



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:13 PM UTC

PDB ID : 2R6C / pdb_00002r6c
Title : Crystal Form BH2
Authors : Bailey, S.; Eliason, W.K.; Steitz, T.A.
Deposited on : 2007-09-05
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

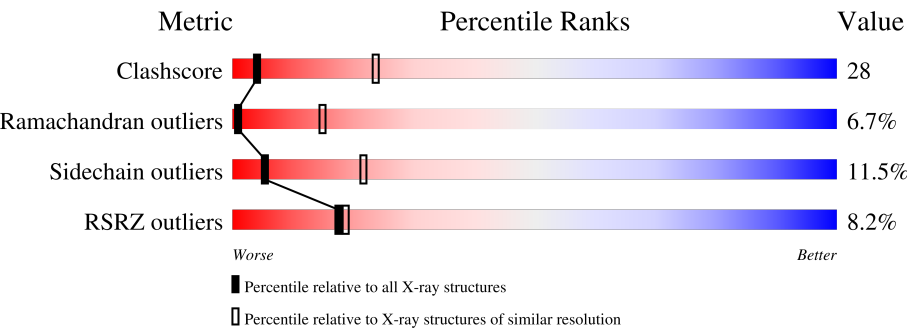
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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))
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	454	4% 42% 27% 8% • 21%
1	B	454	4% 41% 27% 10% • 21%
1	C	454	6% 41% 28% 8% • 21%
1	D	454	5% 38% 30% 9% • 21%
1	E	454	5% 43% 26% 9% • 21%
1	F	454	15% 45% 25% 8% • 21%
2	G	143	10% 57% 30% 8% ••

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Mol	Chain	Length	Quality of chain
2	H	143	7% 51% 36% 8%
2	I	143	4% 51% 36% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19920 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 Replicative helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	B	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	C	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	D	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	E	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			
1	F	358	Total	C	N	O	S	0	0	0
			2759	1737	473	536	13			

- Molecule 2 is a protein called DnaG Primase, Helicase Binding Domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			
2	H	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			
2	I	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			

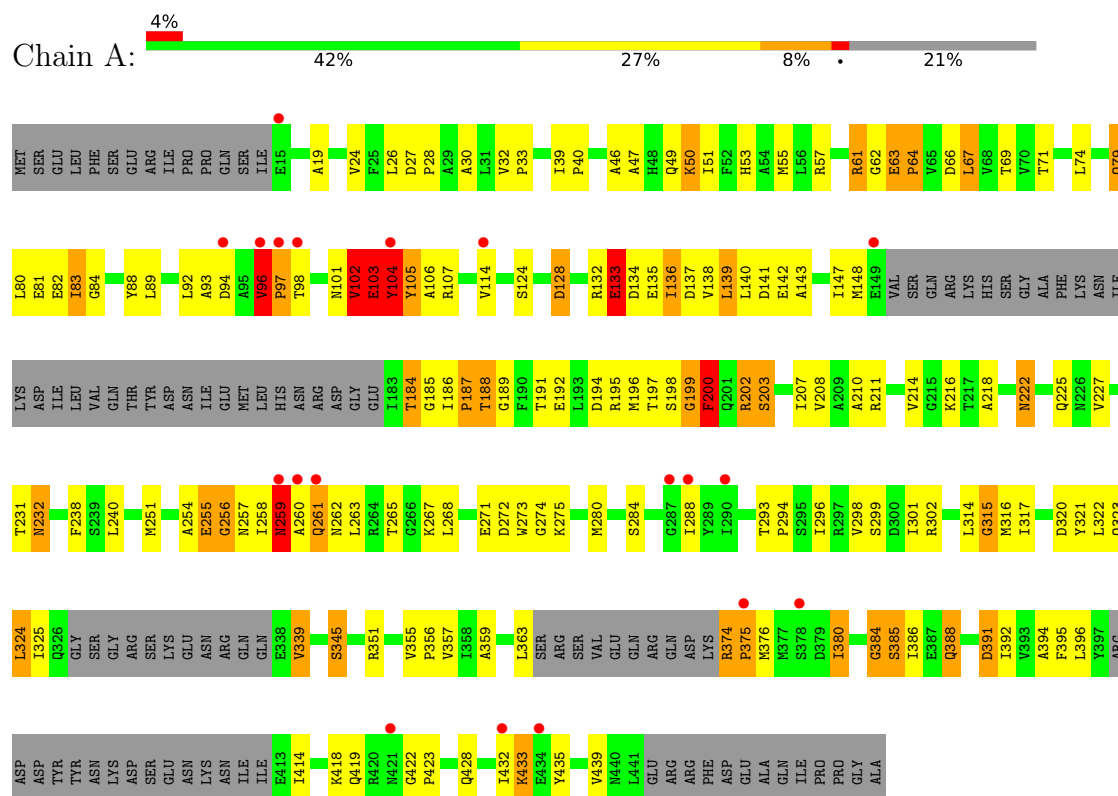
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	530	GLU	ASP	conflict	UNP Q9X4D0
G	531	LEU	VAL	conflict	UNP Q9X4D0
H	530	GLU	ASP	conflict	UNP Q9X4D0
H	531	LEU	VAL	conflict	UNP Q9X4D0
I	530	GLU	ASP	conflict	UNP Q9X4D0
I	531	LEU	VAL	conflict	UNP Q9X4D0

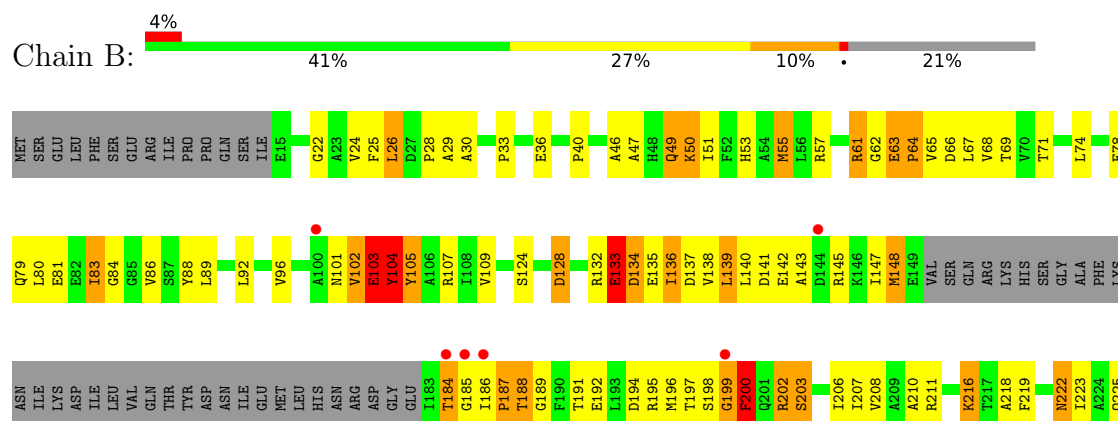
3 Residue-property plots

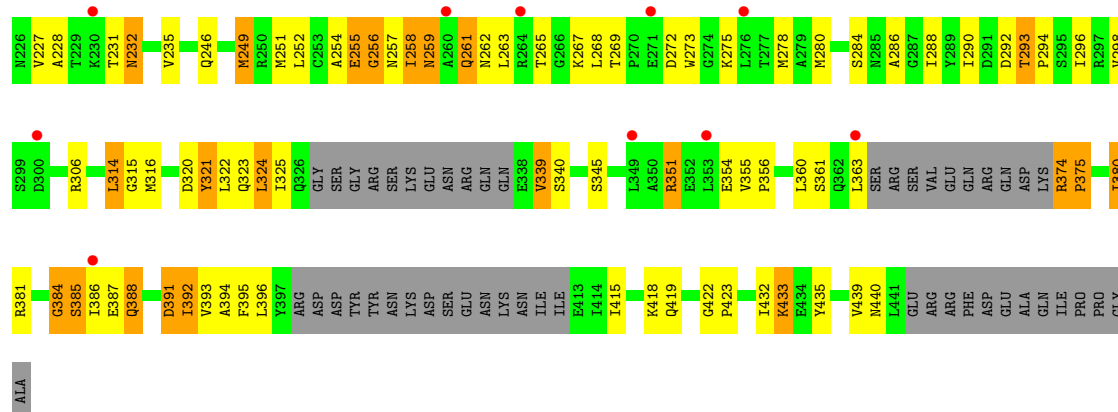
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

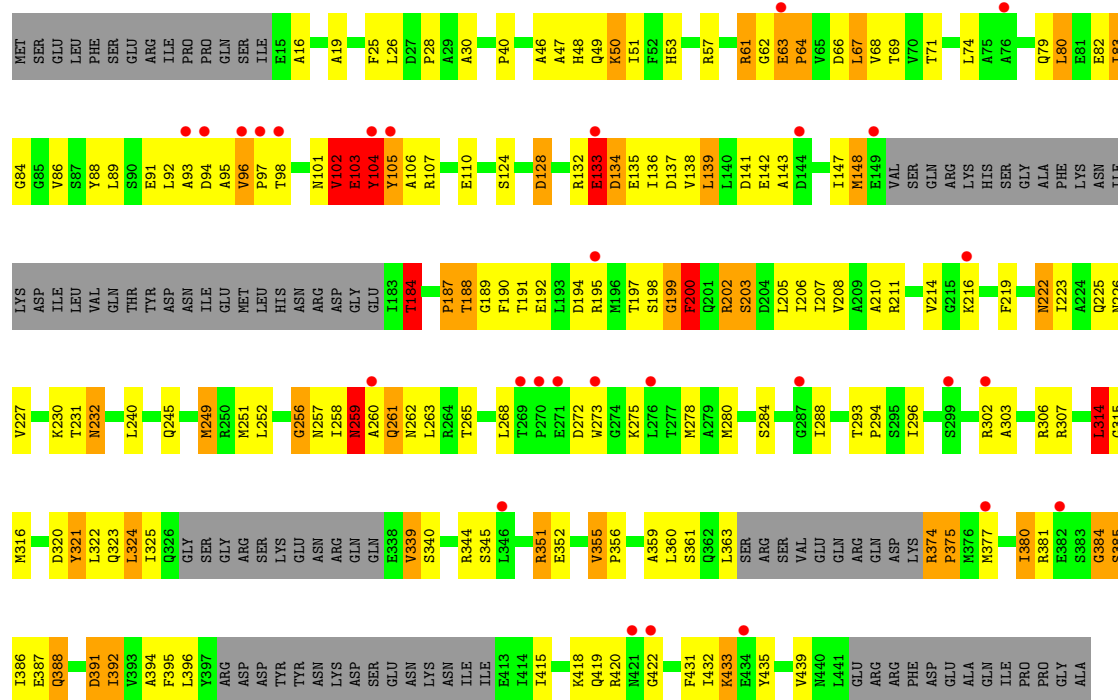
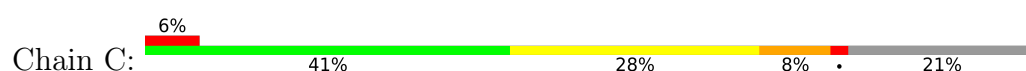


• Molecule 1: Replicative helicase

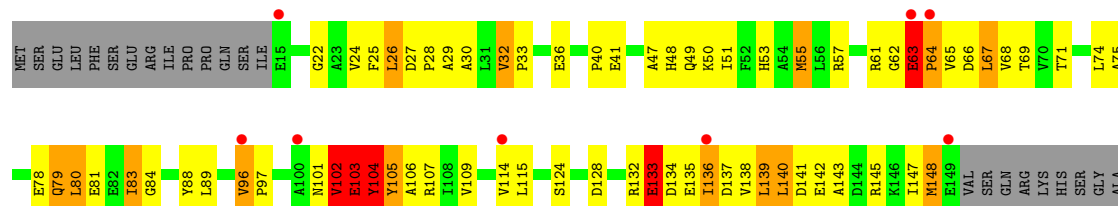


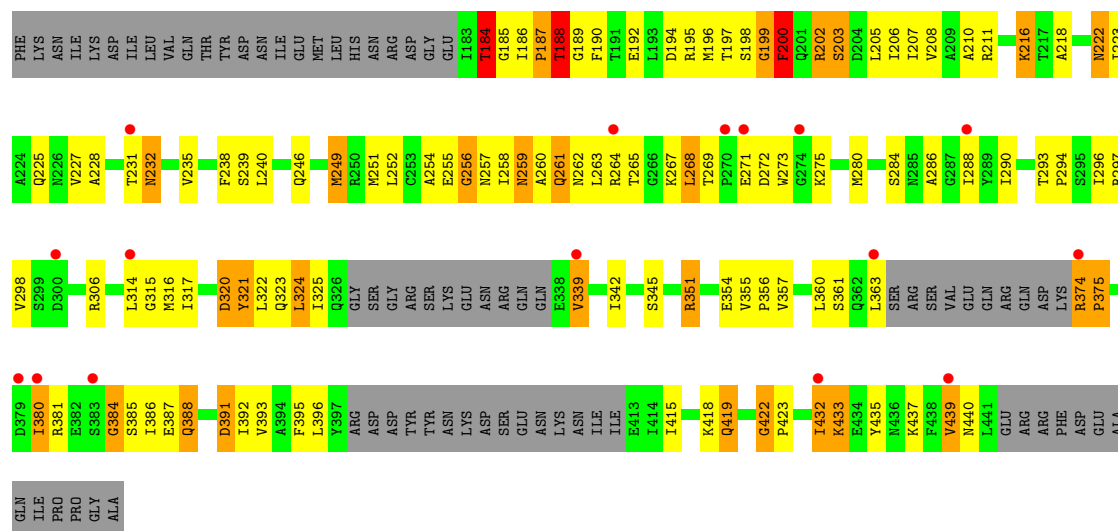


• Molecule 1: Replicative helicase

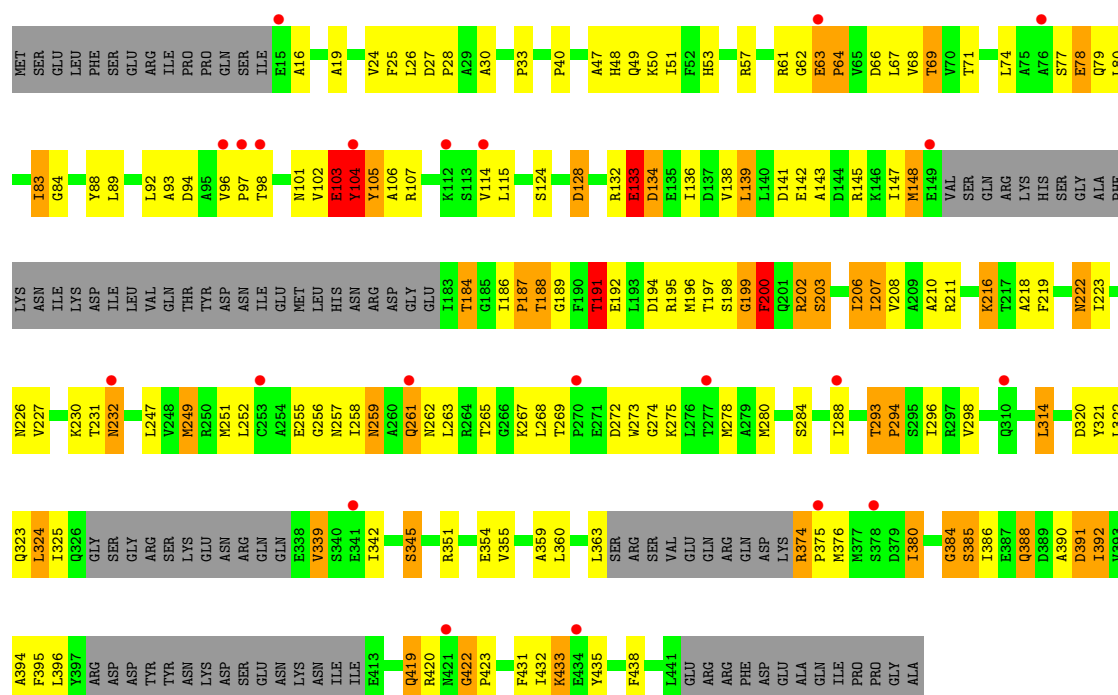


• Molecule 1: Replicative helicase

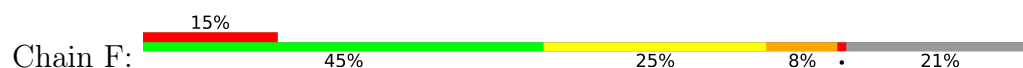


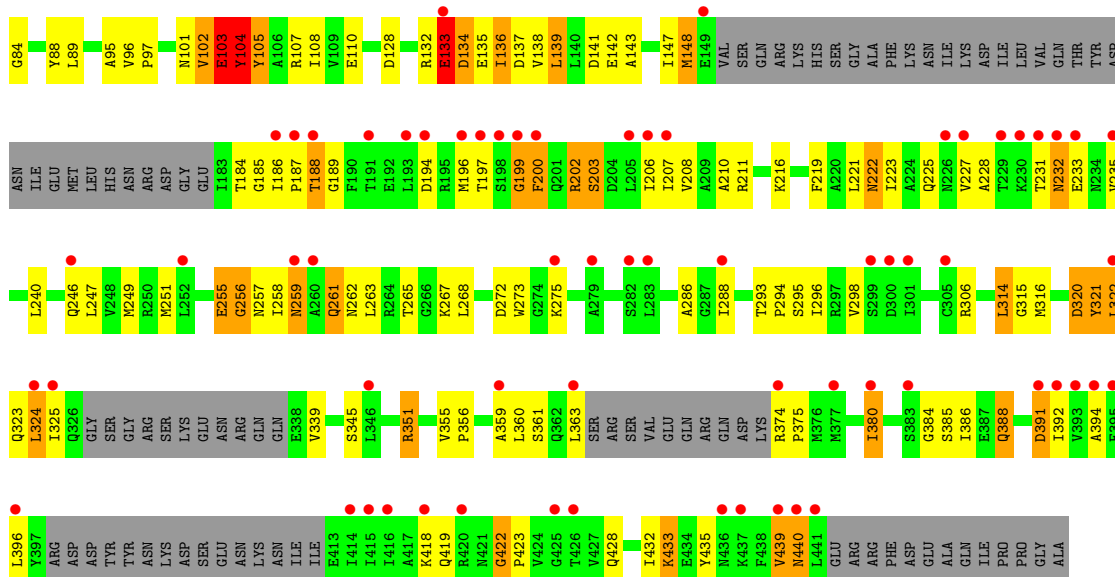


• Molecule 1: Replicative helicase

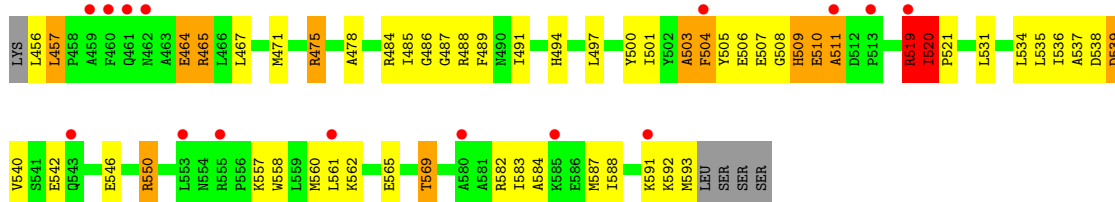


• Molecule 1: Replicative helicase

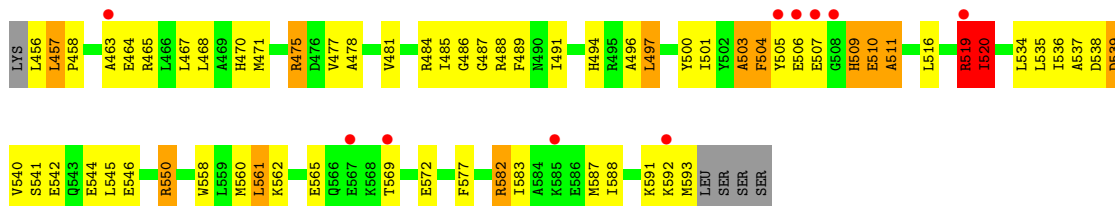




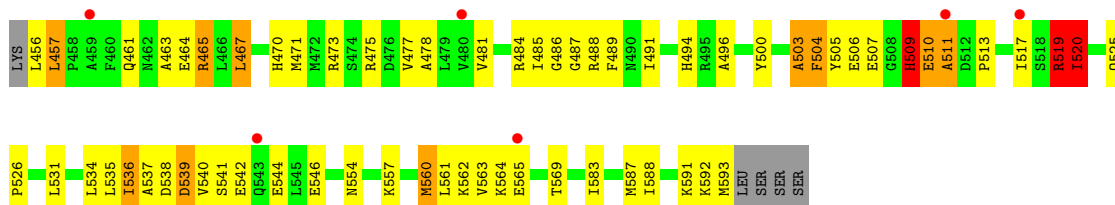
• Molecule 2: DnaG Primase, Helicase Binding Domain



• Molecule 2: DnaG Primase, Helicase Binding Domain



• Molecule 2: DnaG Primase, Helicase Binding Domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.78Å 228.78Å 192.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-4.00) 89.9 (20.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.320 , 0.344 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	127.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 182.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	19920	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% 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	0.65	1/2789 (0.0%)	1.14	21/3770 (0.6%)
1	B	0.61	1/2789 (0.0%)	1.13	21/3770 (0.6%)
1	C	0.64	0/2789	1.16	23/3770 (0.6%)
1	D	0.65	1/2789 (0.0%)	1.16	27/3770 (0.7%)
1	E	0.64	1/2789 (0.0%)	1.14	24/3770 (0.6%)
1	F	0.62	0/2789	1.09	25/3770 (0.7%)
2	G	0.53	0/1134	1.03	7/1514 (0.5%)
2	H	0.58	0/1134	1.03	7/1514 (0.5%)
2	I	0.54	0/1134	1.03	6/1514 (0.4%)
All	All	0.62	4/20136 (0.0%)	1.12	161/27162 (0.6%)

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	1	5
1	B	1	3
1	C	1	5
1	D	2	4
1	E	2	4
1	F	1	2
2	G	0	1
2	H	0	1
2	I	0	1
All	All	8	26

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	32	VAL	CA-CB	-9.01	1.49	1.54
1	E	255	GLU	CA-C	-7.43	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLU	CA-C	-5.44	1.50	1.53
1	A	96	VAL	CA-C	5.21	1.57	1.53

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	261	GLN	N-CA-C	15.34	129.35	111.71
1	C	261	GLN	N-CA-C	13.94	127.75	111.71
1	B	261	GLN	N-CA-C	13.23	127.17	111.82
1	A	261	GLN	N-CA-C	13.15	128.43	112.38
1	C	103	GLU	N-CA-C	12.59	126.80	112.57
1	E	261	GLN	N-CA-C	12.22	127.29	112.38
1	A	260	ALA	N-CA-C	-11.90	101.05	114.62
1	D	260	ALA	N-CA-C	-11.87	101.09	114.62
1	C	260	ALA	N-CA-C	-11.64	100.09	114.75
1	E	103	GLU	N-CA-C	10.93	124.92	112.57
1	A	103	GLU	N-CA-C	9.96	126.26	112.72
2	H	519	ARG	N-CA-C	9.62	131.28	110.80
2	I	519	ARG	N-CA-C	9.49	131.01	110.80
2	G	519	ARG	N-CA-C	9.43	130.89	110.80
1	F	103	GLU	N-CA-C	9.38	125.01	112.25
1	D	103	GLU	N-CA-C	9.25	125.30	112.72
1	D	199	GLY	N-CA-C	-9.22	99.26	112.17
1	A	199	GLY	N-CA-C	-9.14	98.28	112.45
1	C	199	GLY	N-CA-C	-9.14	98.28	112.45
1	E	199	GLY	N-CA-C	-8.97	98.55	112.45
1	E	293	THR	CA-C-N	8.55	130.53	119.84
1	E	293	THR	C-N-CA	8.55	130.53	119.84
1	E	133	GLU	N-CA-C	8.18	128.21	110.80
1	B	199	GLY	N-CA-C	-8.15	99.81	112.45
1	F	261	GLN	N-CA-C	8.06	123.24	113.41
1	D	293	THR	CA-C-N	8.01	129.85	119.84
1	D	293	THR	C-N-CA	8.01	129.85	119.84
1	A	133	GLU	N-CA-C	7.93	127.69	110.80
1	B	133	GLU	N-CA-C	7.78	127.37	110.80
1	F	133	GLU	N-CA-C	7.70	127.21	110.80
1	B	103	GLU	N-CA-C	7.69	123.66	111.81
1	D	133	GLU	N-CA-C	7.62	127.02	110.80
1	C	133	GLU	N-CA-C	7.53	126.83	110.80
1	B	293	THR	CA-C-N	7.45	129.16	119.84
1	B	293	THR	C-N-CA	7.45	129.16	119.84
1	A	321	TYR	N-CA-C	7.43	126.64	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	THR	N-CA-C	7.35	126.45	110.80
1	A	184	THR	N-CA-C	7.23	126.19	110.80
1	A	293	THR	CA-C-N	7.22	128.87	119.84
1	A	293	THR	C-N-CA	7.22	128.87	119.84
1	C	321	TYR	N-CA-C	7.01	125.72	110.80
1	E	321	TYR	N-CA-C	6.89	125.48	110.80
1	D	321	TYR	N-CA-C	6.87	125.43	110.80
1	C	293	THR	CA-C-N	6.77	128.31	119.84
1	C	293	THR	C-N-CA	6.77	128.31	119.84
1	C	184	THR	N-CA-C	6.71	125.08	110.80
1	F	293	THR	CA-C-N	6.63	128.13	119.84
1	F	293	THR	C-N-CA	6.63	128.13	119.84
1	B	103	GLU	CA-C-N	6.62	133.62	121.70
1	B	103	GLU	C-N-CA	6.62	133.62	121.70
1	C	104	TYR	CA-CB-CG	-6.56	102.08	113.90
1	B	255	GLU	O-C-N	6.52	126.36	121.47
1	B	321	TYR	N-CA-C	6.49	124.62	110.80
1	F	78	GLU	N-CA-C	6.48	120.11	111.30
1	D	184	THR	N-CA-C	6.40	124.44	110.80
1	F	103	GLU	CA-C-N	6.40	133.21	121.70
1	F	103	GLU	C-N-CA	6.40	133.21	121.70
1	A	96	VAL	N-CA-C	6.34	114.09	108.63
1	F	104	TYR	CA-CB-CG	-6.34	102.49	113.90
1	F	27	ASP	N-CA-C	6.31	123.75	109.81
1	A	214	VAL	N-CA-C	-6.30	106.66	112.96
1	E	103	GLU	CA-C-N	6.28	133.01	121.70
1	E	103	GLU	C-N-CA	6.28	133.01	121.70
1	B	184	THR	N-CA-C	6.26	124.14	110.80
1	E	255	GLU	O-C-N	6.21	126.80	121.65
2	G	520	ILE	CA-C-N	6.19	127.58	119.84
2	G	520	ILE	C-N-CA	6.19	127.58	119.84
1	A	261	GLN	CA-C-N	6.14	132.74	121.70
1	A	261	GLN	C-N-CA	6.14	132.74	121.70
1	B	78	GLU	N-CA-C	6.13	119.85	111.39
1	E	104	TYR	CA-CB-CG	-6.13	102.87	113.90
1	F	321	TYR	N-CA-C	6.12	123.84	110.80
1	C	422	GLY	CA-C-N	6.09	126.05	119.78
1	C	422	GLY	C-N-CA	6.09	126.05	119.78
1	D	103	GLU	CA-C-N	6.03	132.56	121.70
1	D	103	GLU	C-N-CA	6.03	132.56	121.70
2	I	520	ILE	CA-C-N	6.01	127.36	119.84
2	I	520	ILE	C-N-CA	6.01	127.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	261	GLN	CA-C-N	6.00	132.50	121.70
1	D	261	GLN	C-N-CA	6.00	132.50	121.70
1	C	214	VAL	N-CA-C	-5.98	107.67	113.53
1	A	104	TYR	CA-CB-CG	-5.95	103.19	113.90
1	D	104	TYR	CA-CB-CG	-5.89	103.30	113.90
1	D	267	LYS	N-CA-C	5.88	119.19	110.48
1	B	261	GLN	CA-C-N	5.88	132.28	121.70
1	B	261	GLN	C-N-CA	5.88	132.28	121.70
1	E	261	GLN	CA-C-N	5.84	132.21	121.70
1	E	261	GLN	C-N-CA	5.84	132.21	121.70
1	D	422	GLY	CA-C-N	5.79	125.75	119.78
1	D	422	GLY	C-N-CA	5.79	125.75	119.78
1	E	422	GLY	CA-C-N	5.75	125.70	119.78
1	E	422	GLY	C-N-CA	5.75	125.70	119.78
1	D	78	GLU	N-CA-C	5.74	119.16	111.24
2	I	509	HIS	N-CA-C	5.72	118.06	108.23
1	E	104	TYR	N-CA-CB	5.68	120.16	110.50
1	F	184	THR	N-CA-C	5.67	122.89	110.80
1	C	133	GLU	CA-C-N	5.65	131.87	121.70
1	C	133	GLU	C-N-CA	5.65	131.87	121.70
1	F	199	GLY	N-CA-C	-5.64	102.56	112.77
2	G	519	ARG	CA-C-N	5.64	132.56	122.13
2	G	519	ARG	C-N-CA	5.64	132.56	122.13
1	F	422	GLY	CA-C-N	5.63	125.58	119.78
1	F	422	GLY	C-N-CA	5.63	125.58	119.78
2	I	519	ARG	CA-C-N	5.62	132.52	122.13
2	I	519	ARG	C-N-CA	5.62	132.52	122.13
1	B	29	ALA	N-CA-C	-5.60	106.52	113.19
1	A	133	GLU	CA-C-N	5.59	131.76	121.70
1	A	133	GLU	C-N-CA	5.59	131.76	121.70
1	A	422	GLY	CA-C-N	5.59	125.54	119.78
1	A	422	GLY	C-N-CA	5.59	125.54	119.78
1	F	133	GLU	CA-C-N	5.55	131.70	121.70
1	F	133	GLU	C-N-CA	5.55	131.70	121.70
1	F	261	GLN	CA-C-N	5.54	131.68	121.70
1	F	261	GLN	C-N-CA	5.54	131.68	121.70
1	B	86	VAL	N-CA-C	-5.54	104.81	112.50
1	D	133	GLU	CA-C-N	5.53	131.65	121.70
1	D	133	GLU	C-N-CA	5.53	131.65	121.70
1	C	261	GLN	CA-C-N	5.51	131.61	121.70
1	C	261	GLN	C-N-CA	5.51	131.61	121.70
1	B	267	LYS	N-CA-C	5.50	118.61	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	ALA	N-CA-C	-5.49	106.65	113.19
1	E	133	GLU	CA-C-N	5.47	131.55	121.70
1	E	133	GLU	C-N-CA	5.47	131.55	121.70
1	C	96	VAL	N-CA-C	5.47	114.92	108.96
2	H	577	PHE	N-CA-C	5.47	117.24	111.28
1	E	199	GLY	CA-C-N	5.45	131.51	121.70
1	E	199	GLY	C-N-CA	5.45	131.51	121.70
2	H	519	ARG	CA-C-N	5.44	132.19	122.13
2	H	519	ARG	C-N-CA	5.44	132.19	122.13
1	A	27	ASP	N-CA-C	5.39	121.72	109.81
1	F	267	LYS	N-CA-C	5.38	118.08	110.50
1	B	133	GLU	CA-C-N	5.37	131.37	121.70
1	B	133	GLU	C-N-CA	5.37	131.37	121.70
1	E	267	LYS	N-CA-C	5.36	118.05	110.50
2	H	509	HIS	N-CA-C	5.34	117.39	107.99
1	F	104	TYR	N-CA-CB	5.32	119.54	110.50
1	E	27	ASP	N-CA-C	5.28	121.47	109.81
2	G	520	ILE	N-CA-CB	5.22	118.52	111.21
1	D	190	PHE	N-CA-C	5.21	117.11	108.20
1	B	104	TYR	N-CA-CB	5.21	119.35	110.50
1	D	26	LEU	N-CA-C	5.20	117.75	111.40
1	A	96	VAL	CB-CA-C	5.20	115.78	110.94
1	F	246	GLN	N-CA-C	-5.20	106.89	113.18
1	C	199	GLY	CA-C-N	5.19	131.04	121.70
1	C	199	GLY	C-N-CA	5.19	131.04	121.70
1	D	432	ILE	N-CA-C	5.16	115.83	110.82
2	H	520	ILE	CA-C-N	5.14	126.26	119.84
2	H	520	ILE	C-N-CA	5.14	126.26	119.84
1	F	26	LEU	N-CA-C	5.13	117.66	111.40
1	B	26	LEU	N-CA-C	5.13	117.65	111.40
1	F	104	TYR	CA-C-N	5.13	130.93	121.70
1	F	104	TYR	C-N-CA	5.13	130.93	121.70
1	E	78	GLU	N-CA-C	5.12	118.46	111.39
1	C	103	GLU	CA-C-N	5.12	130.91	121.70
1	C	103	GLU	C-N-CA	5.12	130.91	121.70
2	G	509	HIS	N-CA-C	5.11	117.02	108.23
1	D	138	VAL	N-CA-C	-5.11	105.73	110.53
1	A	267	LYS	N-CA-C	5.10	117.69	110.50
1	D	65	VAL	CB-CA-C	-5.09	104.11	111.19
1	D	27	ASP	N-CA-C	5.09	121.06	109.81
1	C	377	MET	N-CA-C	5.01	116.43	110.97

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	104	TYR	CA
1	B	104	TYR	CA
1	C	104	TYR	CA
1	D	104	TYR	CA
1	D	184	THR	CA
1	E	104	TYR	CA
1	E	184	THR	CA
1	F	104	TYR	CA

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLU	Peptide
1	A	187	PRO	Peptide
1	A	259	ASN	Peptide
1	A	320	ASP	Peptide
1	A	374	ARG	Peptide
1	B	187	PRO	Peptide
1	B	320	ASP	Peptide
1	B	374	ARG	Peptide
1	C	103	GLU	Peptide
1	C	187	PRO	Peptide
1	C	259	ASN	Peptide
1	C	320	ASP	Peptide
1	C	374	ARG	Peptide
1	D	103	GLU	Peptide
1	D	187	PRO	Peptide
1	D	320	ASP	Peptide
1	D	374	ARG	Peptide
1	E	103	GLU	Peptide
1	E	187	PRO	Peptide
1	E	320	ASP	Peptide
1	E	374	ARG	Peptide
1	F	103	GLU	Peptide
1	F	320	ASP	Peptide
2	G	519	ARG	Peptide
2	H	519	ARG	Peptide
2	I	519	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2759	0	2806	168	0
1	B	2759	0	2806	164	0
1	C	2759	0	2805	176	0
1	D	2759	0	2807	194	0
1	E	2759	0	2806	173	0
1	F	2759	0	2807	132	0
2	G	1122	0	1144	63	0
2	H	1122	0	1144	62	0
2	I	1122	0	1144	58	0
All	All	19920	0	20269	1114	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 28.

All (1114) 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:255:GLU:O	1:A:257:ASN:N	1.60	1.34
1:C:188:THR:OG1	1:C:194:ASP:OD1	1.52	1.27
1:C:306:ARG:CZ	1:D:32:VAL:HG21	1.64	1.26
1:D:255:GLU:O	1:D:257:ASN:N	1.70	1.23
1:A:132:ARG:O	1:A:133:GLU:HB2	1.40	1.20
1:E:188:THR:OG1	1:E:194:ASP:OD1	1.60	1.16
1:D:188:THR:OG1	1:D:194:ASP:OD1	1.63	1.14
1:B:132:ARG:O	1:B:133:GLU:HB2	1.46	1.14
1:F:255:GLU:O	1:F:257:ASN:N	1.79	1.14
1:C:227:VAL:O	1:C:231:THR:HG22	1.49	1.13
2:H:475:ARG:NH1	2:H:505:TYR:HB2	1.64	1.12
1:B:63:GLU:H	1:B:64:PRO:HA	0.99	1.11
1:E:104:TYR:HE2	1:F:63:GLU:HB2	1.16	1.10
1:D:63:GLU:H	1:D:64:PRO:HA	1.12	1.08
1:C:132:ARG:O	1:C:133:GLU:HB2	1.43	1.08
1:E:132:ARG:O	1:E:133:GLU:HB2	1.47	1.07
1:F:132:ARG:O	1:F:133:GLU:HB2	1.50	1.07
1:C:94:ASP:HB3	2:H:591:LYS:NZ	1.69	1.06
1:C:94:ASP:HB3	2:H:591:LYS:HZ3	1.09	1.06
1:E:63:GLU:H	1:E:64:PRO:HA	1.13	1.06
1:F:227:VAL:O	1:F:231:THR:HG22	1.56	1.06
1:D:132:ARG:HD2	1:D:139:LEU:HG	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:THR:OG1	1:F:194:ASP:OD1	1.74	1.05
1:A:227:VAL:O	1:A:231:THR:HG22	1.52	1.05
1:B:227:VAL:O	1:B:231:THR:HG22	1.56	1.05
1:D:63:GLU:N	1:D:64:PRO:HA	1.71	1.05
1:A:63:GLU:H	1:A:64:PRO:HA	1.18	1.04
1:D:132:ARG:O	1:D:133:GLU:HB2	1.50	1.04
1:E:257:ASN:C	1:E:435:TYR:CE2	2.35	1.04
1:F:63:GLU:H	1:F:64:PRO:HA	1.17	1.03
1:A:104:TYR:HE2	1:B:63:GLU:HB2	1.17	1.03
1:C:104:TYR:CE2	1:D:63:GLU:HB2	1.93	1.02
1:B:132:ARG:HD2	1:B:139:LEU:HG	1.41	1.02
1:C:133:GLU:N	1:C:134:ASP:HB2	1.74	1.02
2:H:475:ARG:HH12	2:H:505:TYR:HB2	1.23	1.02
1:B:63:GLU:N	1:B:64:PRO:HA	1.71	1.01
1:D:101:ASN:O	1:D:103:GLU:N	1.93	1.01
1:C:63:GLU:H	1:C:64:PRO:HA	1.23	1.01
1:C:257:ASN:C	1:C:435:TYR:CE2	2.39	1.01
1:D:61:ARG:HB2	1:D:62:GLY:HA3	1.43	1.00
1:B:188:THR:OG1	1:B:194:ASP:OD1	1.80	0.99
1:D:257:ASN:C	1:D:435:TYR:CE2	2.40	0.99
1:C:104:TYR:HE2	1:D:63:GLU:HB2	1.23	0.99
1:E:104:TYR:CE2	1:F:63:GLU:HB2	1.96	0.99
1:B:63:GLU:H	1:B:64:PRO:CA	1.77	0.98
1:A:104:TYR:CE2	1:B:63:GLU:HB2	1.99	0.98
1:B:257:ASN:C	1:B:435:TYR:CE2	2.43	0.97
1:A:188:THR:OG1	1:A:194:ASP:OD1	1.83	0.96
1:A:257:ASN:C	1:A:435:TYR:CE2	2.43	0.96
1:D:227:VAL:O	1:D:231:THR:HG22	1.62	0.96
1:E:133:GLU:N	1:E:134:ASP:HB2	1.80	0.96
1:B:133:GLU:N	1:B:134:ASP:HB2	1.80	0.95
1:C:61:ARG:HB2	1:C:62:GLY:HA3	1.45	0.95
1:B:104:TYR:OH	2:G:537:ALA:HB2	1.67	0.94
1:D:63:GLU:H	1:D:64:PRO:CA	1.82	0.93
1:B:62:GLY:HA2	1:B:63:GLU:HB3	1.50	0.93
1:F:63:GLU:N	1:F:64:PRO:HA	1.82	0.93
1:A:61:ARG:HB2	1:A:62:GLY:HA3	1.49	0.93
1:E:257:ASN:C	1:E:435:TYR:HE2	1.77	0.93
1:E:227:VAL:O	1:E:231:THR:HG22	1.68	0.92
1:C:231:THR:HG23	1:C:232:ASN:H	1.33	0.92
1:E:63:GLU:N	1:E:64:PRO:HA	1.83	0.92
1:C:132:ARG:HD2	1:C:139:LEU:HG	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:LEU:O	1:E:325:ILE:HG22	1.70	0.92
1:B:101:ASN:O	1:B:103:GLU:N	2.02	0.91
1:F:61:ARG:HB2	1:F:62:GLY:HA3	1.53	0.90
1:B:66:ASP:H	1:B:69:THR:HG22	1.35	0.90
1:C:322:LEU:O	1:C:325:ILE:HG22	1.70	0.90
1:F:363:LEU:HD23	1:F:380:ILE:HG23	1.51	0.89
2:H:475:ARG:HH12	2:H:505:TYR:CB	1.84	0.89
1:A:104:TYR:HH	1:B:69:THR:HG1	1.17	0.89
1:E:61:ARG:HB2	1:E:62:GLY:HA3	1.54	0.89
1:D:322:LEU:O	1:D:325:ILE:HG22	1.73	0.89
1:A:322:LEU:O	1:A:325:ILE:HG22	1.73	0.89
1:E:63:GLU:H	1:E:64:PRO:CA	1.86	0.89
1:F:132:ARG:HD2	1:F:139:LEU:HG	1.54	0.88
1:E:94:ASP:HB3	2:I:591:LYS:NZ	1.88	0.88
1:F:322:LEU:O	1:F:325:ILE:HG22	1.72	0.88
1:B:322:LEU:O	1:B:325:ILE:HG22	1.72	0.87
1:F:63:GLU:H	1:F:64:PRO:CA	1.87	0.87
2:G:475:ARG:NH1	2:G:505:TYR:HB2	1.89	0.87
1:D:255:GLU:C	1:D:257:ASN:H	1.81	0.87
1:E:93:ALA:HB1	2:I:588:ILE:HD11	1.56	0.87
1:C:302:ARG:HG2	1:C:306:ARG:HH12	1.40	0.87
1:D:66:ASP:H	1:D:69:THR:CG2	1.88	0.87
1:A:63:GLU:H	1:A:64:PRO:CA	1.88	0.86
1:F:67:LEU:O	1:F:71:THR:HG23	1.75	0.86
1:F:101:ASN:O	1:F:103:GLU:N	2.08	0.86
1:B:363:LEU:HD23	1:B:380:ILE:HG23	1.56	0.86
2:H:484:ARG:HH22	2:H:546:GLU:HG2	1.39	0.86
1:A:101:ASN:O	1:A:103:GLU:N	2.10	0.85
1:E:231:THR:HG23	1:E:232:ASN:H	1.40	0.84
1:A:63:GLU:N	1:A:64:PRO:HA	1.89	0.84
1:F:133:GLU:N	1:F:134:ASP:HB2	1.91	0.84
1:B:257:ASN:C	1:B:435:TYR:HE2	1.86	0.84
2:H:475:ARG:HG3	2:H:475:ARG:HH11	1.41	0.84
1:D:133:GLU:N	1:D:134:ASP:HB2	1.93	0.83
1:C:93:ALA:HB1	2:H:588:ILE:HD11	1.61	0.83
2:G:456:LEU:O	2:G:457:LEU:HB2	1.78	0.83
2:I:475:ARG:NH1	2:I:505:TYR:HB2	1.94	0.83
1:E:83:ILE:HG22	1:E:84:GLY:H	1.42	0.83
1:D:231:THR:HG23	1:D:232:ASN:H	1.43	0.83
1:E:101:ASN:O	1:E:103:GLU:N	2.11	0.82
1:E:132:ARG:HD2	1:E:139:LEU:HG	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ASP:H	1:D:69:THR:HG22	1.44	0.81
1:C:63:GLU:N	1:C:64:PRO:HA	1.96	0.81
1:F:66:ASP:H	1:F:69:THR:HG22	1.44	0.81
1:A:67:LEU:O	1:A:71:THR:HG23	1.81	0.81
1:B:66:ASP:H	1:B:69:THR:CG2	1.93	0.80
1:B:62:GLY:HA2	1:B:63:GLU:CB	2.07	0.80
1:C:187:PRO:O	1:C:189:GLY:N	2.14	0.80
1:A:61:ARG:CB	1:A:62:GLY:HA3	2.12	0.80
1:B:227:VAL:O	1:B:231:THR:CG2	2.31	0.79
1:F:66:ASP:H	1:F:69:THR:CG2	1.95	0.79
1:E:94:ASP:HB3	2:I:591:LYS:HZ3	1.47	0.79
1:B:135:GLU:O	1:B:137:ASP:N	2.13	0.79
1:B:231:THR:O	1:B:232:ASN:HB2	1.81	0.79
1:E:258:ILE:O	1:E:259:ASN:HB3	1.81	0.79
2:G:475:ARG:HG3	2:G:475:ARG:HH11	1.47	0.79
1:A:133:GLU:N	1:A:134:ASP:HB2	1.97	0.79
1:A:197:THR:HB	1:A:199:GLY:O	1.81	0.79
1:C:63:GLU:H	1:C:64:PRO:CA	1.95	0.79
1:A:94:ASP:HB3	2:G:591:LYS:NZ	1.98	0.78
1:A:231:THR:HG23	1:A:232:ASN:H	1.49	0.78
1:C:67:LEU:O	1:C:71:THR:HG23	1.83	0.78
1:C:74:LEU:HD22	1:C:83:ILE:HD11	1.65	0.78
1:F:148:MET:HA	1:F:148:MET:CE	2.13	0.78
1:A:66:ASP:H	1:A:69:THR:HG22	1.48	0.78
1:D:61:ARG:CB	1:D:62:GLY:HA3	2.07	0.77
1:B:61:ARG:HB2	1:B:62:GLY:HA3	1.66	0.77
1:C:51:ILE:HD11	1:C:83:ILE:HG21	1.66	0.77
1:F:62:GLY:HA2	1:F:63:GLU:HB3	1.65	0.77
1:B:132:ARG:O	1:B:133:GLU:CB	2.30	0.77
1:E:74:LEU:HD22	1:E:83:ILE:HD11	1.66	0.77
1:C:104:TYR:HH	1:D:69:THR:HG1	1.01	0.77
1:A:363:LEU:HD23	1:A:380:ILE:HG23	1.67	0.76
1:A:62:GLY:HA2	1:A:63:GLU:HB3	1.67	0.76
1:C:315:GLY:O	1:C:356:PRO:HD2	1.85	0.76
1:C:61:ARG:CB	1:C:62:GLY:HA3	2.15	0.76
1:F:71:THR:HG22	1:F:89:LEU:HD12	1.68	0.76
1:A:257:ASN:C	1:A:435:TYR:HE2	1.94	0.76
1:E:62:GLY:HA2	1:E:63:GLU:HB3	1.66	0.75
1:A:222:ASN:HD22	1:A:222:ASN:N	1.85	0.75
1:D:363:LEU:HD23	1:D:380:ILE:HG23	1.65	0.75
1:C:306:ARG:NH2	1:D:32:VAL:HG21	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:ASN:O	1:E:435:TYR:HE2	1.69	0.75
1:A:255:GLU:C	1:A:257:ASN:N	2.44	0.75
1:A:93:ALA:HB1	2:G:588:ILE:HD11	1.67	0.75
1:C:101:ASN:O	1:C:103:GLU:N	2.19	0.75
1:C:187:PRO:C	1:C:189:GLY:H	1.95	0.75
1:C:66:ASP:H	1:C:69:THR:HG22	1.50	0.75
1:B:187:PRO:O	1:B:189:GLY:N	2.19	0.74
1:B:30:ALA:O	1:B:33:PRO:HD2	1.87	0.74
1:F:132:ARG:O	1:F:133:GLU:CB	2.35	0.74
1:E:363:LEU:HD23	1:E:380:ILE:HG23	1.70	0.74
2:G:475:ARG:HH12	2:G:505:TYR:CB	2.00	0.73
1:C:257:ASN:C	1:C:435:TYR:HE2	1.90	0.73
1:D:218:ALA:O	1:D:222:ASN:ND2	2.21	0.73
1:F:135:GLU:O	1:F:137:ASP:N	2.21	0.73
1:A:218:ALA:O	1:A:222:ASN:ND2	2.21	0.73
1:C:104:TYR:H	1:C:107:ARG:H	1.36	0.73
1:B:74:LEU:HD22	1:B:83:ILE:HD11	1.71	0.73
1:C:307:ARG:CZ	1:D:36:GLU:OE2	2.36	0.73
1:E:66:ASP:H	1:E:69:THR:HG22	1.53	0.73
1:E:67:LEU:O	1:E:71:THR:HG23	1.88	0.73
1:E:132:ARG:O	1:E:133:GLU:CB	2.31	0.72
1:F:132:ARG:C	1:F:134:ASP:HB2	2.14	0.72
1:C:363:LEU:HD23	1:C:380:ILE:HG23	1.71	0.72
1:A:104:TYR:H	1:A:107:ARG:H	1.38	0.72
1:A:132:ARG:HD2	1:A:139:LEU:HG	1.70	0.72
1:C:258:ILE:O	1:C:259:ASN:HB3	1.90	0.72
1:E:388:GLN:H	1:E:388:GLN:HE21	1.36	0.72
1:D:135:GLU:O	1:D:137:ASP:N	2.15	0.72
1:A:132:ARG:O	1:A:133:GLU:CB	2.27	0.72
1:A:26:LEU:HD22	2:G:592:LYS:HE3	1.72	0.72
1:D:257:ASN:C	1:D:435:TYR:HE2	1.98	0.72
1:A:94:ASP:HB3	2:G:591:LYS:HZ3	1.54	0.71
1:D:257:ASN:O	1:D:435:TYR:CE2	2.42	0.71
1:F:62:GLY:HA2	1:F:63:GLU:CB	2.19	0.71
1:F:231:THR:HG23	1:F:232:ASN:H	1.55	0.71
1:D:104:TYR:OH	2:H:537:ALA:HB2	1.90	0.71
1:F:74:LEU:HD22	1:F:83:ILE:HD11	1.73	0.71
1:A:268:LEU:HB3	1:A:272:ASP:HB2	1.73	0.71
1:A:74:LEU:HD22	1:A:83:ILE:HD11	1.72	0.71
1:B:218:ALA:O	1:B:222:ASN:ND2	2.24	0.70
1:C:132:ARG:O	1:C:133:GLU:CB	2.30	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:PRO:O	1:D:189:GLY:N	2.24	0.70
1:A:114:VAL:HG11	1:D:140:LEU:HD11	1.72	0.70
1:D:62:GLY:HA2	1:D:63:GLU:HB3	1.71	0.70
1:E:197:THR:HB	1:E:199:GLY:O	1.91	0.70
1:F:148:MET:HA	1:F:148:MET:HE2	1.73	0.70
2:H:484:ARG:NH2	2:H:546:GLU:HG2	2.06	0.70
1:B:257:ASN:O	1:B:435:TYR:HE2	1.74	0.70
1:B:339:VAL:HG13	1:B:384:GLY:HA3	1.73	0.70
1:A:231:THR:O	1:A:232:ASN:HB2	1.90	0.70
2:H:475:ARG:NH1	2:H:505:TYR:CB	2.47	0.70
2:G:475:ARG:NH1	2:G:505:TYR:CB	2.54	0.70
1:C:257:ASN:O	1:C:435:TYR:CE2	2.44	0.69
1:F:227:VAL:O	1:F:231:THR:CG2	2.39	0.69
2:I:475:ARG:HG2	2:I:511:ALA:CB	2.22	0.69
1:A:187:PRO:O	1:A:189:GLY:N	2.24	0.69
1:A:192:GLU:HA	1:A:195:ARG:HG3	1.73	0.69
1:B:47:ALA:HB1	1:B:83:ILE:HG23	1.74	0.69
2:G:487:GLY:HA3	2:G:489:PHE:H	1.57	0.69
1:B:258:ILE:O	1:B:259:ASN:HB3	1.92	0.69
1:C:306:ARG:NH1	1:D:32:VAL:HG21	2.08	0.69
1:A:258:ILE:O	1:A:259:ASN:HB3	1.93	0.69
1:F:28:PRO:C	1:F:30:ALA:H	2.01	0.68
2:H:510:GLU:O	2:H:511:ALA:HB2	1.92	0.68
1:A:62:GLY:CA	1:A:63:GLU:HB3	2.23	0.68
1:B:148:MET:HA	1:B:148:MET:HE2	1.74	0.68
1:B:148:MET:HA	1:B:148:MET:CE	2.24	0.68
1:F:104:TYR:OH	2:I:537:ALA:HB2	1.93	0.68
1:D:51:ILE:HD11	1:D:83:ILE:HG21	1.76	0.68
1:D:388:GLN:HE21	1:D:388:GLN:H	1.40	0.68
1:E:227:VAL:O	1:E:231:THR:CG2	2.41	0.68
1:A:210:ALA:HB2	1:A:396:LEU:HB2	1.76	0.68
1:C:83:ILE:HG22	1:C:84:GLY:H	1.58	0.68
1:E:218:ALA:O	1:E:222:ASN:ND2	2.27	0.68
1:E:268:LEU:HB3	1:E:272:ASP:HB2	1.76	0.68
1:E:273:TRP:C	1:E:275:LYS:H	2.03	0.67
1:A:299:SER:HB3	1:B:36:GLU:HB3	1.75	0.67
1:A:432:ILE:O	1:A:433:LYS:HB2	1.94	0.67
1:C:257:ASN:C	1:C:435:TYR:CD2	2.73	0.67
2:G:491:ILE:HB	2:G:494:HIS:HD2	1.59	0.67
1:F:233:GLU:HG2	1:F:315:GLY:HA3	1.76	0.67
2:H:491:ILE:HB	2:H:494:HIS:HD2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:THR:CB	1:A:199:GLY:O	2.41	0.67
1:E:105:TYR:HE2	1:F:68:VAL:HG12	1.59	0.67
2:H:583:ILE:O	2:H:587:MSE:HG3	1.94	0.67
1:A:388:GLN:H	1:A:388:GLN:HE21	1.43	0.67
1:E:257:ASN:HA	1:E:435:TYR:CD2	2.29	0.67
1:E:192:GLU:HA	1:E:195:ARG:HG3	1.77	0.67
1:C:257:ASN:O	1:C:435:TYR:HE2	1.76	0.66
1:D:231:THR:O	1:D:232:ASN:HB2	1.95	0.66
1:D:258:ILE:O	1:D:259:ASN:HB3	1.95	0.66
1:E:231:THR:O	1:E:232:ASN:HB2	1.94	0.66
2:H:487:GLY:HA3	2:H:489:PHE:H	1.61	0.66
1:B:132:ARG:C	1:B:134:ASP:HB2	2.20	0.66
1:B:262:ASN:OD1	1:B:263:LEU:N	2.29	0.66
1:C:62:GLY:HA2	1:C:63:GLU:HB3	1.75	0.66
1:E:105:TYR:OH	1:F:68:VAL:HB	1.95	0.66
1:A:187:PRO:C	1:A:189:GLY:H	2.04	0.66
1:D:62:GLY:HA2	1:D:63:GLU:CB	2.24	0.66
1:D:187:PRO:C	1:D:189:GLY:H	2.04	0.66
1:E:432:ILE:O	1:E:433:LYS:HB2	1.96	0.66
1:A:47:ALA:HB1	1:A:83:ILE:HG23	1.76	0.66
1:B:222:ASN:N	1:B:222:ASN:HD22	1.93	0.66
1:D:262:ASN:HB3	1:D:265:THR:HG22	1.78	0.66
1:E:83:ILE:HG22	1:E:84:GLY:N	2.10	0.66
1:A:257:ASN:O	1:A:435:TYR:CE2	2.49	0.66
1:B:231:THR:HG23	1:B:232:ASN:H	1.61	0.66
1:C:194:ASP:O	1:C:198:SER:N	2.29	0.66
1:C:222:ASN:N	1:C:222:ASN:HD22	1.93	0.66
1:B:197:THR:HB	1:B:199:GLY:O	1.95	0.65
1:B:257:ASN:O	1:B:435:TYR:CE2	2.48	0.65
1:A:114:VAL:CG1	1:D:140:LEU:HD11	2.26	0.65
1:C:388:GLN:H	1:C:388:GLN:HE21	1.44	0.65
1:D:74:LEU:HD22	1:D:83:ILE:HD11	1.78	0.65
1:E:257:ASN:O	1:E:435:TYR:CE2	2.44	0.65
2:H:491:ILE:HB	2:H:494:HIS:CD2	2.32	0.65
1:D:141:ASP:OD2	1:D:297:ARG:HD3	1.95	0.65
1:E:187:PRO:O	1:E:189:GLY:N	2.28	0.65
2:I:484:ARG:HH22	2:I:546:GLU:HG2	1.60	0.65
1:F:374:ARG:HB3	1:F:375:PRO:HA	1.77	0.65
1:A:273:TRP:C	1:A:275:LYS:H	2.04	0.65
1:D:257:ASN:C	1:D:435:TYR:CD2	2.75	0.65
1:C:432:ILE:O	1:C:433:LYS:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:ASN:C	1:E:435:TYR:CD2	2.75	0.65
2:G:475:ARG:HG2	2:G:511:ALA:CB	2.26	0.65
1:C:19:ALA:HA	1:C:96:VAL:HG21	1.79	0.64
1:E:187:PRO:C	1:E:189:GLY:H	2.05	0.64
1:F:339:VAL:HG13	1:F:384:GLY:HA3	1.79	0.64
1:A:227:VAL:O	1:A:231:THR:CG2	2.38	0.64
1:B:432:ILE:O	1:B:433:LYS:HB2	1.97	0.64
1:C:28:PRO:C	1:C:30:ALA:H	2.05	0.64
1:A:138:VAL:O	1:A:142:GLU:HG2	1.98	0.64
1:D:71:THR:HG22	1:D:89:LEU:HD12	1.79	0.64
1:D:257:ASN:O	1:D:435:TYR:HE2	1.79	0.64
1:F:262:ASN:HB3	1:F:265:THR:HG22	1.80	0.64
2:H:510:GLU:O	2:H:511:ALA:CB	2.44	0.64
1:A:66:ASP:H	1:A:69:THR:CG2	2.11	0.64
1:B:388:GLN:H	1:B:388:GLN:HE21	1.46	0.64
1:F:66:ASP:O	1:F:69:THR:HG22	1.98	0.64
2:I:538:ASP:O	2:I:539:ASP:HB2	1.98	0.64
1:D:197:THR:HB	1:D:199:GLY:O	1.97	0.63
1:D:30:ALA:O	1:D:33:PRO:HD2	1.99	0.63
2:G:486:GLY:H	2:G:488:ARG:HB2	1.64	0.63
1:A:97:PRO:HG2	1:A:98:THR:HG22	1.80	0.63
2:I:456:LEU:O	2:I:457:LEU:HB2	1.98	0.63
1:F:388:GLN:H	1:F:388:GLN:HE21	1.45	0.63
1:D:222:ASN:N	1:D:222:ASN:HD22	1.96	0.63
1:C:26:LEU:HD22	2:H:592:LYS:HE3	1.81	0.62
1:C:431:PHE:CE2	1:C:433:LYS:HG3	2.33	0.62
1:F:63:GLU:N	1:F:64:PRO:CA	2.55	0.62
1:F:262:ASN:OD1	1:F:263:LEU:N	2.31	0.62
1:E:222:ASN:N	1:E:222:ASN:HD22	1.97	0.62
2:G:491:ILE:HB	2:G:494:HIS:CD2	2.34	0.62
1:B:187:PRO:C	1:B:189:GLY:H	2.06	0.62
1:B:273:TRP:C	1:B:275:LYS:H	2.07	0.62
1:E:280:MET:O	1:E:284:SER:HB2	1.99	0.62
1:F:255:GLU:C	1:F:257:ASN:H	2.05	0.62
2:H:562:LYS:HA	2:H:565:GLU:HB3	1.81	0.62
1:A:296:ILE:O	1:A:325:ILE:HG13	1.98	0.62
1:C:66:ASP:H	1:C:69:THR:CG2	2.12	0.62
1:C:197:THR:HB	1:C:199:GLY:O	1.98	0.62
2:H:456:LEU:O	2:H:457:LEU:HB2	2.00	0.62
1:D:432:ILE:O	1:D:433:LYS:HB2	1.99	0.62
1:F:228:ALA:HB1	1:F:286:ALA:HB1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:TYR:HA	1:D:106:ALA:H	1.65	0.62
1:F:210:ALA:HB2	1:F:396:LEU:HB2	1.81	0.62
2:I:475:ARG:HG2	2:I:511:ALA:HB1	1.80	0.62
1:C:148:MET:CE	1:C:148:MET:HA	2.30	0.62
1:D:24:VAL:HG21	1:D:55:MET:HE3	1.80	0.62
1:F:231:THR:O	1:F:232:ASN:HB2	1.99	0.62
2:G:464:GLU:HG3	2:G:489:PHE:CD1	2.35	0.62
1:C:105:TYR:OH	1:D:68:VAL:HB	2.00	0.62
1:C:268:LEU:HB3	1:C:272:ASP:HB2	1.81	0.62
2:G:464:GLU:HG3	2:G:489:PHE:HD1	1.64	0.62
1:A:104:TYR:HA	1:A:106:ALA:N	2.14	0.61
1:A:257:ASN:O	1:A:435:TYR:HE2	1.82	0.61
2:I:464:GLU:HG3	2:I:489:PHE:HD1	1.65	0.61
2:I:560:MSE:O	2:I:562:LYS:N	2.32	0.61
1:A:208:VAL:HG22	1:A:394:ALA:HB3	1.81	0.61
1:F:258:ILE:O	1:F:259:ASN:CB	2.48	0.61
1:D:208:VAL:HB	1:D:360:LEU:HD23	1.81	0.61
1:E:61:ARG:CB	1:E:62:GLY:HA3	2.26	0.61
2:G:510:GLU:O	2:G:511:ALA:CB	2.49	0.61
2:I:519:ARG:H	2:I:520:ILE:HB	1.65	0.61
1:C:105:TYR:HE2	1:D:68:VAL:HG12	1.65	0.61
1:E:28:PRO:C	1:E:30:ALA:H	2.07	0.61
1:D:273:TRP:C	1:D:275:LYS:H	2.08	0.61
1:B:63:GLU:N	1:B:64:PRO:CA	2.48	0.61
1:C:132:ARG:C	1:C:134:ASP:HB2	2.25	0.61
1:E:94:ASP:HB3	2:I:591:LYS:HZ2	1.64	0.61
1:D:63:GLU:N	1:D:64:PRO:CA	2.45	0.61
1:C:231:THR:O	1:C:232:ASN:HB2	2.01	0.60
1:E:197:THR:CB	1:E:199:GLY:O	2.49	0.60
1:C:105:TYR:CE2	1:D:68:VAL:HG12	2.36	0.60
1:A:53:HIS:CE1	1:A:57:ARG:NH1	2.69	0.60
1:A:93:ALA:HB1	2:G:588:ILE:CD1	2.30	0.60
1:A:188:THR:HG22	1:A:200:PHE:CE2	2.37	0.60
1:C:431:PHE:HE2	1:C:433:LYS:HG3	1.65	0.60
2:H:475:ARG:NH1	2:H:475:ARG:HG3	2.15	0.60
1:D:339:VAL:HG13	1:D:384:GLY:HA3	1.82	0.60
1:D:391:ASP:OD1	1:D:391:ASP:N	2.33	0.60
1:D:75:ALA:HB2	1:D:80:LEU:HD12	1.82	0.60
1:B:257:ASN:C	1:B:435:TYR:CD2	2.79	0.60
1:D:132:ARG:O	1:D:133:GLU:CB	2.34	0.60
1:A:104:TYR:HA	1:A:106:ALA:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:562:LYS:HA	2:G:565:GLU:HB3	1.83	0.60
2:I:463:ALA:O	2:I:467:LEU:HB2	2.01	0.60
1:C:64:PRO:O	1:C:69:THR:HG21	2.01	0.59
2:I:562:LYS:HA	2:I:565:GLU:HB3	1.83	0.59
1:A:257:ASN:C	1:A:435:TYR:CD2	2.80	0.59
1:B:392:ILE:HA	1:B:418:LYS:O	2.01	0.59
1:E:93:ALA:HB1	2:I:588:ILE:CD1	2.29	0.59
1:B:374:ARG:HB3	1:B:375:PRO:HA	1.83	0.59
1:A:93:ALA:CB	2:G:588:ILE:HD11	2.31	0.59
1:E:47:ALA:HB1	1:E:83:ILE:HG23	1.84	0.59
1:C:296:ILE:O	1:C:325:ILE:HG13	2.02	0.59
2:G:583:ILE:O	2:G:587:MSE:HG3	2.02	0.59
1:A:262:ASN:HB3	1:A:265:THR:HG22	1.85	0.59
1:C:50:LYS:NZ	1:C:82:GLU:OE2	2.35	0.59
2:H:486:GLY:H	2:H:488:ARG:HB2	1.67	0.59
1:A:83:ILE:HG22	1:A:84:GLY:H	1.68	0.59
2:I:464:GLU:HG3	2:I:489:PHE:CD1	2.38	0.59
1:B:67:LEU:O	1:B:71:THR:HG23	2.02	0.59
2:G:475:ARG:HG2	2:G:511:ALA:HB2	1.84	0.59
2:I:510:GLU:O	2:I:511:ALA:CB	2.49	0.59
2:I:487:GLY:HA3	2:I:489:PHE:H	1.67	0.59
1:B:133:GLU:HG2	1:E:115:LEU:CD1	2.33	0.59
1:D:32:VAL:O	1:D:36:GLU:HG3	2.03	0.59
1:E:93:ALA:CB	2:I:588:ILE:HD11	2.30	0.59
1:A:105:TYR:CE2	1:B:68:VAL:HG12	2.38	0.58
1:A:199:GLY:HA3	1:A:200:PHE:O	2.03	0.58
1:A:257:ASN:HA	1:A:435:TYR:CD2	2.38	0.58
1:D:227:VAL:O	1:D:231:THR:CG2	2.44	0.58
1:E:64:PRO:O	1:E:69:THR:HG21	2.02	0.58
1:E:138:VAL:O	1:E:142:GLU:HG2	2.03	0.58
1:C:93:ALA:CB	2:H:588:ILE:HD11	2.31	0.58
2:G:471:MSE:HB2	2:G:478:ALA:HB2	1.85	0.58
1:F:255:GLU:C	1:F:257:ASN:N	2.60	0.58
2:H:485:ILE:HG22	2:H:487:GLY:HA2	1.86	0.58
1:D:132:ARG:C	1:D:134:ASP:HB2	2.28	0.58
1:B:194:ASP:O	1:B:198:SER:N	2.31	0.58
1:D:249:MET:HA	1:D:252:LEU:HB2	1.86	0.58
1:E:104:TYR:HB3	1:E:105:TYR:HB2	1.84	0.58
1:B:66:ASP:O	1:B:69:THR:HG22	2.04	0.58
1:F:187:PRO:O	1:F:189:GLY:N	2.37	0.58
2:G:465:ARG:HG3	2:G:531:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ASP:C	1:D:143:ALA:H	2.12	0.58
1:E:26:LEU:HD22	2:I:592:LYS:HE3	1.85	0.58
1:B:101:ASN:C	1:B:103:GLU:H	2.06	0.58
1:B:104:TYR:HA	1:B:105:TYR:HB2	1.86	0.58
1:C:207:ILE:HD13	1:C:386:ILE:HG21	1.85	0.58
1:F:74:LEU:HD13	1:F:83:ILE:CD1	2.34	0.58
1:C:188:THR:HG22	1:C:200:PHE:CE2	2.39	0.57
1:D:67:LEU:O	1:D:71:THR:HG23	2.04	0.57
2:G:504:PHE:O	2:G:507:GLU:HB3	2.05	0.57
1:A:202:ARG:O	1:A:203:SER:HB2	2.03	0.57
1:B:88:TYR:O	1:B:92:LEU:HG	2.04	0.57
1:C:208:VAL:HG22	1:C:394:ALA:HB3	1.87	0.57
1:F:61:ARG:CB	1:F:62:GLY:HA3	2.23	0.57
1:A:322:LEU:HB3	1:A:323:GLN:NE2	2.19	0.57
1:C:47:ALA:HB1	1:C:83:ILE:HG23	1.86	0.57
1:E:105:TYR:CE2	1:F:68:VAL:HG12	2.39	0.57
1:B:225:GLN:NE2	1:B:251:MET:HB2	2.19	0.57
1:F:391:ASP:OD1	1:F:391:ASP:N	2.38	0.57
1:B:207:ILE:HD13	1:B:386:ILE:HG21	1.87	0.57
1:F:268:LEU:HB3	1:F:272:ASP:HB2	1.85	0.57
2:I:510:GLU:O	2:I:511:ALA:HB2	2.03	0.57
1:E:257:ASN:CA	1:E:435:TYR:CD2	2.87	0.57
2:G:538:ASP:O	2:G:539:ASP:HB2	2.05	0.57
1:C:104:TYR:HA	1:C:106:ALA:N	2.20	0.57
1:E:148:MET:CE	1:E:148:MET:HA	2.34	0.57
1:B:51:ILE:HD11	1:B:83:ILE:HG21	1.86	0.56
1:A:374:ARG:HB3	1:A:375:PRO:HA	1.86	0.56
1:B:262:ASN:HB3	1:B:265:THR:HG22	1.88	0.56
1:C:138:VAL:O	1:C:142:GLU:HG2	2.05	0.56
1:D:148:MET:HA	1:D:148:MET:CE	2.35	0.56
1:F:196:MET:O	1:F:419:GLN:NE2	2.34	0.56
2:I:475:ARG:HH12	2:I:505:TYR:CB	2.19	0.56
1:A:135:GLU:O	1:A:137:ASP:N	2.33	0.56
1:C:71:THR:HG22	1:C:89:LEU:CD1	2.36	0.56
1:E:101:ASN:C	1:E:103:GLU:H	2.10	0.56
2:H:504:PHE:O	2:H:507:GLU:HB3	2.06	0.56
2:I:475:ARG:NH1	2:I:505:TYR:CB	2.67	0.56
1:A:141:ASP:C	1:A:143:ALA:H	2.14	0.56
1:B:71:THR:HG22	1:B:89:LEU:HD12	1.88	0.56
1:D:53:HIS:CE1	1:D:57:ARG:HD2	2.40	0.56
1:D:296:ILE:O	1:D:325:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:ILE:O	1:E:325:ILE:HG13	2.05	0.56
1:F:258:ILE:O	1:F:259:ASN:HB3	2.06	0.56
1:B:71:THR:HG22	1:B:89:LEU:CD1	2.36	0.56
1:D:223:ILE:HG22	1:D:316:MET:HE1	1.86	0.56
1:D:381:ARG:HD3	1:D:387:GLU:HB2	1.85	0.56
1:F:251:MET:HE1	1:F:288:ILE:HD13	1.87	0.56
1:C:62:GLY:CA	1:C:63:GLU:HB3	2.35	0.56
1:E:66:ASP:H	1:E:69:THR:CG2	2.16	0.56
1:A:302:ARG:HD2	1:B:36:GLU:OE2	2.05	0.55
1:C:262:ASN:OD1	1:C:263:LEU:N	2.39	0.55
1:F:83:ILE:HG22	1:F:84:GLY:H	1.71	0.55
1:A:28:PRO:C	1:A:30:ALA:H	2.14	0.55
2:H:475:ARG:HG2	2:H:511:ALA:CB	2.35	0.55
1:E:105:TYR:CE2	1:F:68:VAL:CG1	2.90	0.55
1:C:227:VAL:O	1:C:231:THR:CG2	2.39	0.55
1:F:79:GLN:O	1:F:83:ILE:HG13	2.07	0.55
1:A:53:HIS:CE1	1:A:57:ARG:HH11	2.25	0.55
1:A:64:PRO:O	1:A:69:THR:HG21	2.06	0.55
1:C:262:ASN:HB3	1:C:265:THR:HG22	1.89	0.55
1:E:194:ASP:O	1:E:198:SER:N	2.29	0.55
1:E:202:ARG:O	1:E:203:SER:HB2	2.06	0.55
1:F:207:ILE:HD11	1:F:361:SER:HB2	1.89	0.55
1:D:40:PRO:O	1:D:49:GLN:HG3	2.05	0.55
1:A:67:LEU:CD1	2:G:584:ALA:HB3	2.36	0.55
1:D:262:ASN:OD1	1:D:263:LEU:N	2.38	0.55
2:G:510:GLU:O	2:G:511:ALA:HB2	2.07	0.55
2:H:519:ARG:H	2:H:520:ILE:HB	1.71	0.55
1:A:207:ILE:HD13	1:A:386:ILE:HG21	1.89	0.55
1:E:53:HIS:CE1	1:E:57:ARG:HD2	2.42	0.55
2:I:583:ILE:O	2:I:587:MSE:HG3	2.06	0.55
1:C:273:TRP:C	1:C:275:LYS:H	2.14	0.55
1:D:196:MET:HE3	1:D:423:PRO:HB2	1.89	0.55
1:B:28:PRO:C	1:B:30:ALA:H	2.13	0.55
1:D:101:ASN:C	1:D:103:GLU:N	2.64	0.55
1:C:93:ALA:HB1	2:H:588:ILE:CD1	2.35	0.54
1:E:262:ASN:OD1	1:E:263:LEU:N	2.40	0.54
2:H:538:ASP:O	2:H:539:ASP:HB2	2.07	0.54
1:A:315:GLY:O	1:A:356:PRO:HD2	2.07	0.54
1:B:257:ASN:HA	1:B:435:TYR:CD2	2.41	0.54
1:C:83:ILE:HG22	1:C:84:GLY:N	2.22	0.54
1:D:200:PHE:CD1	1:D:206:ILE:HD13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLY:CA	1:B:63:GLU:CB	2.83	0.54
1:B:210:ALA:HB2	1:B:396:LEU:HB2	1.90	0.54
1:C:210:ALA:HB2	1:C:396:LEU:HB2	1.87	0.54
1:D:61:ARG:CB	1:D:62:GLY:CA	2.82	0.54
1:A:262:ASN:OD1	1:A:263:LEU:N	2.40	0.54
1:B:197:THR:CB	1:B:199:GLY:O	2.55	0.54
1:E:262:ASN:HB3	1:E:265:THR:HG22	1.88	0.54
1:E:374:ARG:HB3	1:E:375:PRO:HA	1.89	0.54
1:F:202:ARG:O	1:F:203:SER:HB2	2.08	0.54
1:C:103:GLU:N	1:C:104:TYR:CB	2.71	0.54
1:E:19:ALA:HA	1:E:96:VAL:HG21	1.90	0.54
1:E:258:ILE:O	1:E:259:ASN:CB	2.54	0.54
2:H:477:VAL:O	2:H:481:VAL:HG23	2.07	0.54
1:C:202:ARG:O	1:C:203:SER:HB2	2.07	0.54
1:C:257:ASN:HA	1:C:435:TYR:CD2	2.42	0.54
1:D:315:GLY:O	1:D:356:PRO:HD2	2.08	0.54
1:A:71:THR:HG22	1:A:89:LEU:HD12	1.90	0.54
1:B:391:ASP:OD1	1:B:391:ASP:N	2.37	0.54
1:D:194:ASP:O	1:D:198:SER:N	2.38	0.54
2:I:538:ASP:O	2:I:539:ASP:CB	2.56	0.54
1:D:392:ILE:HA	1:D:418:LYS:O	2.08	0.54
1:C:225:GLN:NE2	1:C:251:MET:HB2	2.23	0.54
1:D:64:PRO:O	1:D:69:THR:HG21	2.08	0.54
1:C:259:ASN:OD1	1:C:259:ASN:C	2.51	0.53
1:F:28:PRO:C	1:F:30:ALA:N	2.62	0.53
2:H:471:MSE:HB2	2:H:478:ALA:HB2	1.90	0.53
1:A:222:ASN:HD22	1:A:222:ASN:H	1.56	0.53
1:C:231:THR:HG23	1:C:232:ASN:N	2.13	0.53
1:C:306:ARG:NH2	1:C:352:GLU:OE1	2.41	0.53
1:D:32:VAL:HB	1:D:33:PRO:HD3	1.89	0.53
1:E:51:ILE:HD11	1:E:83:ILE:HG21	1.89	0.53
1:A:105:TYR:HE2	1:B:68:VAL:HG12	1.71	0.53
1:D:202:ARG:HB3	1:D:354:GLU:C	2.32	0.53
1:F:185:GLY:O	1:F:186:ILE:HG13	2.09	0.53
2:I:560:MSE:O	2:I:563:VAL:N	2.36	0.53
2:H:475:ARG:HG2	2:H:511:ALA:HB1	1.90	0.53
1:B:246:GLN:HE22	1:E:376:MET:CE	2.21	0.53
1:D:231:THR:HG23	1:D:232:ASN:N	2.21	0.53
1:E:40:PRO:O	1:E:49:GLN:HG3	2.08	0.53
1:E:257:ASN:CA	1:E:435:TYR:CE2	2.92	0.53
1:F:322:LEU:HD12	1:F:359:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:560:MSE:O	2:G:562:LYS:N	2.42	0.53
2:I:475:ARG:HG2	2:I:511:ALA:HB2	1.90	0.53
1:A:251:MET:HE1	1:A:288:ILE:HG21	1.90	0.53
1:B:268:LEU:HB3	1:B:272:ASP:HB2	1.91	0.53
1:C:374:ARG:HB3	1:C:375:PRO:HA	1.91	0.53
1:E:62:GLY:CA	1:E:63:GLU:HB3	2.35	0.53
1:E:210:ALA:HB2	1:E:396:LEU:HB2	1.91	0.53
1:E:251:MET:HE1	1:E:288:ILE:HG21	1.91	0.53
1:E:259:ASN:C	1:E:259:ASN:OD1	2.51	0.53
1:F:208:VAL:HG22	1:F:394:ALA:HB3	1.90	0.53
1:B:83:ILE:HG22	1:B:84:GLY:H	1.74	0.52
1:E:207:ILE:HA	1:E:359:ALA:O	2.09	0.52
1:D:257:ASN:HA	1:D:435:TYR:CD2	2.45	0.52
1:E:28:PRO:C	1:E:30:ALA:N	2.67	0.52
1:A:51:ILE:HD11	1:A:83:ILE:HG21	1.90	0.52
1:A:105:TYR:OH	1:B:68:VAL:HB	2.09	0.52
1:D:255:GLU:C	1:D:257:ASN:N	2.45	0.52
1:E:431:PHE:CE2	1:E:433:LYS:HG3	2.44	0.52
1:F:71:THR:HG22	1:F:89:LEU:CD1	2.38	0.52
2:H:560:MSE:O	2:H:562:LYS:N	2.43	0.52
1:B:53:HIS:CE1	1:B:57:ARG:HD2	2.45	0.52
1:F:221:LEU:HD21	1:F:247:LEU:HD11	1.91	0.52
1:A:79:GLN:O	1:A:83:ILE:HG13	2.09	0.52
1:E:200:PHE:CD1	1:E:206:ILE:HD13	2.44	0.52
1:F:62:GLY:CA	1:F:63:GLU:CB	2.87	0.52
1:F:235:VAL:HG12	1:F:316:MET:HB2	1.91	0.52
1:E:88:TYR:O	1:E:92:LEU:HG	2.09	0.52
1:A:19:ALA:HA	1:A:96:VAL:HG21	1.92	0.52
1:A:202:ARG:O	1:A:203:SER:CB	2.58	0.52
1:B:185:GLY:O	1:B:186:ILE:HG13	2.09	0.52
1:C:84:GLY:HA3	1:C:88:TYR:HB2	1.92	0.52
1:B:296:ILE:O	1:B:325:ILE:HG13	2.10	0.52
1:C:97:PRO:HG2	1:C:98:THR:HG22	1.92	0.52
1:D:66:ASP:N	1:D:69:THR:HG22	2.21	0.52
2:I:475:ARG:HH11	2:I:475:ARG:HG3	1.75	0.52
1:A:24:VAL:HG21	1:A:55:MET:HE3	1.91	0.52
1:D:432:ILE:HD12	1:D:437:LYS:HE3	1.92	0.52
1:A:83:ILE:CG2	1:A:84:GLY:H	2.22	0.51
1:A:322:LEU:C	1:A:324:LEU:H	2.18	0.51
1:E:25:PHE:CZ	1:E:89:LEU:HD22	2.44	0.51
1:E:231:THR:HG23	1:E:232:ASN:N	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HB	1:A:33:PRO:HD3	1.91	0.51
1:F:148:MET:HA	1:F:148:MET:HE3	1.91	0.51
1:A:339:VAL:HG13	1:A:384:GLY:HA3	1.92	0.51
1:B:105:TYR:O	1:B:109:VAL:HG23	2.09	0.51
1:A:103:GLU:N	1:A:104:TYR:CB	2.74	0.51
1:A:375:PRO:HG2	1:A:395:PHE:HB3	1.93	0.51
1:D:210:ALA:HB2	1:D:396:LEU:HB2	1.91	0.51
1:E:206:ILE:HG23	1:E:392:ILE:HG12	1.92	0.51
1:F:432:ILE:O	1:F:433:LYS:HB2	2.10	0.51
1:C:148:MET:HA	1:C:148:MET:HE2	1.93	0.51
1:C:197:THR:CB	1:C:199:GLY:O	2.58	0.51
1:C:395:PHE:HB2	1:C:415:ILE:HB	1.93	0.51
1:F:139:LEU:O	1:F:143:ALA:HB2	2.10	0.51
2:H:501:ILE:O	2:H:504:PHE:HB3	2.11	0.51
2:H:507:GLU:O	2:H:507:GLU:HG3	2.10	0.51
2:I:477:VAL:O	2:I:481:VAL:HG23	2.11	0.51
1:A:30:ALA:O	1:A:33:PRO:HD2	2.10	0.51
1:A:268:LEU:HB3	1:A:272:ASP:CB	2.38	0.51
1:C:105:TYR:CE2	1:D:68:VAL:CG1	2.94	0.51
1:D:280:MET:O	1:D:284:SER:HB2	2.11	0.51
1:A:194:ASP:O	1:A:198:SER:N	2.39	0.51
1:D:197:THR:CB	1:D:199:GLY:O	2.58	0.51
2:G:475:ARG:HH12	2:G:505:TYR:HB3	1.74	0.51
2:G:519:ARG:H	2:G:520:ILE:HB	1.75	0.51
1:C:257:ASN:CA	1:C:435:TYR:CD2	2.94	0.51
1:E:132:ARG:C	1:E:134:ASP:HB2	2.36	0.51
2:G:538:ASP:O	2:G:539:ASP:CB	2.59	0.51
1:A:104:TYR:OH	1:B:69:THR:OG1	2.05	0.51
1:B:24:VAL:HG21	1:B:55:MET:HE3	1.92	0.50
1:C:135:GLU:O	1:C:137:ASP:N	2.38	0.50
1:C:202:ARG:O	1:C:203:SER:CB	2.59	0.50
1:C:307:ARG:NH2	1:D:36:GLU:OE2	2.43	0.50
1:D:207:ILE:HD13	1:D:386:ILE:HG21	1.93	0.50
1:F:187:PRO:C	1:F:189:GLY:H	2.18	0.50
2:I:486:GLY:H	2:I:488:ARG:HB2	1.76	0.50
1:E:25:PHE:HZ	1:E:89:LEU:HD22	1.75	0.50
1:E:202:ARG:O	1:E:203:SER:CB	2.58	0.50
1:E:385:SER:OG	1:E:386:ILE:N	2.44	0.50
1:D:202:ARG:O	1:D:203:SER:CB	2.60	0.50
1:E:391:ASP:HB3	1:E:420:ARG:HD2	1.93	0.50
1:B:133:GLU:CA	1:B:134:ASP:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:THR:HB	1:F:199:GLY:O	2.10	0.50
1:A:258:ILE:O	1:A:259:ASN:CB	2.59	0.50
1:B:340:SER:CB	1:B:385:SER:HB3	2.41	0.50
1:D:249:MET:HE1	1:D:264:ARG:HE	1.75	0.50
1:F:75:ALA:HB2	1:F:80:LEU:HD12	1.93	0.50
1:D:66:ASP:O	1:D:69:THR:HG22	2.12	0.50
1:D:104:TYR:HA	1:D:106:ALA:N	2.25	0.50
1:E:202:ARG:HB3	1:E:354:GLU:C	2.36	0.50
2:H:487:GLY:CA	2:H:489:PHE:H	2.23	0.50
1:C:71:THR:HG22	1:C:89:LEU:HD12	1.92	0.50
1:C:192:GLU:HA	1:C:195:ARG:HG3	1.92	0.50
1:E:104:TYR:H	1:E:107:ARG:H	1.59	0.50
1:E:219:PHE:HB2	1:E:438:PHE:CE1	2.47	0.50
1:A:66:ASP:O	1:A:69:THR:HG22	2.12	0.50
1:C:96:VAL:HG13	1:C:97:PRO:HD2	1.94	0.50
2:G:467:LEU:O	2:G:471:MSE:HG2	2.11	0.50
2:G:485:ILE:HG22	2:G:487:GLY:HA2	1.94	0.50
2:H:470:HIS:HE1	2:H:537:ALA:O	1.95	0.50
1:B:25:PHE:HZ	1:B:89:LEU:HD22	1.77	0.49
1:B:315:GLY:O	1:B:356:PRO:HD2	2.10	0.49
1:D:139:LEU:O	1:D:143:ALA:HB2	2.12	0.49
1:A:257:ASN:CA	1:A:435:TYR:CD2	2.95	0.49
1:A:385:SER:OG	1:A:386:ILE:N	2.46	0.49
1:C:135:GLU:C	1:C:137:ASP:H	2.19	0.49
1:D:28:PRO:C	1:D:30:ALA:H	2.19	0.49
1:F:207:ILE:HD13	1:F:386:ILE:HG21	1.93	0.49
1:A:140:LEU:HD11	1:D:114:VAL:HG11	1.94	0.49
1:B:208:VAL:HB	1:B:360:LEU:HD23	1.94	0.49
1:C:101:ASN:C	1:C:103:GLU:H	2.17	0.49
1:E:103:GLU:N	1:E:104:TYR:CB	2.76	0.49
2:H:464:GLU:HG3	2:H:489:PHE:HD1	1.77	0.49
1:B:257:ASN:CA	1:B:435:TYR:CD2	2.96	0.49
1:D:25:PHE:HZ	1:D:89:LEU:HD22	1.77	0.49
1:D:259:ASN:OD1	1:D:259:ASN:C	2.56	0.49
1:D:268:LEU:HB3	1:D:272:ASP:HB2	1.93	0.49
1:F:84:GLY:HA3	1:F:88:TYR:HB2	1.95	0.49
1:F:138:VAL:O	1:F:142:GLU:HG2	2.12	0.49
1:F:200:PHE:CD1	1:F:206:ILE:HD13	2.47	0.49
2:I:471:MSE:HB2	2:I:478:ALA:HB2	1.95	0.49
1:C:322:LEU:C	1:C:324:LEU:H	2.21	0.49
1:D:71:THR:HG22	1:D:89:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:LEU:C	1:E:324:LEU:H	2.20	0.49
2:G:475:ARG:HH21	2:G:501:ILE:HG22	1.77	0.49
1:B:83:ILE:CG2	1:B:84:GLY:H	2.25	0.49
1:B:140:LEU:HD11	1:E:114:VAL:HG11	1.95	0.49
1:B:202:ARG:HB3	1:B:354:GLU:C	2.37	0.49
1:B:259:ASN:C	1:B:259:ASN:OD1	2.55	0.49
1:F:222:ASN:HD22	1:F:222:ASN:N	2.11	0.49
1:B:25:PHE:CZ	1:B:89:LEU:HD22	2.48	0.49
1:B:192:GLU:HA	1:B:195:ARG:HG3	1.94	0.49
1:D:142:GLU:HA	1:D:145:ARG:HB3	1.95	0.49
1:D:192:GLU:HA	1:D:195:ARG:HG3	1.94	0.49
1:F:53:HIS:CE1	1:F:57:ARG:NH1	2.81	0.49
1:D:104:TYR:CD2	1:D:104:TYR:O	2.66	0.49
1:D:228:ALA:HB1	1:D:286:ALA:HB1	1.95	0.49
1:E:71:THR:HG22	1:E:89:LEU:HD13	1.93	0.49
1:F:392:ILE:HA	1:F:418:LYS:O	2.12	0.49
1:A:63:GLU:N	1:A:64:PRO:CA	2.59	0.49
1:A:238:PHE:CE2	1:A:301:ILE:HG23	2.48	0.49
1:C:53:HIS:CE1	1:C:57:ARG:NH1	2.81	0.49
1:D:62:GLY:CA	1:D:63:GLU:CB	2.89	0.49
1:D:104:TYR:HD1	1:D:105:TYR:CG	2.31	0.49
1:D:227:VAL:HG21	1:D:316:MET:HE2	1.94	0.49
1:E:97:PRO:HG2	1:E:98:THR:HG22	1.95	0.49
2:I:503:ALA:O	2:I:504:PHE:C	2.56	0.49
1:A:184:THR:OG1	1:A:198:SER:O	2.29	0.49
1:C:84:GLY:HA3	1:C:88:TYR:CB	2.43	0.49
1:D:28:PRO:C	1:D:30:ALA:N	2.71	0.49
1:D:317:ILE:HB	1:D:357:VAL:HG22	1.95	0.49
2:H:464:GLU:HG3	2:H:489:PHE:CD1	2.47	0.49
1:A:53:HIS:CE1	1:A:57:ARG:HD2	2.48	0.48
1:B:28:PRO:C	1:B:30:ALA:N	2.68	0.48
1:B:228:ALA:HB1	1:B:286:ALA:HB1	1.95	0.48
1:D:262:ASN:HB3	1:D:265:THR:CG2	2.43	0.48
1:E:249:MET:HA	1:E:252:LEU:HB2	1.95	0.48
1:A:83:ILE:HG22	1:A:84:GLY:N	2.29	0.48
1:A:132:ARG:C	1:A:134:ASP:HB2	2.38	0.48
1:B:187:PRO:C	1:B:189:GLY:N	2.69	0.48
2:G:487:GLY:CA	2:G:489:PHE:H	2.24	0.48
2:H:503:ALA:O	2:H:504:PHE:C	2.56	0.48
1:A:196:MET:HE3	1:A:423:PRO:HB2	1.95	0.48
1:D:322:LEU:C	1:D:324:LEU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:ARG:NH1	1:F:135:GLU:OE1	2.46	0.48
1:F:141:ASP:C	1:F:143:ALA:H	2.21	0.48
2:G:503:ALA:O	2:G:506:GLU:N	2.46	0.48
2:H:509:HIS:O	2:H:510:GLU:C	2.57	0.48
1:A:273:TRP:C	1:A:275:LYS:N	2.70	0.48
1:B:133:GLU:N	1:B:134:ASP:CB	2.67	0.48
1:D:141:ASP:OD2	1:D:297:ARG:CD	2.59	0.48
1:D:273:TRP:C	1:D:275:LYS:N	2.72	0.48
1:E:104:TYR:OH	1:F:69:THR:OG1	1.87	0.48
1:E:273:TRP:C	1:E:275:LYS:N	2.69	0.48
1:C:226:ASN:O	1:C:230:LYS:HB2	2.14	0.48
1:D:25:PHE:CZ	1:D:89:LEU:HD22	2.49	0.48
1:A:105:TYR:CE2	1:B:68:VAL:CG1	2.96	0.48
1:B:219:PHE:CZ	1:B:223:ILE:HD11	2.48	0.48
1:B:381:ARG:HD3	1:B:387:GLU:HB2	1.96	0.48
1:F:219:PHE:CZ	1:F:223:ILE:HD11	2.48	0.48
1:A:46:ALA:O	1:A:50:LYS:HD2	2.14	0.48
1:B:83:ILE:HG22	1:B:84:GLY:N	2.28	0.48
1:E:322:LEU:HB3	1:E:323:GLN:NE2	2.28	0.48
1:C:258:ILE:N	1:C:435:TYR:CD2	2.82	0.48
1:D:222:ASN:HD22	1:D:222:ASN:H	1.60	0.48
2:G:475:ARG:HG2	2:G:511:ALA:HB1	1.94	0.48
2:H:541:SER:HB3	2:H:544:GLU:HG3	1.96	0.48
1:B:391:ASP:O	1:B:419:GLN:HA	2.14	0.48
1:C:66:ASP:O	1:C:69:THR:HG22	2.14	0.48
1:D:225:GLN:HE22	1:D:254:ALA:HB3	1.78	0.48
2:H:475:ARG:NH1	2:H:475:ARG:CG	2.77	0.48
2:I:504:PHE:O	2:I:507:GLU:HB3	2.14	0.48
1:A:28:PRO:C	1:A:30:ALA:N	2.72	0.47
1:B:251:MET:HE1	1:B:288:ILE:HG21	1.95	0.47
2:H:503:ALA:O	2:H:506:GLU:N	2.45	0.47
1:B:395:PHE:HB2	1:B:415:ILE:HB	1.95	0.47
1:C:104:TYR:HD1	1:C:105:TYR:CG	2.31	0.47
1:D:325:ILE:HG23	1:D:342:ILE:HD13	1.95	0.47
2:G:464:GLU:CG	2:G:489:PHE:HD1	2.27	0.47
2:G:487:GLY:HA3	2:G:489:PHE:N	2.27	0.47
2:I:465:ARG:HG3	2:I:531:LEU:HD21	1.95	0.47
1:A:271:GLU:O	1:A:275:LYS:HB2	2.14	0.47
1:C:280:MET:O	1:C:284:SER:HB2	2.14	0.47
1:C:392:ILE:HA	1:C:418:LYS:O	2.14	0.47
1:D:132:ARG:NH1	1:D:135:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:GLN:NE2	1:D:251:MET:HB2	2.29	0.47
1:E:216:LYS:HA	1:E:396:LEU:HD12	1.96	0.47
1:B:222:ASN:HD22	1:B:222:ASN:H	1.61	0.47
1:B:227:VAL:HG21	1:B:316:MET:HE2	1.96	0.47
1:D:235:VAL:HG12	1:D:316:MET:HB2	1.96	0.47
1:D:251:MET:HE1	1:D:288:ILE:HG21	1.96	0.47
1:E:63:GLU:N	1:E:64:PRO:CA	2.56	0.47
1:A:392:ILE:HA	1:A:418:LYS:O	2.14	0.47
1:D:257:ASN:CA	1:D:435:TYR:CD2	2.98	0.47
1:E:104:TYR:CD2	1:E:104:TYR:C	2.90	0.47
1:F:32:VAL:HB	1:F:33:PRO:HD3	1.96	0.47
1:F:101:ASN:C	1:F:103:GLU:N	2.72	0.47
2:H:538:ASP:O	2:H:539:ASP:CB	2.61	0.47
1:A:50:LYS:NZ	1:A:82:GLU:OE2	2.48	0.47
1:A:185:GLY:O	1:A:186:ILE:HG13	2.13	0.47
1:B:66:ASP:N	1:B:69:THR:HG22	2.16	0.47
1:B:104:TYR:HB3	1:B:105:TYR:HB2	1.95	0.47
1:C:391:ASP:O	1:C:419:GLN:HA	2.15	0.47
1:F:83:ILE:CG2	1:F:84:GLY:H	2.26	0.47
1:A:101:ASN:C	1:A:103:GLU:N	2.73	0.47
1:D:66:ASP:OD1	1:D:69:THR:HG22	2.15	0.47
1:D:105:TYR:O	1:D:109:VAL:HG23	2.15	0.47
1:D:184:THR:OG1	1:D:198:SER:O	2.30	0.47
2:I:503:ALA:O	2:I:506:GLU:N	2.46	0.47
1:A:104:TYR:HD1	1:A:105:TYR:CG	2.33	0.47
1:A:231:THR:HG23	1:A:232:ASN:N	2.25	0.47
1:D:323:GLN:HE21	1:D:361:SER:HA	1.79	0.47
2:G:507:GLU:O	2:G:507:GLU:HG3	2.15	0.47
2:H:463:ALA:O	2:H:467:LEU:HB2	2.14	0.47
1:C:258:ILE:O	1:C:259:ASN:CB	2.61	0.47
1:D:298:VAL:HG11	1:D:345:SER:HB3	1.96	0.47
1:F:202:ARG:O	1:F:203:SER:CB	2.63	0.47
2:I:513:PRO:O	2:I:517:ILE:HG12	2.15	0.47
1:A:391:ASP:OD1	1:A:391:ASP:N	2.43	0.47
1:B:223:ILE:O	1:B:227:VAL:HG23	2.15	0.47
1:C:216:LYS:HB2	1:C:360:LEU:HD22	1.97	0.47
1:D:207:ILE:CD1	1:D:386:ILE:HG21	2.45	0.47
1:E:83:ILE:CG2	1:E:84:GLY:H	2.09	0.47
1:E:104:TYR:HD1	1:E:105:TYR:CG	2.32	0.47
1:E:208:VAL:HG22	1:E:394:ALA:HB3	1.96	0.47
1:C:66:ASP:OD1	1:C:66:ASP:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:MET:HE1	1:E:288:ILE:HD13	1.96	0.46
1:B:196:MET:O	1:B:419:GLN:NE2	2.40	0.46
1:B:322:LEU:C	1:B:324:LEU:H	2.22	0.46
1:F:208:VAL:HA	1:F:394:ALA:O	2.15	0.46
1:D:374:ARG:HB3	1:D:375:PRO:HA	1.96	0.46
1:B:258:ILE:O	1:B:259:ASN:CB	2.62	0.46
1:C:86:VAL:HG22	2:H:572:GLU:HG3	1.98	0.46
2:G:475:ARG:NH1	2:G:475:ARG:HG3	2.20	0.46
1:C:104:TYR:N	1:C:107:ARG:H	2.09	0.46
1:D:187:PRO:C	1:D:189:GLY:N	2.69	0.46
1:D:202:ARG:O	1:D:203:SER:HB2	2.15	0.46
1:D:256:GLY:O	1:D:257:ASN:C	2.57	0.46
2:I:509:HIS:O	2:I:510:GLU:C	2.58	0.46
1:A:132:ARG:NH1	1:A:135:GLU:OE1	2.48	0.46
1:A:141:ASP:C	1:A:143:ALA:N	2.73	0.46
1:A:259:ASN:OD1	1:A:259:ASN:C	2.58	0.46
1:B:235:VAL:HG12	1:B:316:MET:HB2	1.98	0.46
1:D:141:ASP:C	1:D:143:ALA:N	2.74	0.46
1:E:62:GLY:HA2	1:E:63:GLU:CB	2.33	0.46
1:F:251:MET:CE	1:F:288:ILE:HD13	2.45	0.46
1:F:257:ASN:C	1:F:435:TYR:CE2	2.93	0.46
1:F:315:GLY:O	1:F:356:PRO:HD2	2.16	0.46
1:C:25:PHE:CZ	1:C:89:LEU:HD22	2.51	0.46
1:C:104:TYR:HA	1:C:106:ALA:H	1.79	0.46
1:E:339:VAL:HG13	1:E:384:GLY:HA3	1.98	0.46
1:F:188:THR:HG22	1:F:200:PHE:CE2	2.51	0.46
2:G:503:ALA:O	2:G:504:PHE:C	2.57	0.46
2:G:550:ARG:CB	2:G:550:ARG:HH11	2.28	0.46
1:B:66:ASP:O	1:B:67:LEU:C	2.59	0.46
1:C:28:PRO:C	1:C:30:ALA:N	2.68	0.46
1:F:240:LEU:HD22	1:F:295:SER:HA	1.97	0.46
2:H:467:LEU:HD12	2:H:467:LEU:HA	1.85	0.46
1:A:280:MET:O	1:A:284:SER:HB2	2.15	0.46
1:A:88:TYR:O	1:A:92:LEU:HG	2.16	0.45
1:B:196:MET:HE3	1:B:423:PRO:HB2	1.97	0.45
1:B:222:ASN:ND2	1:B:222:ASN:N	2.63	0.45
1:C:62:GLY:CA	1:C:63:GLU:CB	2.93	0.45
1:C:101:ASN:HB2	1:C:105:TYR:CD1	2.51	0.45
1:D:128:ASP:HB3	1:D:139:LEU:HD21	1.96	0.45
1:D:200:PHE:CD1	1:D:200:PHE:N	2.83	0.45
1:E:187:PRO:C	1:E:189:GLY:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:THR:O	1:E:194:ASP:HB2	2.16	0.45
1:F:64:PRO:HB2	1:F:65:VAL:H	1.64	0.45
2:H:471:MSE:O	2:H:475:ARG:HD2	2.16	0.45
2:I:491:ILE:HB	2:I:494:HIS:CD2	2.51	0.45
2:I:519:ARG:O	2:I:519:ARG:HD3	2.16	0.45
2:I:541:SER:HB3	2:I:544:GLU:HG3	1.98	0.45
1:B:104:TYR:HD1	1:B:105:TYR:CG	2.34	0.45
1:C:351:ARG:HH11	1:C:351:ARG:HB2	1.80	0.45
1:D:322:LEU:HB3	1:D:323:GLN:NE2	2.31	0.45
2:G:565:GLU:O	2:G:569:THR:HG22	2.15	0.45
2:I:487:GLY:HA2	2:I:488:ARG:HB2	1.97	0.45
1:A:61:ARG:CB	1:A:62:GLY:CA	2.90	0.45
1:D:135:GLU:C	1:D:137:ASP:N	2.74	0.45
1:F:322:LEU:C	1:F:324:LEU:H	2.24	0.45
2:G:519:ARG:HD3	2:G:519:ARG:O	2.17	0.45
1:B:249:MET:HA	1:B:252:LEU:HB2	1.98	0.45
1:B:280:MET:O	1:B:284:SER:HB2	2.17	0.45
1:D:185:GLY:O	1:D:186:ILE:HG13	2.17	0.45
1:D:246:GLN:HG2	1:D:246:GLN:O	2.17	0.45
1:E:84:GLY:HA3	1:E:88:TYR:CB	2.46	0.45
1:F:298:VAL:HG11	1:F:345:SER:HB3	1.98	0.45
1:A:67:LEU:HD12	2:G:584:ALA:HB3	1.98	0.45
1:C:219:PHE:CZ	1:C:223:ILE:HD11	2.51	0.45
1:D:322:LEU:C	1:D:324:LEU:N	2.73	0.45
1:E:322:LEU:C	1:E:324:LEU:N	2.74	0.45
1:F:104:TYR:CD1	1:F:104:TYR:C	2.91	0.45
1:A:104:TYR:CD2	1:A:104:TYR:O	2.69	0.45
1:B:200:PHE:CD1	1:B:206:ILE:HD13	2.52	0.45
1:C:187:PRO:C	1:C:189:GLY:N	2.62	0.45
1:E:48:HIS:NE2	1:E:88:TYR:OH	2.37	0.45
1:F:51:ILE:HD11	1:F:83:ILE:HG21	1.99	0.45
1:F:233:GLU:CG	1:F:315:GLY:HA3	2.43	0.45
2:G:475:ARG:HH11	2:G:475:ARG:CG	2.23	0.45
2:H:487:GLY:HA3	2:H:489:PHE:N	2.27	0.45
1:E:208:VAL:HB	1:E:360:LEU:HD23	1.99	0.45
1:E:273:TRP:O	1:E:275:LYS:N	2.47	0.45
1:A:256:GLY:O	1:A:257:ASN:C	2.60	0.45
1:D:104:TYR:CD1	1:D:104:TYR:C	2.81	0.45
2:I:470:HIS:HE1	2:I:537:ALA:O	2.00	0.45
1:B:202:ARG:O	1:B:203:SER:CB	2.64	0.45
1:B:439:VAL:HG12	1:B:440:ASN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LEU:HD13	1:D:83:ILE:CD1	2.47	0.45
1:E:251:MET:CE	1:E:288:ILE:HD13	2.47	0.45
1:E:298:VAL:HG11	1:E:345:SER:HB3	1.99	0.45
1:F:439:VAL:HG12	1:F:440:ASN:H	1.82	0.45
1:A:200:PHE:CD1	1:A:200:PHE:N	2.85	0.45
1:C:385:SER:OG	1:C:386:ILE:N	2.49	0.45
1:F:296:ILE:O	1:F:325:ILE:HG13	2.17	0.45
1:B:101:ASN:C	1:B:103:GLU:N	2.67	0.44
1:C:133:GLU:CA	1:C:134:ASP:HB2	2.46	0.44
1:C:200:PHE:CD1	1:C:206:ILE:HD13	2.52	0.44
1:C:222:ASN:N	1:C:222:ASN:ND2	2.62	0.44
1:C:322:LEU:HB3	1:C:323:GLN:NE2	2.31	0.44
2:I:473:ARG:HD2	2:I:536:ILE:HD11	1.99	0.44
1:C:231:THR:CG2	1:C:232:ASN:H	2.15	0.44
1:C:316:MET:HG2	1:C:356:PRO:HG2	1.99	0.44
1:A:298:VAL:HG11	1:A:345:SER:HB3	2.00	0.44
1:D:196:MET:O	1:D:419:GLN:NE2	2.43	0.44
1:E:142:GLU:HA	1:E:145:ARG:HB3	1.99	0.44
1:E:219:PHE:CZ	1:E:223:ILE:HD11	2.52	0.44
1:F:104:TYR:H	1:F:107:ARG:HB2	1.82	0.44
1:A:257:ASN:CA	1:A:435:TYR:CE2	3.00	0.44
1:C:105:TYR:O	1:C:106:ALA:C	2.60	0.44
1:D:104:TYR:H	1:D:107:ARG:H	1.65	0.44
1:E:104:TYR:HA	1:E:106:ALA:N	2.33	0.44
1:F:187:PRO:C	1:F:189:GLY:N	2.75	0.44
1:F:197:THR:CB	1:F:199:GLY:O	2.65	0.44
1:C:104:TYR:HB3	1:C:105:TYR:HB2	2.00	0.44
1:C:391:ASP:OD1	1:C:391:ASP:N	2.46	0.44
1:E:77:SER:C	1:E:78:GLU:HG2	2.42	0.44
1:E:374:ARG:HD2	1:E:376:MET:HE3	1.99	0.44
1:F:83:ILE:HG22	1:F:84:GLY:N	2.32	0.44
2:H:496:ALA:O	2:H:500:TYR:HD2	2.00	0.44
1:A:104:TYR:OH	1:B:63:GLU:HG3	2.17	0.44
1:C:88:TYR:O	1:C:92:LEU:HG	2.18	0.44
1:D:133:GLU:N	1:D:134:ASP:CB	2.74	0.44
1:E:16:ALA:HA	1:F:68:VAL:HG11	2.00	0.44
2:G:582:ARG:HE	2:G:582:ARG:HB3	1.56	0.44
1:A:207:ILE:HA	1:A:359:ALA:O	2.17	0.44
1:C:48:HIS:NE2	1:C:88:TYR:OH	2.42	0.44
1:C:83:ILE:CG2	1:C:84:GLY:H	2.17	0.44
1:C:303:ALA:HB1	1:D:36:GLU:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:GLN:N	1:C:323:GLN:CD	2.76	0.44
1:C:207:ILE:HA	1:C:359:ALA:O	2.17	0.44
1:E:66:ASP:O	1:E:69:THR:HG22	2.18	0.44
1:E:98:THR:HG23	1:E:101:ASN:HD21	1.83	0.44
1:E:133:GLU:CA	1:E:134:ASP:HB2	2.48	0.44
1:F:273:TRP:C	1:F:275:LYS:H	2.26	0.44
1:C:40:PRO:O	1:C:49:GLN:HG3	2.17	0.44
1:E:84:GLY:HA3	1:E:88:TYR:HB3	2.00	0.44
1:E:322:LEU:O	1:E:324:LEU:N	2.51	0.44
1:A:102:VAL:C	1:A:104:TYR:HB3	2.43	0.43
1:A:322:LEU:C	1:A:324:LEU:N	2.74	0.43
1:A:396:LEU:CD2	1:A:414:ILE:HG12	2.48	0.43
1:B:225:GLN:HE22	1:B:254:ALA:HB3	1.82	0.43
1:E:200:PHE:CD1	1:E:200:PHE:N	2.85	0.43
1:F:46:ALA:O	1:F:47:ALA:C	2.61	0.43
1:C:104:TYR:OH	1:D:63:GLU:HG3	2.18	0.43
1:C:340:SER:HB3	1:C:385:SER:HB3	2.00	0.43
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.83	0.43
1:E:422:GLY:HA3	1:E:423:PRO:HD3	1.82	0.43
2:I:565:GLU:O	2:I:569:THR:HG22	2.18	0.43
1:A:101:ASN:HB2	1:A:105:TYR:CD1	2.53	0.43
1:B:292:ASP:O	1:B:293:THR:C	2.60	0.43
1:C:94:ASP:HB3	2:H:591:LYS:HZ2	1.69	0.43
1:E:226:ASN:O	1:E:230:LYS:HB2	2.19	0.43
1:F:251:MET:HE1	1:F:288:ILE:HG21	1.99	0.43
1:F:351:ARG:HH11	1:F:351:ARG:HB2	1.82	0.43
1:F:422:GLY:HA3	1:F:423:PRO:HD3	1.83	0.43
1:A:104:TYR:N	1:A:107:ARG:H	2.12	0.43
1:B:46:ALA:O	1:B:47:ALA:C	2.61	0.43
1:B:53:HIS:CE1	1:B:57:ARG:NH1	2.86	0.43
1:B:61:ARG:HB2	1:B:62:GLY:CA	2.44	0.43
1:B:216:LYS:HA	1:B:396:LEU:HD12	2.00	0.43
1:B:256:GLY:O	1:B:257:ASN:C	2.61	0.43
1:C:381:ARG:HD3	1:C:387:GLU:HB2	2.00	0.43
1:D:47:ALA:HB1	1:D:83:ILE:HG23	2.00	0.43
1:E:62:GLY:CA	1:E:63:GLU:CB	2.95	0.43
2:G:465:ARG:CG	2:G:531:LEU:HD21	2.46	0.43
1:C:61:ARG:CB	1:C:62:GLY:CA	2.93	0.43
1:C:135:GLU:C	1:C:137:ASP:N	2.77	0.43
1:C:323:GLN:HE21	1:C:361:SER:HA	1.83	0.43
1:E:101:ASN:HB2	1:E:105:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:GLN:HE21	1:F:361:SER:HA	1.83	0.43
1:A:124:SER:O	1:A:128:ASP:HB2	2.19	0.43
1:A:384:GLY:O	1:A:385:SER:C	2.61	0.43
1:B:138:VAL:O	1:B:142:GLU:HG2	2.19	0.43
1:B:202:ARG:O	1:B:203:SER:HB2	2.19	0.43
1:C:101:ASN:C	1:C:103:GLU:N	2.76	0.43
1:D:84:GLY:HA3	1:D:88:TYR:CB	2.49	0.43
1:E:101:ASN:C	1:E:103:GLU:N	2.70	0.43
1:F:249:MET:HE3	1:F:249:MET:HB2	1.94	0.43
1:A:101:ASN:HB3	1:A:104:TYR:CD1	2.53	0.43
1:A:187:PRO:C	1:A:189:GLY:N	2.69	0.43
1:A:316:MET:HG2	1:A:356:PRO:HG2	2.01	0.43
1:B:22:GLY:HA3	1:B:96:VAL:HG21	2.00	0.43
1:D:102:VAL:O	1:D:104:TYR:HA	2.19	0.43
1:D:124:SER:O	1:D:128:ASP:HB2	2.18	0.43
2:G:501:ILE:O	2:G:504:PHE:HB3	2.18	0.43
2:G:558:TRP:C	2:G:560:MSE:N	2.75	0.43
1:A:67:LEU:HD21	1:A:89:LEU:HB3	2.00	0.43
1:C:251:MET:HE1	1:C:288:ILE:HG21	2.00	0.43
1:D:133:GLU:CA	1:D:134:ASP:HB2	2.48	0.43
1:B:273:TRP:C	1:B:275:LYS:N	2.72	0.43
1:D:79:GLN:O	1:D:83:ILE:HG13	2.18	0.43
1:D:255:GLU:HB3	1:D:256:GLY:H	1.61	0.43
1:E:148:MET:HA	1:E:148:MET:HE2	2.00	0.43
2:G:484:ARG:HH22	2:G:546:GLU:HG2	1.84	0.43
1:D:439:VAL:HG12	1:D:440:ASN:H	1.84	0.43
1:E:24:VAL:C	1:E:26:LEU:H	2.27	0.43
2:I:461:GLN:HG3	2:I:491:ILE:HD11	2.00	0.43
1:A:376:MET:CE	1:D:246:GLN:HE22	2.32	0.42
1:B:61:ARG:CB	1:B:62:GLY:HA3	2.34	0.42
1:E:101:ASN:HB3	1:E:104:TYR:CD1	2.53	0.42
1:E:247:LEU:C	1:E:247:LEU:HD23	2.44	0.42
1:F:24:VAL:HG21	1:F:55:MET:HE3	2.00	0.42
1:A:210:ALA:CB	1:A:396:LEU:HB2	2.48	0.42
1:B:40:PRO:O	1:B:49:GLN:HG3	2.19	0.42
1:C:340:SER:CB	1:C:385:SER:HB3	2.49	0.42
1:E:391:ASP:O	1:E:419:GLN:HA	2.19	0.42
2:H:546:GLU:O	2:H:550:ARG:HB2	2.19	0.42
1:B:298:VAL:HG11	1:B:345:SER:HB3	2.00	0.42
1:C:101:ASN:HB2	1:C:102:VAL:H	1.69	0.42
1:D:207:ILE:HG23	1:D:393:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:565:GLU:O	2:H:569:THR:HG22	2.19	0.42
1:A:40:PRO:O	1:A:49:GLN:HG3	2.19	0.42
1:A:140:LEU:HD11	1:D:114:VAL:CG1	2.50	0.42
1:B:207:ILE:HG23	1:B:393:VAL:HG13	2.01	0.42
1:C:98:THR:HG23	1:C:101:ASN:HD21	1.85	0.42
1:C:306:ARG:NH2	1:D:32:VAL:CG2	2.79	0.42
1:F:96:VAL:HA	1:F:97:PRO:HD3	1.92	0.42
2:G:487:GLY:HA2	2:G:488:ARG:HB2	2.01	0.42
1:A:322:LEU:O	1:A:324:LEU:N	2.52	0.42
1:B:141:ASP:C	1:B:143:ALA:H	2.28	0.42
1:C:339:VAL:HG13	1:C:384:GLY:HA3	2.00	0.42
1:D:186:ILE:HA	1:D:187:PRO:HD3	1.92	0.42
1:D:258:ILE:N	1:D:435:TYR:CD2	2.87	0.42
1:E:104:TYR:CD2	1:E:104:TYR:O	2.72	0.42
2:G:486:GLY:N	2:G:488:ARG:HB2	2.33	0.42
1:C:141:ASP:C	1:C:143:ALA:H	2.28	0.42
1:D:83:ILE:CG2	1:D:84:GLY:H	2.30	0.42
1:D:395:PHE:HB2	1:D:415:ILE:HB	2.01	0.42
1:E:268:LEU:HB3	1:E:272:ASP:CB	2.46	0.42
2:G:487:GLY:HA3	2:G:489:PHE:HD2	1.85	0.42
1:B:135:GLU:C	1:B:137:ASP:N	2.77	0.42
1:C:249:MET:HA	1:C:252:LEU:HB2	2.01	0.42
1:D:41:GLU:OE1	1:D:41:GLU:N	2.51	0.42
1:D:84:GLY:HA3	1:D:88:TYR:HB2	2.02	0.42
1:E:26:LEU:HD23	1:E:26:LEU:HA	1.76	0.42
1:E:141:ASP:C	1:E:143:ALA:H	2.28	0.42
1:F:84:GLY:HA3	1:F:88:TYR:CB	2.49	0.42
2:H:468:LEU:HD23	2:H:497:LEU:HD13	2.01	0.42
2:H:486:GLY:N	2:H:488:ARG:HB2	2.33	0.42
2:H:516:LEU:HD23	2:H:516:LEU:HA	1.93	0.42
1:A:225:GLN:HE22	1:A:254:ALA:HB3	1.85	0.42
1:B:185:GLY:C	1:B:186:ILE:HG13	2.44	0.42
1:C:25:PHE:HZ	1:C:89:LEU:HD22	1.84	0.42
1:C:258:ILE:N	1:C:435:TYR:CE2	2.85	0.42
1:E:105:TYR:CZ	1:F:68:VAL:HB	2.55	0.42
1:B:351:ARG:HB2	1:B:351:ARG:HH11	1.85	0.42
1:C:273:TRP:C	1:C:275:LYS:N	2.78	0.42
1:C:314:LEU:HD13	1:C:355:VAL:HG21	2.02	0.42
1:C:391:ASP:HB3	1:C:420:ARG:NH1	2.34	0.42
2:H:582:ARG:HE	2:H:582:ARG:HB3	1.45	0.42
1:A:62:GLY:CA	1:A:63:GLU:CB	2.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ALA:C	1:B:33:PRO:HD2	2.45	0.42
1:B:142:GLU:HA	1:B:145:ARG:HB3	2.01	0.42
1:B:292:ASP:OD1	1:B:292:ASP:N	2.50	0.42
1:B:322:LEU:C	1:B:324:LEU:N	2.77	0.42
1:C:91:GLU:O	1:C:95:ALA:HB2	2.20	0.42
1:C:124:SER:O	1:C:128:ASP:HB2	2.19	0.42
1:D:238:PHE:O	1:D:320:ASP:N	2.46	0.42
1:E:196:MET:HE3	1:E:423:PRO:HB2	2.01	0.42
1:F:105:TYR:H	1:F:108:ILE:HD12	1.85	0.42
1:F:320:ASP:HA	1:F:360:LEU:HD12	2.01	0.42
2:G:467:LEU:HD12	2:G:467:LEU:HA	1.91	0.42
2:I:487:GLY:HA3	2:I:489:PHE:N	2.33	0.42
1:B:84:GLY:HA3	1:B:88:TYR:CB	2.50	0.41
1:B:375:PRO:HG2	1:B:395:PHE:HB3	2.01	0.41
1:D:22:GLY:HA3	1:D:96:VAL:HG21	2.02	0.41
1:F:61:ARG:HB2	1:F:62:GLY:CA	2.39	0.41
2:H:457:LEU:HA	2:H:458:PRO:HD3	1.83	0.41
2:I:560:MSE:C	2:I:562:LYS:N	2.75	0.41
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.93	0.41
1:D:375:PRO:HG2	1:D:395:PHE:HB3	2.02	0.41
1:E:30:ALA:O	1:E:33:PRO:HD2	2.20	0.41
1:E:222:ASN:HD22	1:E:222:ASN:H	1.67	0.41
1:E:293:THR:HA	1:E:294:PRO:HD2	1.76	0.41
1:F:74:LEU:HD13	1:F:83:ILE:HD11	2.02	0.41
1:F:104:TYR:HD1	1:F:105:TYR:CG	2.37	0.41
2:G:505:TYR:O	2:G:508:GLY:N	2.52	0.41
1:C:322:LEU:C	1:C:324:LEU:N	2.79	0.41
1:D:216:LYS:HA	1:D:396:LEU:HD12	2.01	0.41
1:E:323:GLN:CD	1:E:323:GLN:H	2.27	0.41
2:G:500:TYR:CZ	2:G:521:PRO:HD3	2.55	0.41
2:I:525:GLN:N	2:I:526:PRO:HD2	2.34	0.41
2:I:560:MSE:C	2:I:562:LYS:H	2.28	0.41
2:I:564:LYS:HE3	2:I:587:MSE:HG2	2.01	0.41
1:C:184:THR:OG1	1:C:198:SER:O	2.33	0.41
1:C:344:ARG:HH11	1:D:61:ARG:CG	2.33	0.41
1:D:104:TYR:CD1	1:D:105:TYR:N	2.88	0.41
2:G:557:LYS:O	2:G:560:MSE:HB3	2.19	0.41
1:B:64:PRO:HB2	1:B:65:VAL:H	1.63	0.41
1:B:200:PHE:CD1	1:B:200:PHE:N	2.87	0.41
2:I:496:ALA:O	2:I:500:TYR:HD2	2.03	0.41
1:B:64:PRO:O	1:B:69:THR:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLN:HE22	1:E:376:MET:HE1	1.84	0.41
1:D:96:VAL:HA	1:D:97:PRO:HD3	1.90	0.41
1:D:271:GLU:O	1:D:275:LYS:HB2	2.21	0.41
1:E:186:ILE:HA	1:E:187:PRO:HD3	1.89	0.41
1:E:375:PRO:HG2	1:E:395:PHE:HB3	2.03	0.41
2:G:509:HIS:O	2:G:510:GLU:C	2.63	0.41
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.93	0.41
1:D:239:SER:O	1:D:240:LEU:C	2.63	0.41
1:E:104:TYR:HA	1:E:106:ALA:H	1.85	0.41
2:I:554:ASN:HB2	2:I:557:LYS:HD2	2.02	0.41
1:B:422:GLY:HA3	1:B:423:PRO:HD3	1.84	0.41
1:C:46:ALA:O	1:C:47:ALA:C	2.64	0.41
1:C:190:PHE:O	1:C:191:THR:C	2.64	0.41
1:E:103:GLU:N	1:E:104:TYR:HB2	2.36	0.41
1:E:216:LYS:HA	1:E:396:LEU:CD1	2.51	0.41
1:F:225:GLN:NE2	1:F:251:MET:HB2	2.36	0.41
1:A:103:GLU:N	1:A:104:TYR:HB2	2.36	0.41
1:A:188:THR:CG2	1:A:200:PHE:CE2	3.04	0.41
1:A:317:ILE:HB	1:A:357:VAL:HG22	2.02	0.41
1:B:208:VAL:HG22	1:B:394:ALA:HB3	2.02	0.41
1:B:323:GLN:HE21	1:B:361:SER:HA	1.85	0.41
1:C:256:GLY:O	1:C:257:ASN:C	2.64	0.41
1:D:48:HIS:HE2	1:D:88:TYR:HH	1.69	0.41
1:D:257:ASN:CA	1:D:435:TYR:CE2	3.04	0.41
1:D:259:ASN:OD1	1:D:262:ASN:CG	2.64	0.41
1:D:351:ARG:HB2	1:D:351:ARG:HH11	1.86	0.41
1:E:222:ASN:ND2	1:E:222:ASN:N	2.66	0.41
1:E:384:GLY:O	1:E:385:SER:C	2.64	0.41
1:F:101:ASN:C	1:F:103:GLU:H	2.13	0.41
2:G:475:ARG:NH1	2:G:475:ARG:CG	2.83	0.41
1:A:273:TRP:O	1:A:275:LYS:N	2.53	0.41
1:B:188:THR:HG22	1:B:200:PHE:CE2	2.56	0.41
1:B:340:SER:HB3	1:B:385:SER:HB3	2.03	0.41
1:C:94:ASP:CB	2:H:591:LYS:NZ	2.61	0.41
1:E:104:TYR:OH	1:F:63:GLU:HG3	2.21	0.41
1:E:124:SER:O	1:E:128:ASP:HB2	2.20	0.41
1:E:325:ILE:HG23	1:E:342:ILE:HD13	2.03	0.41
1:F:95:ALA:HA	2:I:457:LEU:O	2.20	0.41
1:F:255:GLU:CG	1:F:256:GLY:H	2.33	0.41
2:I:484:ARG:NH2	2:I:546:GLU:HG2	2.32	0.41
1:B:124:SER:O	1:B:128:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:MET:HA	1:D:148:MET:HE3	2.03	0.40
1:E:24:VAL:C	1:E:26:LEU:N	2.78	0.40
1:E:188:THR:HG22	1:E:200:PHE:CE2	2.57	0.40
1:E:258:ILE:N	1:E:435:TYR:CE2	2.85	0.40
1:E:391:ASP:HB3	1:E:420:ARG:NH1	2.36	0.40
1:F:66:ASP:O	1:F:67:LEU:C	2.63	0.40
1:F:432:ILE:HG22	1:F:435:TYR:H	1.85	0.40
2:I:464:GLU:CG	2:I:489:PHE:HD1	2.33	0.40
1:A:39:ILE:HB	1:A:40:PRO:HD2	2.03	0.40
1:A:105:TYR:OH	1:B:66:ASP:OD1	2.37	0.40
1:A:323:GLN:CD	1:A:323:GLN:H	2.28	0.40
1:C:16:ALA:HA	1:D:68:VAL:HG11	2.03	0.40
2:I:485:ILE:HG22	2:I:487:GLY:HA2	2.04	0.40
1:A:396:LEU:HD23	1:A:414:ILE:HG12	2.03	0.40
1:C:148:MET:HA	1:C:148:MET:HE3	2.03	0.40
1:D:422:GLY:HA3	1:D:423:PRO:HD3	1.80	0.40
1:A:323:GLN:CD	1:A:323:GLN:N	2.78	0.40
1:B:67:LEU:HD23	1:B:67:LEU:HA	1.94	0.40
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.88	0.40
1:D:439:VAL:HG12	1:D:440:ASN:N	2.36	0.40
2:H:558:TRP:C	2:H:560:MSE:N	2.80	0.40
1:B:46:ALA:HB1	1:B:50:LYS:HE3	2.03	0.40
1:D:202:ARG:HB3	1:D:354:GLU:O	2.21	0.40
1:D:381:ARG:HA	1:D:381:ARG:HD2	1.91	0.40
1:E:207:ILE:HG22	1:E:390:ALA:HB1	2.04	0.40
2:H:475:ARG:NH1	2:H:504:PHE:HD2	2.20	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	348/454 (77%)	284 (82%)	41 (12%)	23 (7%)	1	15
1	B	348/454 (77%)	285 (82%)	40 (12%)	23 (7%)	1	15
1	C	348/454 (77%)	283 (81%)	40 (12%)	25 (7%)	1	13
1	D	348/454 (77%)	285 (82%)	42 (12%)	21 (6%)	1	16
1	E	348/454 (77%)	283 (81%)	42 (12%)	23 (7%)	1	15
1	F	348/454 (77%)	289 (83%)	38 (11%)	21 (6%)	1	16
2	G	136/143 (95%)	113 (83%)	13 (10%)	10 (7%)	1	13
2	H	136/143 (95%)	109 (80%)	17 (12%)	10 (7%)	1	13
2	I	136/143 (95%)	111 (82%)	14 (10%)	11 (8%)	1	11
All	All	2496/3153 (79%)	2042 (82%)	287 (12%)	167 (7%)	1	15

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	188	THR
1	A	200	PHE
1	A	203	SER
1	A	232	ASN
1	A	256	GLY
1	A	259	ASN
1	A	385	SER
1	B	63	GLU
1	B	102	VAL
1	B	104	TYR
1	B	188	THR
1	B	200	PHE
1	B	203	SER
1	B	232	ASN
1	B	256	GLY
1	B	259	ASN
1	B	385	SER
1	C	63	GLU
1	C	104	TYR
1	C	188	THR
1	C	200	PHE
1	C	203	SER
1	C	232	ASN
1	C	256	GLY
1	C	259	ASN

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Mol	Chain	Res	Type
1	C	385	SER
1	D	102	VAL
1	D	136	ILE
1	D	188	THR
1	D	200	PHE
1	D	203	SER
1	D	232	ASN
1	D	256	GLY
1	D	385	SER
1	E	63	GLU
1	E	104	TYR
1	E	188	THR
1	E	200	PHE
1	E	203	SER
1	E	232	ASN
1	E	256	GLY
1	E	259	ASN
1	E	385	SER
1	F	63	GLU
1	F	102	VAL
1	F	104	TYR
1	F	188	THR
1	F	203	SER
1	F	232	ASN
1	F	256	GLY
1	F	259	ASN
1	F	385	SER
2	G	504	PHE
2	G	510	GLU
2	G	511	ALA
2	G	534	LEU
2	G	535	LEU
2	G	539	ASP
2	H	504	PHE
2	H	510	GLU
2	H	511	ALA
2	H	535	LEU
2	H	539	ASP
2	I	504	PHE
2	I	510	GLU
2	I	511	ALA
2	I	534	LEU

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Mol	Chain	Res	Type
2	I	539	ASP
1	A	83	ILE
1	A	102	VAL
1	A	104	TYR
1	A	133	GLU
1	A	433	LYS
1	B	83	ILE
1	B	133	GLU
1	B	136	ILE
1	B	433	LYS
1	C	83	ILE
1	C	102	VAL
1	C	133	GLU
1	C	384	GLY
1	D	63	GLU
1	D	83	ILE
1	D	133	GLU
1	D	184	THR
1	D	259	ASN
1	D	433	LYS
1	E	83	ILE
1	E	102	VAL
1	E	133	GLU
1	E	433	LYS
1	F	83	ILE
1	F	133	GLU
1	F	136	ILE
2	G	503	ALA
2	H	503	ALA
2	H	534	LEU
2	I	561	LEU
1	A	294	PRO
1	B	184	THR
1	C	134	ASP
1	D	104	TYR
1	D	105	TYR
1	D	294	PRO
1	D	321	TYR
1	E	184	THR
1	E	294	PRO
1	F	294	PRO
1	F	440	ASN

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Mol	Chain	Res	Type
2	I	503	ALA
2	I	535	LEU
1	A	105	TYR
1	A	384	GLY
1	B	64	PRO
1	B	105	TYR
1	B	294	PRO
1	B	384	GLY
1	C	240	LEU
1	C	294	PRO
1	C	321	TYR
1	C	433	LYS
1	D	384	GLY
1	E	105	TYR
1	E	134	ASP
1	E	384	GLY
1	F	64	PRO
1	F	105	TYR
1	F	200	PHE
1	F	321	TYR
2	G	457	LEU
2	G	561	LEU
2	H	561	LEU
1	A	136	ILE
1	A	240	LEU
1	B	134	ASP
1	B	314	LEU
1	C	105	TYR
1	C	184	THR
1	C	314	LEU
1	C	375	PRO
1	E	191	THR
1	E	314	LEU
1	F	134	ASP
1	F	314	LEU
1	F	433	LYS
2	H	457	LEU
2	I	457	LEU
2	I	560	MSE
1	B	321	TYR
1	D	375	PRO
1	E	274	GLY

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Mol	Chain	Res	Type
1	A	274	GLY
1	A	315	GLY
1	B	375	PRO
2	G	520	ILE
2	H	520	ILE
1	A	97	PRO
1	C	68	VAL
1	C	136	ILE
1	E	68	VAL
2	I	520	ILE
1	A	375	PRO
1	A	64	PRO
1	C	64	PRO
1	E	64	PRO
1	D	64	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	297/386 (77%)	262 (88%)	35 (12%)	5	21
1	B	297/386 (77%)	257 (86%)	40 (14%)	4	18
1	C	297/386 (77%)	265 (89%)	32 (11%)	6	24
1	D	297/386 (77%)	257 (86%)	40 (14%)	4	18
1	E	297/386 (77%)	263 (89%)	34 (11%)	5	22
1	F	297/386 (77%)	265 (89%)	32 (11%)	6	24
2	G	117/116 (101%)	106 (91%)	11 (9%)	8	29
2	H	117/116 (101%)	104 (89%)	13 (11%)	6	23
2	I	117/116 (101%)	108 (92%)	9 (8%)	12	35
All	All	2133/2664 (80%)	1887 (88%)	246 (12%)	5	22

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	61	ARG
1	A	67	LEU
1	A	79	GLN
1	A	80	LEU
1	A	81	GLU
1	A	96	VAL
1	A	102	VAL
1	A	103	GLU
1	A	128	ASP
1	A	133	GLU
1	A	136	ILE
1	A	139	LEU
1	A	147	ILE
1	A	148	MET
1	A	191	THR
1	A	200	PHE
1	A	202	ARG
1	A	211	ARG
1	A	216	LYS
1	A	222	ASN
1	A	255	GLU
1	A	261	GLN
1	A	314	LEU
1	A	324	LEU
1	A	339	VAL
1	A	345	SER
1	A	351	ARG
1	A	355	VAL
1	A	380	ILE
1	A	388	GLN
1	A	391	ASP
1	A	419	GLN
1	A	428	GLN
1	A	439	VAL
1	B	26	LEU
1	B	49	GLN
1	B	50	LYS
1	B	55	MET
1	B	61	ARG
1	B	79	GLN
1	B	80	LEU
1	B	81	GLU

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Mol	Chain	Res	Type
1	B	102	VAL
1	B	103	GLU
1	B	104	TYR
1	B	107	ARG
1	B	128	ASP
1	B	136	ILE
1	B	139	LEU
1	B	147	ILE
1	B	148	MET
1	B	191	THR
1	B	200	PHE
1	B	202	ARG
1	B	211	ARG
1	B	216	LYS
1	B	222	ASN
1	B	249	MET
1	B	255	GLU
1	B	258	ILE
1	B	261	GLN
1	B	269	THR
1	B	278	MET
1	B	290	ILE
1	B	306	ARG
1	B	314	LEU
1	B	324	LEU
1	B	339	VAL
1	B	351	ARG
1	B	355	VAL
1	B	380	ILE
1	B	388	GLN
1	B	391	ASP
1	B	392	ILE
1	C	50	LYS
1	C	61	ARG
1	C	67	LEU
1	C	79	GLN
1	C	80	LEU
1	C	102	VAL
1	C	110	GLU
1	C	128	ASP
1	C	133	GLU
1	C	139	LEU

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Mol	Chain	Res	Type
1	C	147	ILE
1	C	148	MET
1	C	200	PHE
1	C	202	ARG
1	C	205	LEU
1	C	211	ARG
1	C	222	ASN
1	C	245	GLN
1	C	249	MET
1	C	261	GLN
1	C	278	MET
1	C	314	LEU
1	C	324	LEU
1	C	339	VAL
1	C	345	SER
1	C	351	ARG
1	C	355	VAL
1	C	380	ILE
1	C	388	GLN
1	C	391	ASP
1	C	392	ILE
1	C	439	VAL
1	D	26	LEU
1	D	50	LYS
1	D	55	MET
1	D	63	GLU
1	D	67	LEU
1	D	79	GLN
1	D	80	LEU
1	D	81	GLU
1	D	96	VAL
1	D	102	VAL
1	D	103	GLU
1	D	104	TYR
1	D	136	ILE
1	D	139	LEU
1	D	140	LEU
1	D	147	ILE
1	D	148	MET
1	D	188	THR
1	D	200	PHE
1	D	202	ARG

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Mol	Chain	Res	Type
1	D	205	LEU
1	D	211	ARG
1	D	216	LYS
1	D	222	ASN
1	D	249	MET
1	D	261	GLN
1	D	268	LEU
1	D	269	THR
1	D	290	ILE
1	D	306	ARG
1	D	314	LEU
1	D	324	LEU
1	D	339	VAL
1	D	351	ARG
1	D	355	VAL
1	D	380	ILE
1	D	388	GLN
1	D	391	ASP
1	D	419	GLN
1	D	439	VAL
1	E	50	LYS
1	E	69	THR
1	E	79	GLN
1	E	80	LEU
1	E	104	TYR
1	E	128	ASP
1	E	133	GLU
1	E	136	ILE
1	E	139	LEU
1	E	147	ILE
1	E	148	MET
1	E	191	THR
1	E	200	PHE
1	E	202	ARG
1	E	206	ILE
1	E	207	ILE
1	E	211	ARG
1	E	216	LYS
1	E	222	ASN
1	E	249	MET
1	E	261	GLN
1	E	269	THR

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Mol	Chain	Res	Type
1	E	278	MET
1	E	314	LEU
1	E	324	LEU
1	E	339	VAL
1	E	345	SER
1	E	351	ARG
1	E	355	VAL
1	E	380	ILE
1	E	388	GLN
1	E	391	ASP
1	E	392	ILE
1	E	419	GLN
1	F	26	LEU
1	F	50	LYS
1	F	61	ARG
1	F	67	LEU
1	F	79	GLN
1	F	80	LEU
1	F	81	GLU
1	F	102	VAL
1	F	104	TYR
1	F	110	GLU
1	F	128	ASP
1	F	136	ILE
1	F	139	LEU
1	F	147	ILE
1	F	148	MET
1	F	202	ARG
1	F	211	ARG
1	F	216	LYS
1	F	222	ASN
1	F	255	GLU
1	F	261	GLN
1	F	306	ARG
1	F	314	LEU
1	F	322	LEU
1	F	324	LEU
1	F	351	ARG
1	F	355	VAL
1	F	380	ILE
1	F	388	GLN
1	F	391	ASP

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Mol	Chain	Res	Type
1	F	428	GLN
1	F	439	VAL
2	G	464	GLU
2	G	465	ARG
2	G	475	ARG
2	G	497	LEU
2	G	519	ARG
2	G	536	ILE
2	G	540	VAL
2	G	542	GLU
2	G	550	ARG
2	G	569	THR
2	G	593	MSE
2	H	465	ARG
2	H	475	ARG
2	H	497	LEU
2	H	519	ARG
2	H	520	ILE
2	H	536	ILE
2	H	540	VAL
2	H	542	GLU
2	H	545	LEU
2	H	550	ARG
2	H	561	LEU
2	H	582	ARG
2	H	593	MSE
2	I	465	ARG
2	I	467	LEU
2	I	509	HIS
2	I	519	ARG
2	I	520	ILE
2	I	536	ILE
2	I	540	VAL
2	I	542	GLU
2	I	593	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	53	HIS
1	A	201	GLN

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Mol	Chain	Res	Type
1	A	222	ASN
1	A	225	GLN
1	A	323	GLN
1	A	388	GLN
1	B	53	HIS
1	B	79	GLN
1	B	201	GLN
1	B	222	ASN
1	B	225	GLN
1	B	245	GLN
1	B	246	GLN
1	B	261	GLN
1	B	323	GLN
1	B	362	GLN
1	B	388	GLN
1	C	53	HIS
1	C	79	GLN
1	C	201	GLN
1	C	222	ASN
1	C	225	GLN
1	C	245	GLN
1	C	261	GLN
1	C	323	GLN
1	C	388	GLN
1	D	53	HIS
1	D	79	GLN
1	D	201	GLN
1	D	222	ASN
1	D	225	GLN
1	D	246	GLN
1	D	261	GLN
1	D	323	GLN
1	D	362	GLN
1	D	388	GLN
1	E	53	HIS
1	E	79	GLN
1	E	201	GLN
1	E	222	ASN
1	E	225	GLN
1	E	323	GLN
1	E	388	GLN
1	F	53	HIS

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Mol	Chain	Res	Type
1	F	79	GLN
1	F	225	GLN
1	F	226	ASN
1	F	261	GLN
1	F	285	ASN
1	F	323	GLN
1	F	362	GLN
1	F	388	GLN
2	G	470	HIS
2	G	494	HIS
2	G	509	HIS
2	H	470	HIS
2	H	482	GLN
2	H	494	HIS
2	H	509	HIS
2	H	554	ASN
2	H	566	GLN
2	I	470	HIS
2	I	494	HIS
2	I	509	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	358/454 (78%)	0.51	19 (5%)	32 27	156, 167, 168, 170	0
1	B	358/454 (78%)	0.51	16 (4%)	38 30	163, 167, 168, 175	0
1	C	358/454 (78%)	0.63	29 (8%)	18 19	157, 167, 168, 170	0
1	D	358/454 (78%)	0.60	24 (6%)	24 22	163, 167, 168, 182	0
1	E	358/454 (78%)	0.53	22 (6%)	27 24	163, 167, 168, 170	0
1	F	358/454 (78%)	1.19	67 (18%)	3 6	162, 167, 168, 187	0
2	G	132/143 (92%)	0.88	15 (11%)	10 13	163, 167, 168, 169	0
2	H	132/143 (92%)	0.75	10 (7%)	20 20	162, 167, 168, 169	0
2	I	132/143 (92%)	0.71	6 (4%)	38 30	163, 167, 168, 169	0
All	All	2544/3153 (80%)	0.68	208 (8%)	17 19	156, 167, 168, 187	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	393	VAL	10.3
1	F	197	THR	9.1
1	A	261	GLN	8.2
1	F	199	GLY	7.6
1	F	231	THR	6.7
1	F	205	LEU	6.3
1	F	193	LEU	6.0
1	C	270	PRO	6.0
2	G	513	PRO	6.0
2	G	553	LEU	6.0
1	F	392	ILE	6.0
1	A	260	ALA	5.4
1	C	104	TYR	5.4
1	F	207	ILE	5.2
1	F	305	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	380	ILE	4.8
1	F	233	GLU	4.6
2	H	506	GLU	4.6
1	C	76	ALA	4.4
1	F	391	ASP	4.3
1	C	97	PRO	4.2
1	A	96	VAL	4.1
1	F	322	LEU	4.0
1	F	416	ILE	3.8
1	E	149	GLU	3.8
1	A	421	ASN	3.8
1	F	198	SER	3.8
1	E	104	TYR	3.7
1	F	324	LEU	3.7
1	F	418	LYS	3.7
1	C	96	VAL	3.6
1	F	436	ASN	3.6
1	B	353	LEU	3.6
1	F	227	VAL	3.6
2	H	519	ARG	3.6
1	A	288	ILE	3.5
1	C	421	ASN	3.5
1	F	194	ASP	3.4
1	F	415	ILE	3.4
1	D	149	GLU	3.4
1	F	200	PHE	3.4
1	F	188	THR	3.4
1	C	271	GLU	3.4
2	H	592	LYS	3.4
1	F	394	ALA	3.3
2	H	507	GLU	3.3
1	B	199	GLY	3.2
1	C	149	GLU	3.2
2	H	569	THR	3.2
1	F	230	LYS	3.2
1	A	375	PRO	3.1
1	B	185	GLY	3.1
1	E	96	VAL	3.1
1	F	441	LEU	3.1
1	D	100	ALA	3.1
1	E	375	PRO	3.1
2	I	517	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	133	GLU	3.0
1	D	363	LEU	3.0
1	A	434	GLU	3.0
1	D	432	ILE	2.9
1	C	260	ALA	2.9
1	F	377	MET	2.9
1	A	432	ILE	2.9
1	D	271	GLU	2.9
1	F	383	SER	2.9
1	F	414	ILE	2.9
1	D	439	VAL	2.9
2	H	585	LYS	2.9
1	F	325	ILE	2.8
1	D	380	ILE	2.8
1	F	288	ILE	2.8
1	F	187	PRO	2.8
1	D	270	PRO	2.8
1	B	184	THR	2.7
1	B	260	ALA	2.7
2	H	567	GLU	2.7
2	G	580	ALA	2.7
2	I	543	GLN	2.7
1	C	276	LEU	2.7
1	F	300	ASP	2.6
1	F	301	ILE	2.6
1	A	97	PRO	2.6
1	A	15	GLU	2.6
1	F	133	GLU	2.6
1	C	98	THR	2.6
1	F	206	ILE	2.6
1	C	195	ARG	2.6
1	D	136	ILE	2.6
1	D	379	ASP	2.6
2	I	480	VAL	2.6
2	G	460	PHE	2.6
1	F	440	ASN	2.6
1	F	283	LEU	2.6
1	B	230	LYS	2.6
1	F	275	LYS	2.6
1	D	114	VAL	2.5
1	F	259	ASN	2.5
1	D	374	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	260	ALA	2.5
1	F	395	PHE	2.5
1	F	191	THR	2.5
1	F	420	ARG	2.5
1	E	15	GLU	2.5
1	E	261	GLN	2.5
2	G	591	LYS	2.5
1	F	363	LEU	2.5
2	G	459	ALA	2.5
1	A	290	ILE	2.5
1	C	377	MET	2.5
2	G	555	ARG	2.5
1	C	144	ASP	2.5
1	C	287	GLY	2.5
1	C	63	GLU	2.4
1	F	439	VAL	2.4
1	F	346	LEU	2.4
1	D	63	GLU	2.4
1	D	383	SER	2.4
1	E	341	GLU	2.4
1	F	196	MET	2.4
1	C	273	TRP	2.4
1	A	104	TYR	2.4
1	C	422	GLY	2.4
2	H	508	GLY	2.4
1	F	396	LEU	2.4
1	F	226	ASN	2.4
1	B	271	GLU	2.4
1	E	270	PRO	2.4
1	B	100	ALA	2.4
1	D	274	GLY	2.4
2	G	461	GLN	2.4
1	B	186	ILE	2.4
2	I	565	GLU	2.3
1	B	363	LEU	2.3
1	A	149	GLU	2.3
1	F	235	VAL	2.3
1	F	149	GLU	2.3
1	D	231	THR	2.3
1	B	276	LEU	2.3
1	E	97	PRO	2.3
1	F	246	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	76	ALA	2.3
1	E	434	GLU	2.3
1	F	65	VAL	2.3
1	E	98	THR	2.3
1	D	64	PRO	2.3
2	H	505	TYR	2.3
1	D	96	VAL	2.3
1	D	339	VAL	2.2
1	E	232	ASN	2.2
1	C	216	LYS	2.2
1	A	114	VAL	2.2
1	C	269	THR	2.2
1	F	279	ALA	2.2
1	E	310	GLN	2.2
2	G	504	PHE	2.2
1	F	437	LYS	2.2
1	E	277	THR	2.2
1	D	288	ILE	2.2
1	E	112	LYS	2.2
2	G	462	ASN	2.2
1	E	378	SER	2.2
1	D	314	LEU	2.2
1	D	15	GLU	2.2
1	B	144	ASP	2.1
1	A	259	ASN	2.1
1	B	349	LEU	2.1
1	C	93	ALA	2.1
2	I	511	ALA	2.1
1	E	421	ASN	2.1
1	F	229	THR	2.1
1	E	114	VAL	2.1
2	G	519	ARG	2.1
1	C	346	LEU	2.1
1	E	288	ILE	2.1
1	D	300	ASP	2.1
1	C	105	TYR	2.1
2	G	511	ALA	2.1
1	F	186	ILE	2.1
1	C	302	ARG	2.1
1	A	98	THR	2.1
1	C	434	GLU	2.1
1	E	63	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	252	LEU	2.1
1	F	282	SER	2.1
1	B	264	ARG	2.1
1	F	425	GLY	2.1
1	F	426	THR	2.1
1	B	386	ILE	2.1
2	G	543	GLN	2.1
1	F	299	SER	2.1
2	G	585	LYS	2.0
1	A	94	ASP	2.0
1	A	287	GLY	2.0
1	F	359	ALA	2.0
1	F	63	GLU	2.0
1	A	378	SER	2.0
1	F	374	ARG	2.0
1	C	94	ASP	2.0
2	I	459	ALA	2.0
1	F	232	ASN	2.0
1	C	382	GLU	2.0
1	C	299	SER	2.0
2	H	463	ALA	2.0
1	B	300	ASP	2.0
1	D	264	ARG	2.0
1	E	253	CYS	2.0
2	G	561	LEU	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.