A:93:ARG:N	1:A:94:GLY:HA3	2.27	0.49
1:B:136:PRO:O	1:B:137:LEU:HB3	2.13	0.49
1:B:246:PRO:HB3	1:B:247:ALA:HB2	1.92	0.49
1:B:27:TYR:CB	1:B:28:ALA:CA	2.91	0.49
1:B:878:TYR:HB3	1:B:879:PRO:HD3	1.93	0.49
1:D:843:SER:O	1:D:844:ARG:HB2	2.13	0.49
1:D:93:ARG:N	1:D:94:GLY:HA3	2.28	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: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:N	1:D:530:ASN:OD1	2.45	0.48
1:D:588:PHE:CD2	1:D:652:PRO:HG3	2.48	0.48
1:C:953:ALA:O	1:C:955:ALA:N	2.45	0.48
1:A:78:ASP:O	1:A:79:MET:C	2.51	0.48
1:B:46:LEU:HD12	1:B:201:ARG:CZ	2.42	0.48
1:A:840:THR:CG2	1:A:840:THR:O	2.60	0.48
1:B:843:SER:O	1:B:844:ARG:HB2	2.13	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:A:490:ASN:OD1	1:A:490:ASN:C	2.51	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:B:673:ARG:HA	1:B:676:GLY:C	2.34	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:861:GLU:HG2	1:B:941:TYR:CZ	2.49	0.47
1:C:375:ASP:N	1:C:375:ASP:OD1	2.47	0.47
1:C:479:GLY:O	1:D:1000:TYR:HE2	1.97	0.47
1:C:94:GLY:HA2	1:C:95:LYS:HB2	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:N	1:B:24:MET:SD	2.74	0.47
1:C:58:HIS:CD2	1:C:98:PRO:HB3	2.50	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:N	1:A:317:ASP:OD1	2.48	0.47
1:B:425:ARG:HD2	1:B:589:PRO:O	2.15	0.47
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:A:132:SER:CA	1:A:133:LYS:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD23	1:A:87:THR:CG2	2.45	0.47
1:C:820:ALA:HB1	1:C:821:ALA:CA	2.45	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:321:SER:OG	1:C:617:ASP:HA	2.14	0.47
1:C:38:PRO:HB2	1:C:40:TRP:CE3	2.50	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:D:68:LEU:CA	1:D:69:ARG:HB2	2.45	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:O	1:B:199:VAL:HG12	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:A:511:GLN:OE1	1:A:808:MET:HG2	2.15	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:B:484:LEU:HG	1:B:882:VAL:HG11	1.97	0.46
1:D:203:TRP:HB3	1:D:236:PHE:HB3	1.97	0.46
1:D:559:SER:HA	1:D:607:LYS:HD2	1.97	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:B:497:PHE:HA	1:B:987:TYR:OH	2.16	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:363:LYS:HE3	1:B:387:LYS:HE3	1.96	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:C:177:SER:O	1:C:181:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:VAL:O	1:C:199:VAL:HG12	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:506:ARG:HA	1:C:821:ALA:O	2.15	0.46
1:C:497:PHE:HA	1:C:987:TYR:OH	2.16	0.46
1:D:806:LYS:CB	1:D:807:VAL:CB	2.93	0.46
1:A:432:MET:C	1:A:432:MET:SD	2.95	0.46
1:A:55:ILE:HD11	1:A:83:TRP:CD1	2.51	0.46
1:B:177:SER:O	1:B:181:ASP:HB2	2.16	0.46
1:A:343:ARG:HH22	1:B:568:ASP:HB2	1.81	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:B:329:ASP:HB3	1:B:628:ASP:HB2	1.98	0.46
1:C:985:LEU:CD2	1:D:1000:TYR:CZ	2.97	0.46
1:A:248:PRO:HA	1:A:249:LEU:HA	1.71	0.45
1:A:29:ARG:O	1:A:30:LEU:HB2	2.15	0.45
1:A:756:ARG:NH2	1:D:775:TRP:O	2.48	0.45
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:C:996:PHE:C	1:C:996:PHE:CD1	2.89	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:B:268:PRO:O	1:B:269:VAL:C	2.55	0.45
1:C:985:LEU:HD13	1:C:986:MET:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:MET:CE	1:A:609:VAL:O	2.64	0.45
1:A:79:MET:HG3	1:A:83:TRP:CE2	2.51	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:421:VAL:HG13	1:B:589:PRO:HA	1.99	0.45
1:B:69:ARG:HG3	1:B:70:TYR:N	2.31	0.45
1:B:946:PRO:O	1:B:950:TRP:HD1	2.00	0.45
1:D:946:PRO:O	1:D:950:TRP:HD1	1.99	0.45
1:A:133:LYS:N	1:A:135:GLY:HA3	2.32	0.45
1:A:94:GLY:HA2	1:A:95:LYS:CB	2.47	0.45
1:A:953:ALA:O	1:A:954:GLY:C	2.55	0.45
1:C:248:PRO:HA	1:C:249:LEU:HA	1.72	0.45
1:C:24:MET:SD	1:C:24:MET:N	2.75	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:523:GLU:HA	1:A:526:ARG:HG2	1.99	0.45
1:A:427:LYS:N	1:A:645:ASN:O	2.47	0.45
1:B:673:ARG:C	1:B:676:GLY:H	2.21	0.45
1:D:714:VAL:O	1:D:718:ASN:HB2	2.17	0.45
1:D:985:LEU:HD13	1:D:986:MET:N	2.32	0.45
1:A:48:LEU:C	1:A:48:LEU:HD12	2.38	0.44
1:A:565:ASP:OD2	1:A:568:ASP:N	2.50	0.44
1:A:717:HIS:HE2	1:A:766:GLU:CD	2.19	0.44
1:A:980:LEU:N	1:A:980:LEU:HD12	2.32	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: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:184:ALA:HA	1:A:185:ALA:HB2	1.98	0.44
1:A:29:ARG:O	1:A:30:LEU:CB	2.65	0.44
1:A:996:PHE:C	1:A:996:PHE:CD1	2.90	0.44
1:C:30:LEU:HD22	1:C:190:TRP:CD2	2.51	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:HB2	1:A:189:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:140:LEU:HD23	1:A:142:MET:CE	2.47	0.44
1:A:979:PRO:HD2	1:B:959:PHE:CZ	2.52	0.44
1:B:977:GLY:O	1:B:979:PRO:HD3	2.17	0.44
1:A:355:ILE:HD11	1:A:402:ILE:CG2	2.47	0.44
1:A:325:LYS:HE3	1:A:622:ASP:OD2	2.17	0.44
1:B:894:PRO:HB2	1:B:910:ALA:HA	2.00	0.44
1:B:94:GLY:HA2	1:B:95:LYS:CB	2.48	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
1:B:289:LYS:O	1:B:293:ARG:HG2	2.18	0.44
1:B:953:ALA:O	1:B:954:GLY:C	2.55	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:194:LYS:CE	1:A:195:PRO:HD2	2.41	0.44
1:A:660:TYR:N	1:A:660:TYR:CD1	2.86	0.44
1:A:441:MET:HE3	1:A:792:VAL:CG1	2.48	0.44
1:A:441:MET:HE3	1:A:792:VAL:HG13	1.99	0.44
1:B:755:ARG:HA	1:B:759:LEU:HB2	1.99	0.44
1:C:263:THR:CB	1:C:264:ARG:HE	2.31	0.44
1:C:29:ARG:O	1:C:30:LEU:HB2	2.17	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:A:79:MET:O	1:A:83:TRP:N	2.36	0.43
1:B:211:ALA:HB2	1:B:231:LYS:O	2.17	0.43
1:D:541:MET:HE3	1:D:632:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ARG:CZ	1:D:774:VAL:HG21	2.49	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: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:C:27:TYR:N	1:C:186:GLN:HG2	2.33	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:506:ARG:HA	1:B:821:ALA:O	2.18	0.43
1:B:535:ARG:HB2	1:B:639:ASP:HB2	2.00	0.43
1:B:287:HIS:HB2	1:B:690:MET:HG3	2.00	0.43
1:B:820:ALA:HB1	1:B:821:ALA:CA	2.47	0.43
1:A:184:ALA:CA	1:A:185:ALA:CB	2.90	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: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:986:MET:CE	1:B:462:ARG:HD3	2.48	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:C:808:MET:HB3	1:C:809:GLN:HB2	2.01	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:B:113:ASN:O	1:B:114:PHE:HB2	2.19	0.43
1:B:87:THR:HA	1:B:88:GLN:C	2.38	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: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:D:270:SER:HA	1:D:687:VAL:HG11	2.01	0.43
1:A:886:HIS:CD2	1:A:890:CYS:SG	3.11	0.42
1:A:94:GLY:HA2	1:A:95:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:VAL:HG13	1:C:589:PRO:HA	2.01	0.42
1:D:953:ALA:O	1:D:954:GLY:C	2.57	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: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:69:ARG:CG	1:A:70:TYR:N	2.81	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:321:SER:O	1:A:322:PRO:C	2.45	0.42
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.85	0.42
1:A:561:LYS:HD3	1:A:563:ARG:NH1	2.34	0.42
1:A:85:SER:N	1:A:86:LEU:HB2	2.35	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: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:760:GLY:HA3	1:B:761:GLY:HA3	1.75	0.42
1:C:621:ALA:HB2	1:C:629:TYR:CZ	2.55	0.42
1:C:812:ARG:C	1:C:817:ASP:N	2.72	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:837:LYS:C	1:A:840:THR:CG2	2.88	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:538:TYR:CZ	1:D:635:TRP:HB2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:152:ARG:HH22	1:A:360:GLY:N	2.18	0.42
1:A:25:GLU:CB	1:A:26:VAL:HG22	2.50	0.42
1:A:355:ILE:HD12	1:A:404:SER:O	2.19	0.42
1:A:539:MET:HE2	1:A:610:ILE:HB	2.01	0.42
1:A:620:LEU:O	1:A:621:ALA:C	2.57	0.42
1:C:155:ARG:NH2	1:C:401:GLU:OE2	2.53	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: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:D:94:GLY:HA2	1:D:95:LYS:CB	2.50	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:86:LEU:N	1:A:87:THR:C	2.74	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:808:MET:H	1:D:809:GLN:HB3	1.84	0.41
1:D:94:GLY:HA2	1:D:95:LYS:HB2	2.01	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:B:86:LEU:N	1:B:87:THR:C	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:978:MET:O	1:A:980:LEU:HD12	2.20	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: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:B:982:VAL:O	1:B:983:THR:C	2.58	0.41
1:D:455:VAL:O	1:D:505:ARG:CG	2.68	0.41
1:D:660:TYR:N	1:D:660:TYR:CD1	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:794:LYS:CB	1:D:795:PRO:HD3	2.50	0.41
1:A:804:LEU:O	1:A:807:VAL:CG1	2.69	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:766:GLU:H	1:A:766:GLU:CD	2.23	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:C:25:GLU:N	1:C:26:VAL:C	2.74	0.41
1:D:660:TYR:CE2	1:D:754:LEU:HA	2.55	0.41
1:D:85:SER:N	1:D:86:LEU:HB2	2.36	0.41
1:A:1000:TYR:O	1:A:1000:TYR:CD1	2.73	0.41
1:A:343:ARG:NH2	1:B:568:ASP:O	2.54	0.41
1:B:173:LEU:HA	1:B:174:ASN:HA	1.82	0.41
1:A:986:MET:HE2	1:B:499:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LEU:O	1:B:731:THR:CB	2.68	0.41
1:D:129:PHE:CZ	1:D:168:PRO:HB2	2.56	0.41
1:A:329:ASP:HB3	1:A:628:ASP:HB2	2.03	0.41
1:A:943:LYS:CB	1:A:944:THR:CB	2.89	0.41
1:B:31:GLN:CB	1:B:32:ASN:CB	2.95	0.41
1:B:333:ARG:NE	1:B:380:GLU:OE2	2.40	0.41
1:C:113:ASN:O	1:C:114:PHE:HB2	2.21	0.41
1:D:491:LYS:O	1:D:494:VAL:HB	2.20	0.41
1:D:575:THR:OG1	1:D:576:ASP:N	2.54	0.41
1:D:808:MET:HB3	1:D:809:GLN:HB2	2.03	0.41
1:C:981:LEU:HB2	1:D:962:ALA:HB1	2.02	0.41
1:C:245:ARG:HD2	1:C:245:ARG:O	2.21	0.41
1:C:69:ARG:HG3	1:C:70:TYR:N	2.35	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:HG	1:A:367:LEU:H	1.84	0.40
1:A:521:ARG:HB3	1:A:521:ARG:HE	1.61	0.40
1:A:532:HIS:CG	1:A:533:VAL:N	2.88	0.40
1:A:555:HIS:C	1:A:555:HIS:CD2	2.94	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:A:368:MET:HE2	1:A:368:MET:HB2	1.87	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:A:675:THR:CG2	1:A:682:ALA:HA	2.51	0.40
1:A:986:MET:HE2	1:B:500:ASN:HA	2.04	0.40
1:B:25:GLU:HB2	1:B:26:VAL:CG2	2.52	0.40
1:B:428:ASP:CG	1:B:431:ARG:HB2	2.41	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:247:ALA:HB1	1:A:248:PRO:HD2	2.04	0.40
1:A:894:PRO:HD3	1:A:929:TRP:CE2	2.57	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:B:86:LEU:HB3	1:B:87:THR:CB	2.51	0.40
1:C:794:LYS:CB	1:C:795:PRO:HD3	2.51	0.40
1:C:953:ALA:O	1:C:954:GLY:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	904/1034 (87%)	779 (86%)	90 (10%)	35 (4%)	3	22
1	B	888/1034 (86%)	779 (88%)	84 (10%)	25 (3%)	5	29
1	C	888/1034 (86%)	786 (88%)	75 (8%)	27 (3%)	4	28
1	D	886/1034 (86%)	787 (89%)	71 (8%)	28 (3%)	4	26
All	All	3566/4136 (86%)	3131 (88%)	320 (9%)	115 (3%)	4	26

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	A	88	GLN
1	A	133	LYS
1	A	137	LEU
1	A	184	ALA
1	A	243	ASP
1	A	413	ALA

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Mol	Chain	Res	Type
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
1	A	844	ARG
1	B	95	LYS
1	B	99	GLU
1	B	117	ARG

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Mol	Chain	Res	Type
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
1	B	764	SER
1	C	89	LEU
1	D	69	ARG
1	D	89	LEU

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Mol	Chain	Res	Type
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%)	695 (90%)	80 (10%)	7	29
1	B	646/856 (76%)	578 (90%)	68 (10%)	7	28
1	C	650/856 (76%)	573 (88%)	77 (12%)	5	23
1	D	645/856 (75%)	569 (88%)	76 (12%)	5	23
All	All	2716/3424 (79%)	2415 (89%)	301 (11%)	6	25

All (301) 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	36	LYS
1	A	39	ARG
1	A	40	TRP
1	A	48	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	317	ASP
1	A	341	LYS
1	A	349	SER
1	A	392	ASP
1	A	394	ASP
1	A	415	ASN
1	A	416	LEU
1	A	432	MET
1	A	446	LYS
1	A	452	LYS
1	A	457	ARG
1	A	459	LEU
1	A	468	CYS
1	A	469	THR

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Mol	Chain	Res	Type
1	A	483	PHE
1	A	495	LEU
1	A	521	ARG
1	A	530	ASN
1	A	544	ASP
1	A	560	SER
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	717	HIS
1	A	728	LEU
1	A	740	SER
1	A	742	GLN
1	A	745	LEU
1	A	756	ARG
1	A	767	ASP
1	A	780	GLU
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	949	VAL
1	A	951	GLN
1	A	959	PHE
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

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Mol	Chain	Res	Type
1	B	117	ARG
1	B	126	SER
1	B	145	LEU
1	B	153	LEU
1	B	195	PRO
1	B	197	SER
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	341	LYS
1	B	363	LYS
1	B	375	ASP
1	B	392	ASP
1	B	394	ASP
1	B	411	PRO
1	B	416	LEU
1	B	427	LYS
1	B	431	ARG
1	B	452	LYS
1	B	455	VAL
1	B	468	CYS
1	B	469	THR
1	B	483	PHE
1	B	495	LEU
1	B	510	ILE
1	B	527	THR
1	B	530	ASN
1	B	544	ASP
1	B	564	ASP
1	B	569	THR
1	B	570	THR
1	B	573	LEU
1	B	613	PRO
1	B	620	LEU
1	B	647	THR

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Mol	Chain	Res	Type
1	B	678	THR
1	B	683	ARG
1	B	689	ASP
1	B	740	SER
1	B	741	LYS
1	B	742	GLN
1	B	767	ASP
1	B	775	TRP
1	B	804	LEU
1	B	808	MET
1	B	817	ASP
1	B	840	THR
1	B	844	ARG
1	B	861	GLU
1	B	877	THR
1	B	916	PRO
1	B	926	THR
1	B	949	VAL
1	B	951	GLN
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	84	ARG
1	C	90	ASP
1	C	126	SER
1	C	139	LEU
1	C	145	LEU
1	C	153	LEU
1	C	181	ASP
1	C	195	PRO
1	C	197	SER
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

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Mol	Chain	Res	Type
1	C	316	THR
1	C	319	ILE
1	C	336	ARG
1	C	341	LYS
1	C	375	ASP
1	C	392	ASP
1	C	411	PRO
1	C	416	LEU
1	C	427	LYS
1	C	451	GLN
1	C	452	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	577	CYS
1	C	613	PRO
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	710	TYR
1	C	728	LEU
1	C	740	SER
1	C	742	GLN
1	C	773	ASP
1	C	775	TRP

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Mol	Chain	Res	Type
1	C	802	GLU
1	C	804	LEU
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	951	GLN
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	99	GLU
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
1	D	319	ILE
1	D	341	LYS
1	D	375	ASP
1	D	392	ASP
1	D	411	PRO
1	D	416	LEU
1	D	427	LYS
1	D	446	LYS
1	D	452	LYS
1	D	455	VAL

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Mol	Chain	Res	Type
1	D	468	CYS
1	D	469	THR
1	D	483	PHE
1	D	495	LEU
1	D	510	ILE
1	D	521	ARG
1	D	527	THR
1	D	530	ASN
1	D	532	HIS
1	D	538	TYR
1	D	544	ASP
1	D	560	SER
1	D	564	ASP
1	D	570	THR
1	D	573	LEU
1	D	576	ASP
1	D	577	CYS
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	689	ASP
1	D	727	LEU
1	D	728	LEU
1	D	731	THR
1	D	740	SER
1	D	741	LYS
1	D	742	GLN
1	D	750	SER
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	839	LEU
1	D	840	THR
1	D	861	GLU
1	D	877	THR
1	D	916	PRO

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Mol	Chain	Res	Type
1	D	926	THR
1	D	949	VAL
1	D	951	GLN
1	D	981	LEU
1	D	985	LEU
1	D	998	LYS
1	D	1003	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	31	GLN
1	A	196	HIS
1	A	202	GLN
1	A	397	HIS
1	A	463	GLN
1	A	478	HIS
1	A	555	HIS
1	A	684	HIS
1	A	709	ASN
1	B	202	GLN
1	B	310	ASN
1	B	463	GLN
1	B	555	HIS
1	B	963	GLN
1	C	58	HIS
1	C	202	GLN
1	C	295	GLN
1	C	417	GLN
1	C	463	GLN
1	D	202	GLN
1	D	417	GLN
1	D	447	GLN
1	D	463	GLN
1	D	555	HIS

5.3.3 RNA ⓘ

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 carbohydrates 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%)	-0.00	42 (4%) 33 21	11, 21, 94, 177	0
1	B	922/1034 (89%)	0.34	98 (10%) 6 3	9, 25, 146, 228	0
1	C	922/1034 (89%)	1.16	188 (20%) 1 1	25, 71, 152, 347	0
1	D	922/1034 (89%)	1.55	232 (25%) 0 0	24, 71, 221, 430	0
All	All	3690/4136 (89%)	0.76	560 (15%) 2 1	9, 53, 158, 430	0

All (560) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	823	HIS	21.4
1	D	936	THR	18.9
1	D	955	ALA	18.8
1	D	940	ALA	16.8
1	D	935	SER	16.5
1	B	894	PRO	15.9
1	C	46	LEU	15.8
1	C	111	THR	15.7
1	D	953	ALA	15.5
1	D	951	GLN	15.2
1	D	838	ALA	15.0
1	D	837	LYS	14.7
1	D	91	VAL	14.6
1	B	893	GLU	14.4
1	D	954	GLY	13.9
1	D	894	PRO	13.6
1	D	950	TRP	12.9
1	D	824	SER	12.8
1	D	829	LEU	12.6
1	D	930	ALA	12.6
1	D	97	PHE	12.4

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Mol	Chain	Res	Type	RSRZ
1	C	110	LEU	12.3
1	D	937	ALA	12.2
1	D	808	MET	12.1
1	D	836	PHE	11.7
1	B	836	PHE	11.5
1	D	948	PHE	11.5
1	C	48	LEU	11.2
1	D	835	ASN	11.1
1	D	481	VAL	11.1
1	D	952	MET	10.9
1	B	847	ARG	10.7
1	D	834	GLU	10.5
1	C	93	ARG	10.5
1	D	934	ALA	10.4
1	D	931	LEU	10.1
1	C	966	SER	10.1
1	C	40	TRP	10.1
1	D	44	ALA	10.0
1	C	45	PRO	10.0
1	D	90	ASP	9.8
1	C	77	SER	9.8
1	D	43	ALA	9.5
1	C	200	GLY	9.5
1	C	73	SER	9.4
1	C	113	ASN	9.1
1	D	45	PRO	9.0
1	D	811	SER	8.9
1	B	484	LEU	8.8
1	C	52	LEU	8.7
1	B	837	LYS	8.5
1	B	951	GLN	8.4
1	B	848	ALA	8.4
1	B	922	GLY	8.4
1	C	78	ASP	8.3
1	C	76	THR	8.3
1	B	934	ALA	8.3
1	D	825	TRP	8.2
1	B	885	LEU	8.2
1	D	413	ALA	8.2
1	D	828	ASP	8.0
1	C	988	ALA	8.0
1	D	466	ASN	8.0

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Mol	Chain	Res	Type	RSRZ
1	C	112	GLY	8.0
1	D	810	ALA	7.9
1	C	55	ILE	7.9
1	B	884	GLN	7.8
1	B	937	ALA	7.8
1	D	492	GLY	7.7
1	D	841	ALA	7.6
1	B	829	LEU	7.5
1	D	493	GLU	7.5
1	D	821	ALA	7.5
1	C	50	TRP	7.4
1	B	838	ALA	7.4
1	C	178	ILE	7.3
1	C	460	GLN	7.3
1	A	83	TRP	7.2
1	C	35	PRO	7.2
1	D	945	ASN	7.1
1	C	301	THR	7.0
1	D	509	TYR	7.0
1	D	473	SER	6.8
1	D	800	GLU	6.8
1	C	47	ALA	6.7
1	D	77	SER	6.6
1	A	77	SER	6.6
1	D	480	GLN	6.6
1	D	37	PHE	6.5
1	D	141	ASP	6.5
1	D	947	LYS	6.5
1	D	531	ILE	6.5
1	D	819	ASP	6.4
1	D	932	LEU	6.4
1	A	179	LEU	6.3
1	D	956	GLN	6.3
1	D	839	LEU	6.2
1	D	89	LEU	6.2
1	D	893	GLU	6.2
1	C	34	TRP	6.1
1	C	97	PHE	6.1
1	A	176	PRO	6.1
1	A	975	SER	6.1
1	C	49	ALA	6.0
1	D	76	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	804	LEU	6.0
1	D	488	PRO	5.9
1	D	179	LEU	5.9
1	B	888	LYS	5.9
1	D	142	MET	5.8
1	C	79	MET	5.7
1	D	942	TYR	5.7
1	D	182	GLY	5.7
1	C	105	ALA	5.5
1	D	139	LEU	5.5
1	D	938	PHE	5.5
1	C	199	VAL	5.4
1	D	530	ASN	5.4
1	B	517	LEU	5.3
1	D	916	PRO	5.3
1	C	843	SER	5.3
1	C	201	ARG	5.2
1	A	107	ALA	5.2
1	A	47	ALA	5.2
1	C	195	PRO	5.1
1	D	479	GLY	5.1
1	D	186	GLN	5.1
1	B	824	SER	5.1
1	D	83	TRP	5.0
1	C	96	SER	5.0
1	C	186	GLN	5.0
1	C	107	ALA	5.0
1	A	108	ALA	5.0
1	D	92	PHE	5.0
1	D	860	VAL	5.0
1	B	864	TRP	5.0
1	C	92	PHE	4.9
1	D	504	ASP	4.9
1	D	865	LYS	4.9
1	D	946	PRO	4.9
1	A	82	LEU	4.9
1	D	277	LEU	4.9
1	B	952	MET	4.9
1	C	701	PRO	4.9
1	A	59	CYS	4.9
1	D	501	SER	4.9
1	A	181	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	526	ARG	4.8
1	D	941	TYR	4.8
1	D	468	CYS	4.8
1	B	892	ILE	4.8
1	C	369	ASP	4.8
1	B	909	THR	4.8
1	C	818	ASP	4.8
1	C	589	PRO	4.7
1	D	507	GLN	4.7
1	C	676	GLY	4.7
1	D	661	LEU	4.7
1	D	887	ALA	4.7
1	D	807	VAL	4.7
1	D	178	ILE	4.7
1	A	97	PHE	4.7
1	D	472	ARG	4.6
1	D	144	PRO	4.6
1	D	145	LEU	4.6
1	C	817	ASP	4.6
1	C	244	PHE	4.6
1	D	181	ASP	4.6
1	C	432	MET	4.5
1	D	863	GLU	4.5
1	C	41	LEU	4.5
1	D	1003	ARG	4.5
1	C	56	CYS	4.5
1	C	82	LEU	4.5
1	D	939	LYS	4.5
1	C	323	ALA	4.5
1	B	938	PHE	4.5
1	D	822	ALA	4.5
1	A	922	GLY	4.5
1	C	61	VAL	4.4
1	D	412	ALA	4.4
1	C	394	ASP	4.4
1	C	205	ALA	4.4
1	C	242	HIS	4.4
1	C	921	ARG	4.4
1	D	496	SER	4.4
1	C	166	LEU	4.4
1	C	99	GLU	4.4
1	C	1002	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	833	PHE	4.3
1	D	140	LEU	4.3
1	A	175	ALA	4.3
1	B	955	ALA	4.3
1	D	500	ASN	4.3
1	D	662	GLY	4.3
1	B	846	LEU	4.2
1	B	497	PHE	4.2
1	B	820	ALA	4.2
1	C	840	THR	4.2
1	A	61	VAL	4.2
1	D	926	THR	4.2
1	D	885	LEU	4.2
1	D	28	ALA	4.1
1	B	890	CYS	4.1
1	C	810	ALA	4.1
1	C	837	LYS	4.1
1	B	857	LEU	4.1
1	D	31	GLN	4.1
1	C	476	VAL	4.0
1	B	887	ALA	4.0
1	D	180	LYS	4.0
1	B	83	TRP	4.0
1	D	913	LEU	4.0
1	D	826	ASP	4.0
1	D	866	VAL	4.0
1	D	96	SER	3.9
1	A	78	ASP	3.9
1	D	668	PHE	3.9
1	D	490	ASN	3.9
1	B	845	SER	3.9
1	D	966	SER	3.9
1	D	335	SER	3.9
1	C	827	PRO	3.9
1	C	59	CYS	3.9
1	B	810	ALA	3.8
1	C	932	LEU	3.8
1	C	504	ASP	3.8
1	D	914	GLU	3.8
1	D	34	TRP	3.8
1	D	47	ALA	3.8
1	C	27	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	917	PHE	3.8
1	B	891	ALA	3.8
1	D	957	LEU	3.8
1	D	74	TRP	3.7
1	C	481	VAL	3.7
1	D	963	GLN	3.7
1	D	560	SER	3.7
1	A	52	LEU	3.7
1	D	56	CYS	3.7
1	D	806	LYS	3.7
1	C	809	GLN	3.6
1	D	886	HIS	3.6
1	C	138	PHE	3.6
1	D	944	THR	3.6
1	C	472	ARG	3.6
1	A	66	PRO	3.6
1	D	912	LEU	3.6
1	A	818	ASP	3.6
1	C	85	SER	3.6
1	B	830	ALA	3.6
1	A	55	ILE	3.6
1	A	178	ILE	3.6
1	C	304	THR	3.6
1	B	921	ARG	3.6
1	B	507	GLN	3.6
1	C	516	ASP	3.6
1	B	945	ASN	3.5
1	B	947	LYS	3.5
1	C	808	MET	3.5
1	A	180	LYS	3.5
1	D	850	LEU	3.5
1	B	914	GLU	3.5
1	C	108	ALA	3.5
1	B	877	THR	3.5
1	A	62	ASP	3.5
1	B	136	PRO	3.5
1	B	913	LEU	3.4
1	C	100	ARG	3.4
1	C	114	PHE	3.4
1	C	53	THR	3.4
1	C	346	LEU	3.4
1	A	45	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	489	GLU	3.4
1	D	494	VAL	3.4
1	D	878	TYR	3.4
1	D	464	TRP	3.4
1	D	644	GLU	3.4
1	C	545	PHE	3.4
1	A	79	MET	3.4
1	D	184	ALA	3.4
1	B	879	PRO	3.4
1	D	65	ASP	3.4
1	C	57	LEU	3.3
1	D	801	LEU	3.3
1	D	852	ALA	3.3
1	C	130	ASN	3.3
1	D	183	GLY	3.3
1	B	839	LEU	3.3
1	D	476	VAL	3.3
1	B	809	GLN	3.3
1	C	820	ALA	3.3
1	D	392	ASP	3.3
1	B	41	LEU	3.3
1	D	35	PRO	3.3
1	A	99	GLU	3.2
1	D	469	THR	3.2
1	C	723	ASP	3.2
1	C	204	GLN	3.2
1	D	587	HIS	3.2
1	B	63	LEU	3.2
1	D	769	ALA	3.2
1	D	809	GLN	3.2
1	D	450	SER	3.2
1	B	835	ASN	3.2
1	C	989	GLY	3.2
1	B	948	PHE	3.2
1	C	126	SER	3.1
1	C	371	ALA	3.1
1	C	38	PRO	3.1
1	D	175	ALA	3.1
1	C	264	ARG	3.1
1	B	856	ALA	3.1
1	D	984	PRO	3.1
1	D	50	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	66	PRO	3.1
1	C	54	ARG	3.1
1	C	700	GLN	3.1
1	D	960	ILE	3.1
1	A	819	ASP	3.1
1	A	976	ASP	3.1
1	C	94	GLY	3.1
1	D	849	VAL	3.1
1	B	58	HIS	3.1
1	A	974	GLY	3.1
1	D	882	VAL	3.1
1	B	882	VAL	3.0
1	C	585	PRO	3.0
1	D	857	LEU	3.0
1	D	910	ALA	3.0
1	D	78	ASP	3.0
1	D	525	LEU	3.0
1	C	847	ARG	3.0
1	B	956	GLN	3.0
1	C	279	LEU	3.0
1	D	276	LEU	3.0
1	D	856	ALA	3.0
1	D	38	PRO	3.0
1	D	73	SER	3.0
1	D	308	GLU	3.0
1	A	811	SER	3.0
1	B	135	GLY	3.0
1	C	927	SER	3.0
1	D	169	SER	3.0
1	C	305	VAL	2.9
1	B	858	GLY	2.9
1	B	863	GLU	2.9
1	B	958	ALA	2.9
1	D	187	VAL	2.9
1	C	975	SER	2.9
1	B	482	PRO	2.9
1	B	936	THR	2.9
1	D	88	GLN	2.9
1	C	859	ALA	2.9
1	D	411	PRO	2.9
1	B	851	GLU	2.9
1	C	131	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	497	PHE	2.9
1	C	1001	LEU	2.9
1	A	98	PRO	2.9
1	D	199	VAL	2.9
1	B	911	ALA	2.9
1	C	335	SER	2.8
1	B	886	HIS	2.8
1	D	719	ASN	2.8
1	D	467	GLU	2.8
1	D	820	ALA	2.8
1	B	118	GLY	2.8
1	C	300	LYS	2.8
1	B	841	ALA	2.8
1	B	876	LEU	2.8
1	C	145	LEU	2.8
1	C	944	THR	2.8
1	C	81	ALA	2.8
1	D	979	PRO	2.8
1	C	324	GLY	2.8
1	C	987	TYR	2.8
1	D	417	GLN	2.8
1	D	520	GLN	2.8
1	B	865	LYS	2.8
1	B	227	LYS	2.7
1	D	558	PHE	2.7
1	C	307	PHE	2.7
1	D	423	GLU	2.7
1	C	36	LYS	2.7
1	C	520	GLN	2.7
1	B	826	ASP	2.7
1	B	840	THR	2.7
1	D	350	ASP	2.7
1	A	67	THR	2.7
1	C	362	ALA	2.7
1	C	149	GLU	2.7
1	D	962	ALA	2.7
1	D	478	HIS	2.7
1	D	768	PRO	2.7
1	C	117	ARG	2.7
1	C	322	PRO	2.7
1	A	65	ASP	2.7
1	D	176	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	910	ALA	2.6
1	D	414	LEU	2.6
1	B	817	ASP	2.6
1	B	920	ASP	2.6
1	C	179	LEU	2.6
1	C	517	LEU	2.6
1	B	518	GLN	2.6
1	B	514	ALA	2.6
1	C	393	ALA	2.6
1	C	75	ALA	2.6
1	C	265	ALA	2.6
1	C	680	ALA	2.6
1	B	111	THR	2.6
1	D	482	PRO	2.6
1	C	807	VAL	2.6
1	D	929	TRP	2.6
1	C	779	GLY	2.6
1	A	177	SER	2.6
1	D	113	ASN	2.6
1	B	64	GLU	2.6
1	C	391	ASP	2.6
1	D	660	TYR	2.5
1	D	33	ILE	2.5
1	D	718	ASN	2.5
1	B	932	LEU	2.5
1	D	30	LEU	2.5
1	A	977	GLY	2.5
1	C	282	ASN	2.5
1	B	134	THR	2.5
1	D	112	GLY	2.5
1	D	52	LEU	2.5
1	C	274	ASP	2.5
1	C	722	SER	2.5
1	D	353	SER	2.5
1	D	508	LYS	2.5
1	C	433	ARG	2.5
1	C	127	LEU	2.5
1	C	640	PRO	2.5
1	D	958	ALA	2.5
1	D	483	PHE	2.5
1	B	950	TRP	2.5
1	C	51	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	104	GLU	2.5
1	C	198	LEU	2.4
1	D	310	ASN	2.4
1	D	390	CYS	2.4
1	B	510	ILE	2.4
1	C	798	ASP	2.4
1	D	598	VAL	2.4
1	C	602	GLN	2.4
1	D	920	ASP	2.4
1	C	193	GLU	2.4
1	D	701	PRO	2.4
1	B	72	PRO	2.4
1	C	858	GLY	2.4
1	D	595	VAL	2.4
1	B	263	THR	2.4
1	C	856	ALA	2.4
1	D	333	ARG	2.4
1	D	862	HIS	2.4
1	C	80	ALA	2.4
1	D	104	GLU	2.4
1	C	62	ASP	2.4
1	B	57	LEU	2.4
1	C	118	GLY	2.4
1	C	136	PRO	2.4
1	C	155	ARG	2.4
1	A	676	GLY	2.4
1	C	182	GLY	2.4
1	D	614	ALA	2.4
1	B	478	HIS	2.4
1	D	46	LEU	2.4
1	D	134	THR	2.4
1	C	26	VAL	2.3
1	C	299	SER	2.3
1	C	681	ALA	2.3
1	D	513	LEU	2.3
1	D	111	THR	2.3
1	A	54	ARG	2.3
1	B	825	TRP	2.3
1	D	210	ASP	2.3
1	C	314	HIS	2.3
1	D	602	GLN	2.3
1	C	957	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	543	VAL	2.3
1	C	133	LYS	2.3
1	C	738	ASP	2.3
1	D	983	THR	2.3
1	B	248	PRO	2.3
1	D	151	CYS	2.3
1	D	105	ALA	2.3
1	D	64	GLU	2.3
1	C	243	ASP	2.3
1	A	48	LEU	2.2
1	D	470	ASN	2.2
1	D	855	ASN	2.2
1	C	203	TRP	2.2
1	C	378	TRP	2.2
1	C	668	PHE	2.2
1	D	978	MET	2.2
1	C	74	TRP	2.2
1	B	483	PHE	2.2
1	C	689	ASP	2.2
1	B	907	ALA	2.2
1	B	935	SER	2.2
1	D	53	THR	2.2
1	B	59	CYS	2.2
1	C	845	SER	2.2
1	D	588	PHE	2.2
1	D	75	ALA	2.2
1	A	136	PRO	2.2
1	D	645	ASN	2.2
1	C	475	ARG	2.2
1	C	838	ALA	2.2
1	C	503	PHE	2.2
1	C	43	ALA	2.2
1	B	781	PRO	2.2
1	D	26	VAL	2.2
1	C	32	ASN	2.1
1	C	154	THR	2.1
1	D	463	GLN	2.1
1	C	192	THR	2.1
1	C	917	PHE	2.1
1	D	840	THR	2.1
1	C	327	MET	2.1
1	C	720	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	641	ASP	2.1
1	A	58	HIS	2.1
1	C	184	ALA	2.1
1	A	809	GLN	2.1
1	B	130	ASN	2.1
1	C	1000	TYR	2.1
1	B	42	HIS	2.1
1	B	503	PHE	2.1
1	C	811	SER	2.1
1	D	460	GLN	2.1
1	A	810	ALA	2.1
1	B	764	SER	2.1
1	D	108	ALA	2.1
1	D	57	LEU	2.1
1	C	470	ASN	2.1
1	B	929	TRP	2.0
1	C	202	GLN	2.0
1	C	125	ALA	2.0
1	C	537	ALA	2.0
1	B	477	ARG	2.0
1	D	94	GLY	2.0
1	C	196	HIS	2.0
1	C	321	SER	2.0
1	C	841	ALA	2.0
1	D	928	TYR	2.0
1	C	918	LEU	2.0
1	D	1002	ALA	2.0
1	C	281	GLN	2.0
1	C	775	TRP	2.0
1	D	512	ASP	2.0
1	C	183	GLY	2.0
1	C	474	GLU	2.0
1	D	278	GLN	2.0
1	C	42	HIS	2.0
1	D	667	THR	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 carbohydrates 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.