



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:29 PM UTC

PDB ID : 7QX8 / pdb_00007qx8
Title : Crystal structure of serine hydroxymethyltransferase, isoform 7 from *Arabidopsis thaliana* (SHM7)
Authors : Ruszkowski, M.; Grzechowiak, M.; Sekula, B.
Deposited on : 2022-01-26
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

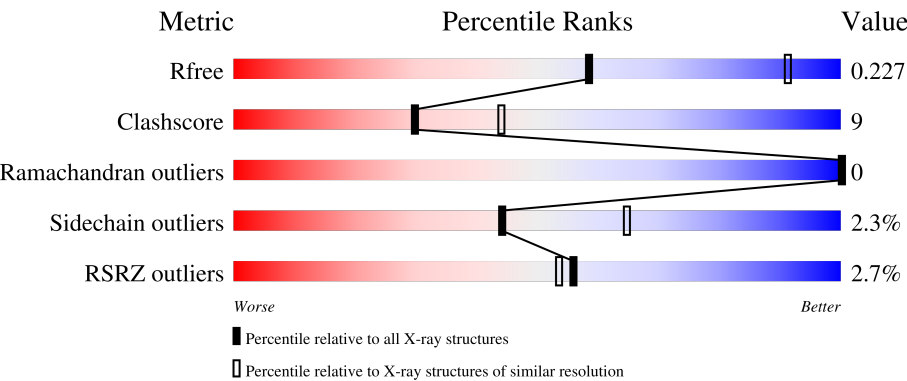
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	479	2% 78% 13% 8%
1	B	479	2% 79% 13% 8%
1	C	479	2% 78% 15% 7%
1	D	479	% 72% 18% 9%
1	E	479	3% 76% 16% 8%

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Mol	Chain	Length	Quality of chain
1	F	479	2% 75% 16% • 7%
1	G	479	3% 73% 19% • 7%
1	H	479	7% 76% 15% • 9%
1	I	479	% 77% 15% 8%
1	J	479	% 75% 18% 7%
1	K	479	4% 71% 19% • 9%
1	L	479	2% 76% 16% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41696 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 Serine hydroxymethyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3454	2183	608	638	25			
1	B	443	Total	C	N	O	S	0	0	0
			3454	2181	608	640	25			
1	C	447	Total	C	N	O	S	0	0	0
			3486	2199	613	649	25			
1	D	438	Total	C	N	O	S	0	1	0
			3429	2167	603	634	25			
1	E	442	Total	C	N	O	S	0	1	0
			3460	2186	609	640	25			
1	F	444	Total	C	N	O	S	0	1	0
			3467	2186	612	644	25			
1	G	444	Total	C	N	O	S	0	0	0
			3460	2183	609	643	25			
1	H	438	Total	C	N	O	S	0	1	0
			3431	2169	604	633	25			
1	I	442	Total	C	N	O	S	0	1	0
			3456	2182	610	639	25			
1	J	444	Total	C	N	O	S	0	0	0
			3461	2185	609	642	25			
1	K	437	Total	C	N	O	S	0	1	0
			3419	2158	604	632	25			
1	L	443	Total	C	N	O	S	0	1	0
			3463	2187	610	641	25			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	SER	-	expression tag	UNP Q84WV0
A	121	ASN	-	expression tag	UNP Q84WV0
A	122	ALA	-	expression tag	UNP Q84WV0
B	120	SER	-	expression tag	UNP Q84WV0
B	121	ASN	-	expression tag	UNP Q84WV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	122	ALA	-	expression tag	UNP Q84WV0
C	120	SER	-	expression tag	UNP Q84WV0
C	121	ASN	-	expression tag	UNP Q84WV0
C	122	ALA	-	expression tag	UNP Q84WV0
D	120	SER	-	expression tag	UNP Q84WV0
D	121	ASN	-	expression tag	UNP Q84WV0
D	122	ALA	-	expression tag	UNP Q84WV0
E	120	SER	-	expression tag	UNP Q84WV0
E	121	ASN	-	expression tag	UNP Q84WV0
E	122	ALA	-	expression tag	UNP Q84WV0
F	120	SER	-	expression tag	UNP Q84WV0
F	121	ASN	-	expression tag	UNP Q84WV0
F	122	ALA	-	expression tag	UNP Q84WV0
G	120	SER	-	expression tag	UNP Q84WV0
G	121	ASN	-	expression tag	UNP Q84WV0
G	122	ALA	-	expression tag	UNP Q84WV0
H	120	SER	-	expression tag	UNP Q84WV0
H	121	ASN	-	expression tag	UNP Q84WV0
H	122	ALA	-	expression tag	UNP Q84WV0
I	120	SER	-	expression tag	UNP Q84WV0
I	121	ASN	-	expression tag	UNP Q84WV0
I	122	ALA	-	expression tag	UNP Q84WV0
J	120	SER	-	expression tag	UNP Q84WV0
J	121	ASN	-	expression tag	UNP Q84WV0
J	122	ALA	-	expression tag	UNP Q84WV0
K	120	SER	-	expression tag	UNP Q84WV0
K	121	ASN	-	expression tag	UNP Q84WV0
K	122	ALA	-	expression tag	UNP Q84WV0
L	120	SER	-	expression tag	UNP Q84WV0
L	121	ASN	-	expression tag	UNP Q84WV0
L	122	ALA	-	expression tag	UNP Q84WV0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	24	Total O 24 24	0	0
2	C	35	Total O 35 35	0	0
2	D	12	Total O 12 12	0	0

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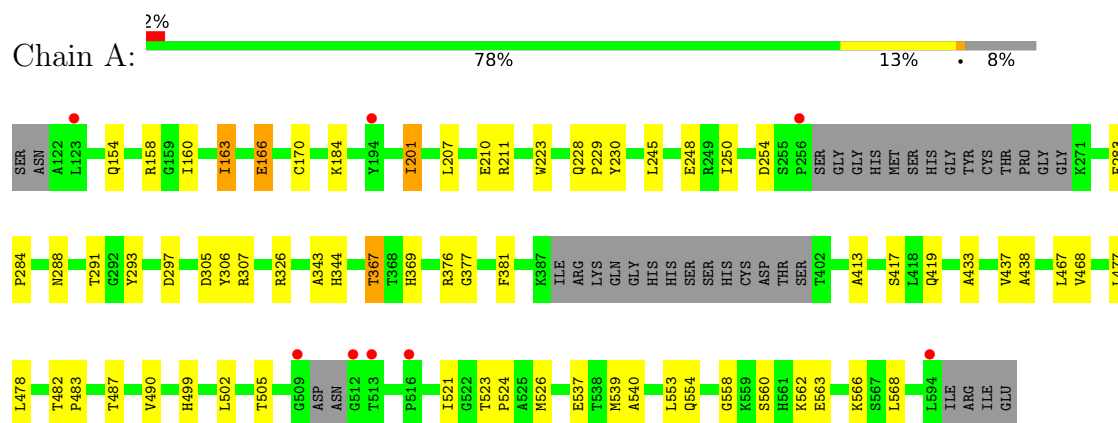
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	30	Total 30	O 30	0	0
2	F	18	Total 18	O 18	0	0
2	G	15	Total 15	O 15	0	0
2	H	6	Total 6	O 6	0	0
2	I	24	Total 24	O 24	0	0
2	J	26	Total 26	O 26	0	0
2	K	14	Total 14	O 14	0	0
2	L	20	Total 20	O 20	0	0

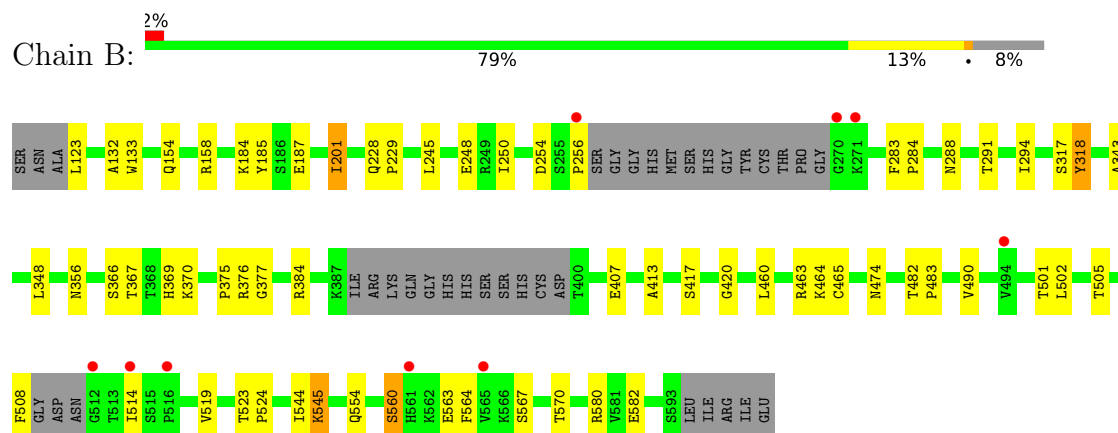
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

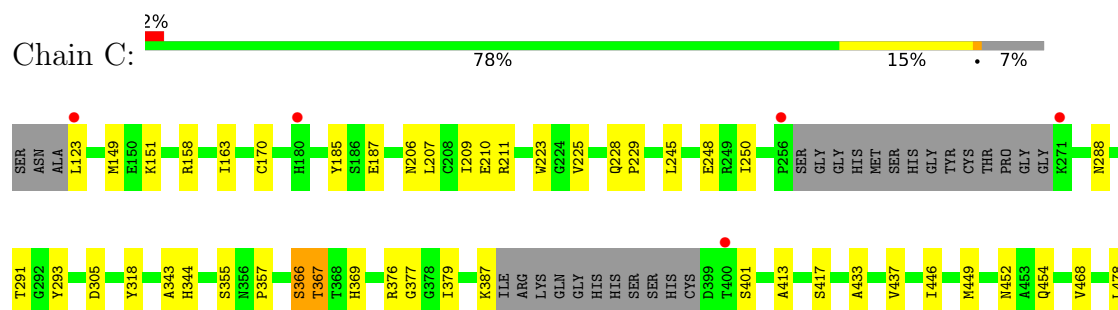
• Molecule 1: Serine hydroxymethyltransferase 7



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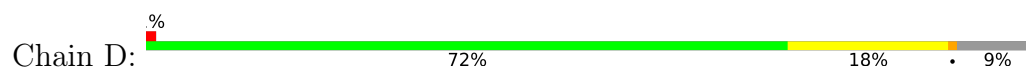


• Molecule 1: Serine hydroxymethyltransferase 7

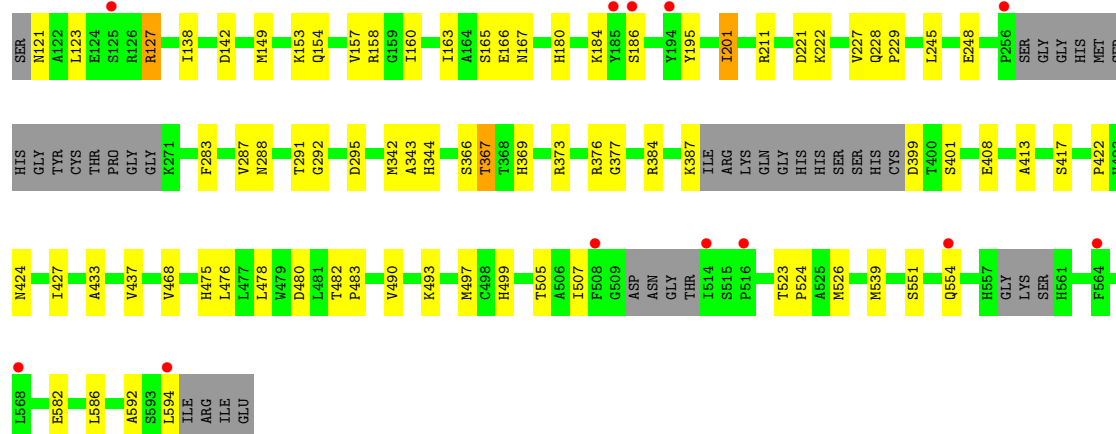
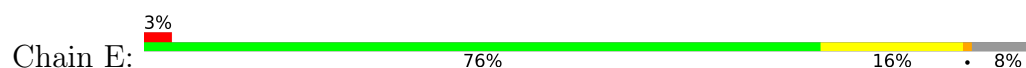




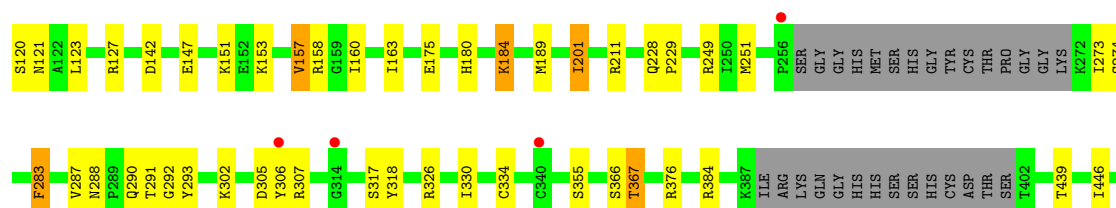
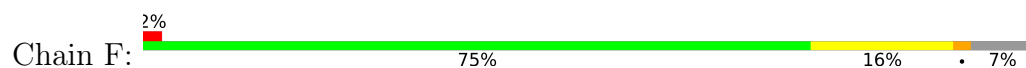
• Molecule 1: Serine hydroxymethyltransferase 7

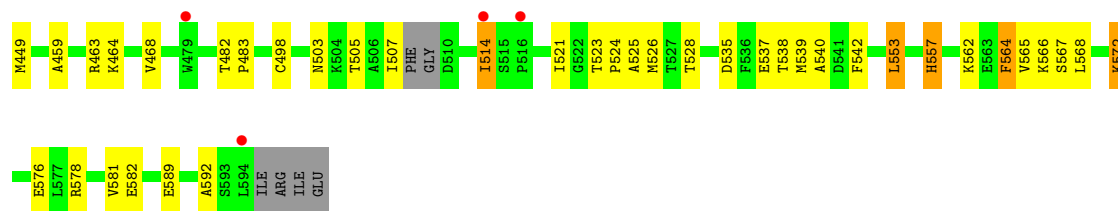


• Molecule 1: Serine hydroxymethyltransferase 7

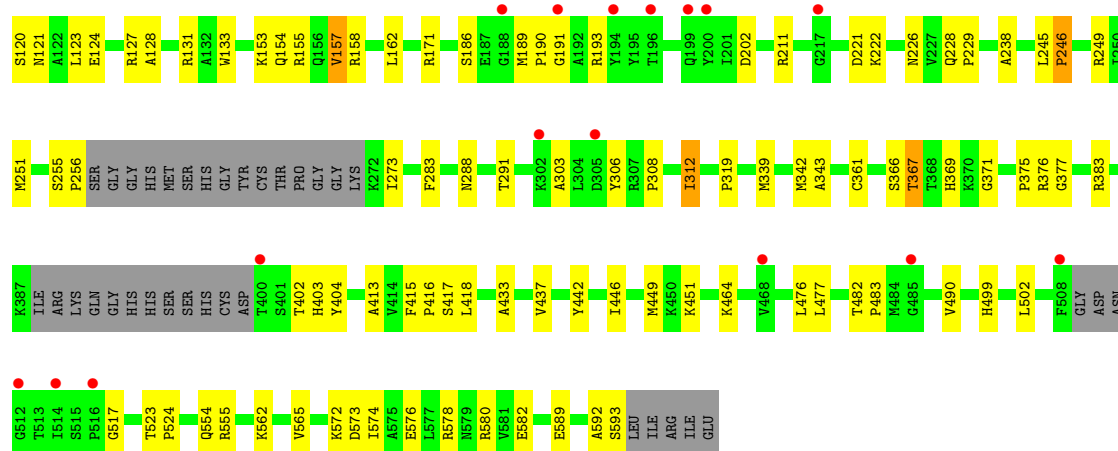
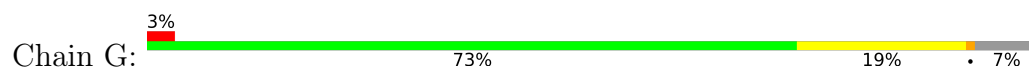


• Molecule 1: Serine hydroxymethyltransferase 7

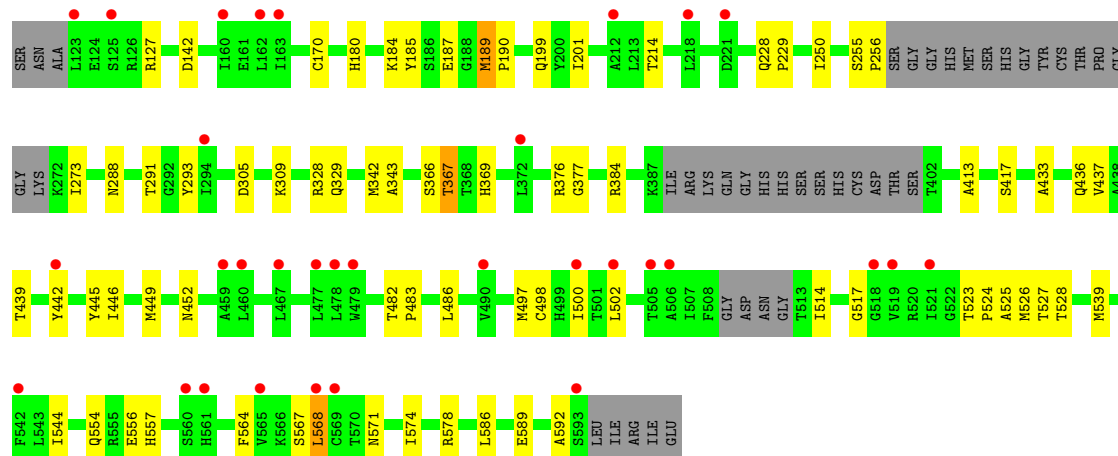
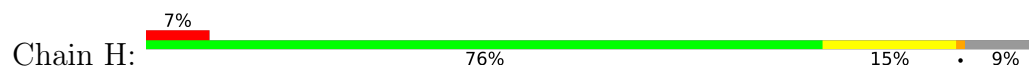




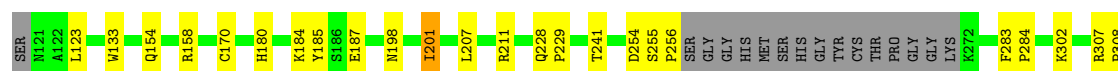
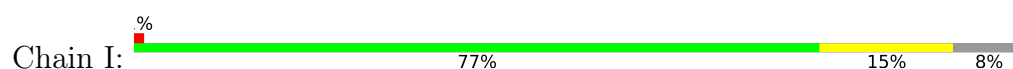
• Molecule 1: Serine hydroxymethyltransferase 7

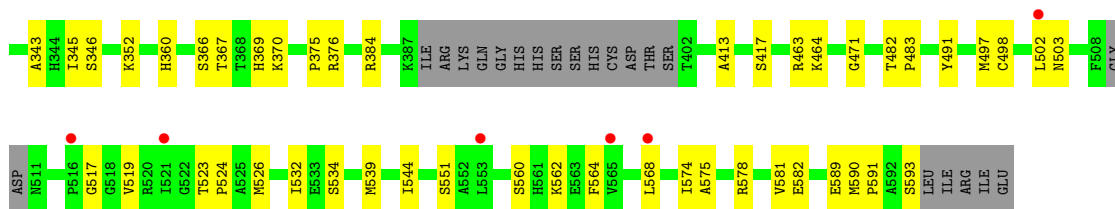


• Molecule 1: Serine hydroxymethyltransferase 7

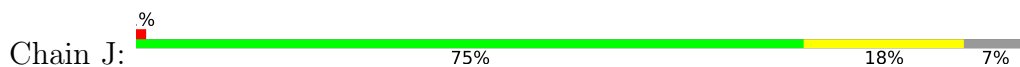


• Molecule 1: Serine hydroxymethyltransferase 7

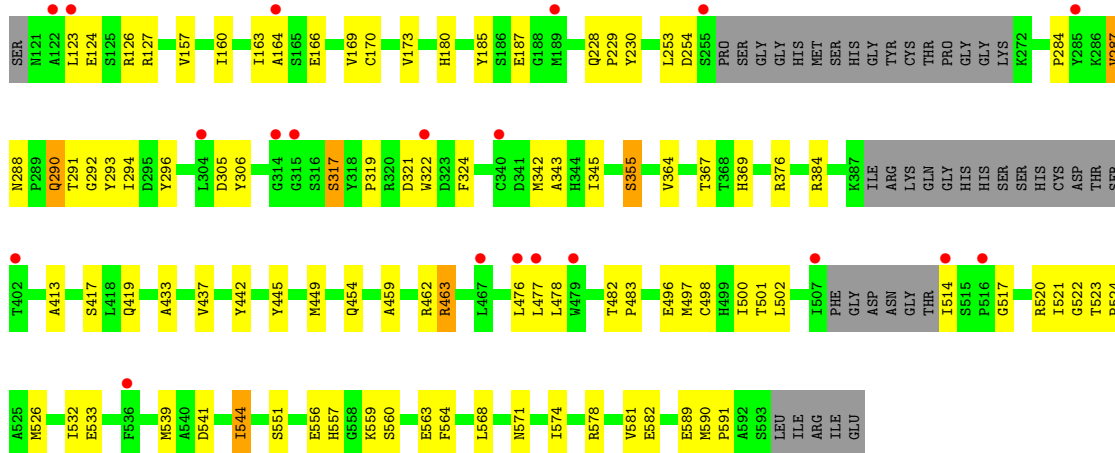




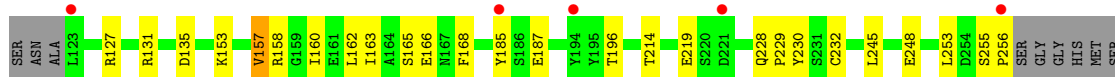
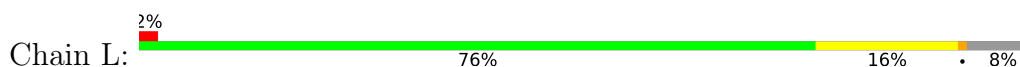
• Molecule 1: Serine hydroxymethyltransferase 7

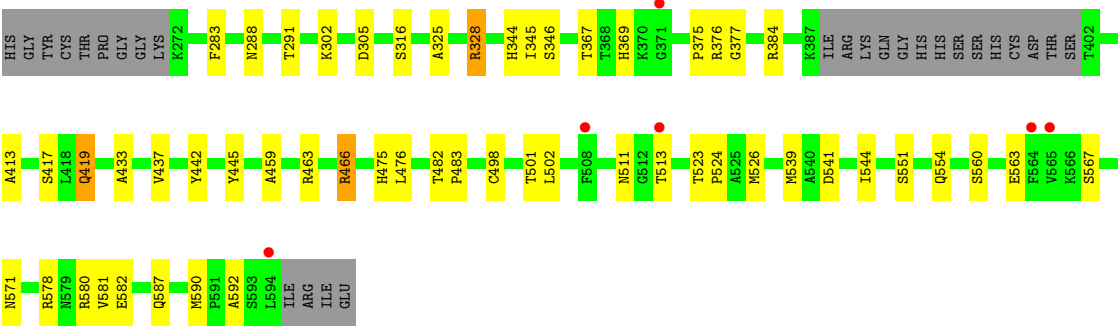


• Molecule 1: Serine hydroxymethyltransferase 7



• Molecule 1: Serine hydroxymethyltransferase 7





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.83Å 123.95Å 290.54Å 90.00° 93.17° 90.00°	Depositor
Resolution (Å)	58.00 – 2.74 58.00 – 2.74	Depositor EDS
% Data completeness (in resolution range)	65.2 (58.00-2.74) 65.3 (58.00-2.74)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.227 0.188 , 0.227	Depositor DCC
R_{free} test set	1220 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41696	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.07	4/3524 (0.1%)	1.46	4/4757 (0.1%)
1	B	1.02	1/3524 (0.0%)	1.48	5/4757 (0.1%)
1	C	1.07	3/3557 (0.1%)	1.49	9/4804 (0.2%)
1	D	1.02	2/3501 (0.1%)	1.47	4/4726 (0.1%)
1	E	1.06	2/3533 (0.1%)	1.46	5/4770 (0.1%)
1	F	1.01	0/3540	1.47	4/4781 (0.1%)
1	G	1.02	2/3530 (0.1%)	1.51	4/4767 (0.1%)
1	H	0.98	0/3505	1.47	4/4733 (0.1%)
1	I	1.05	3/3530 (0.1%)	1.49	9/4767 (0.2%)
1	J	1.08	4/3531 (0.1%)	1.48	2/4768 (0.0%)
1	K	0.99	0/3491	1.47	0/4713
1	L	1.03	1/3538 (0.0%)	1.48	4/4779 (0.1%)
All	All	1.03	22/42304 (0.1%)	1.48	54/57122 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	499	HIS	CE1-NE2	7.71	1.40	1.32
1	E	499	HIS	CE1-NE2	6.86	1.39	1.32
1	L	344	HIS	CE1-NE2	6.85	1.39	1.32
1	B	420	GLY	C-O	6.66	1.31	1.24
1	J	344	HIS	CE1-NE2	6.39	1.39	1.32
1	A	163	ILE	C-O	6.29	1.30	1.24
1	A	499	HIS	CE1-NE2	6.29	1.38	1.32
1	C	344	HIS	CE1-NE2	6.22	1.38	1.32
1	I	360	HIS	CE1-NE2	5.87	1.38	1.32
1	J	246	PRO	C-O	-5.84	1.16	1.23
1	D	426	HIS	CE1-NE2	5.77	1.38	1.32
1	A	166	GLU	C-O	5.66	1.30	1.23
1	C	357	PRO	C-O	-5.65	1.17	1.24
1	D	244	LEU	C-O	5.60	1.31	1.23
1	C	163	ILE	C-O	5.51	1.29	1.24
1	J	426	HIS	CE1-NE2	5.34	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	471	GLY	C-O	5.28	1.31	1.24
1	G	319	PRO	C-O	-5.25	1.18	1.23
1	I	307	ARG	N-CA	5.21	1.50	1.46
1	A	344	HIS	CE1-NE2	5.15	1.37	1.32
1	G	246	PRO	C-O	-5.10	1.17	1.23
1	E	344	HIS	CE1-NE2	5.04	1.37	1.32

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	367	THR	CA-CB-OG1	-6.49	99.86	109.60
1	C	318	TYR	CB-CA-C	6.30	118.57	110.13
1	I	370	LYS	O-C-N	6.30	126.38	120.71
1	B	370	LYS	O-C-N	6.17	126.26	120.71
1	I	593	SER	CA-C-O	-6.11	110.42	120.80
1	E	422	PRO	CA-C-O	-6.02	114.66	122.12
1	C	454	GLN	N-CA-C	-5.81	104.86	111.07
1	D	501	THR	CB-CA-C	5.79	119.58	110.19
1	J	386	PRO	CB-CA-C	-5.76	103.55	111.21
1	E	221	ASP	CA-CB-CG	5.76	118.36	112.60
1	F	318	TYR	CB-CA-C	5.66	116.15	109.47
1	H	592	ALA	CA-C-N	5.59	131.76	121.70
1	H	592	ALA	C-N-CA	5.59	131.76	121.70
1	I	241	THR	CA-CB-OG1	-5.56	101.27	109.60
1	G	273	ILE	CA-C-O	-5.52	116.01	120.70
1	I	375	PRO	CA-C-O	-5.52	115.27	122.12
1	G	404	TYR	CA-C-O	-5.52	115.54	121.56
1	L	165	SER	CA-C-N	5.49	128.89	120.82
1	L	165	SER	C-N-CA	5.49	128.89	120.82
1	G	367	THR	CA-CB-OG1	-5.49	101.37	109.60
1	L	501	THR	CB-CA-C	5.48	119.07	110.19
1	E	367	THR	CB-CA-C	5.46	118.54	109.53
1	D	370	LYS	O-C-N	5.36	125.54	120.71
1	F	439	THR	CA-CB-OG1	-5.36	101.56	109.60
1	B	318	TYR	CB-CA-C	5.30	116.25	110.15
1	C	223	TRP	CA-C-N	5.30	126.28	121.82
1	C	223	TRP	C-N-CA	5.30	126.28	121.82
1	C	366	SER	O-C-N	5.27	128.56	123.29
1	A	367	THR	CA-CB-OG1	-5.24	101.74	109.60
1	E	344	HIS	CA-CB-CG	-5.23	108.57	113.80
1	A	223	TRP	CA-C-N	5.21	126.19	121.82
1	A	223	TRP	C-N-CA	5.21	126.19	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	LYS	CA-C-O	-5.21	116.37	119.55
1	C	379	ILE	CA-C-O	-5.19	116.60	120.96
1	B	132	ALA	O-C-N	5.19	127.63	122.08
1	J	593	SER	CB-CA-C	5.15	119.19	110.79
1	I	308	PRO	CA-C-O	-5.12	115.43	121.67
1	A	381	PHE	CA-C-O	-5.11	115.13	120.80
1	G	375	PRO	CA-C-O	-5.10	115.79	122.12
1	I	551	SER	CA-C-N	5.09	127.10	120.28
1	I	551	SER	C-N-CA	5.09	127.10	120.28
1	C	566	LYS	CA-C-N	5.09	127.35	120.38
1	C	566	LYS	C-N-CA	5.09	127.35	120.38
1	D	288	ASN	CB-CA-C	5.09	118.03	109.69
1	H	214	THR	CA-CB-OG1	-5.07	101.99	109.60
1	B	501	THR	CB-CA-C	5.04	118.36	110.19
1	E	165	SER	O-C-N	5.03	127.26	122.03
1	F	566	LYS	CA-C-N	5.03	127.02	120.28
1	F	566	LYS	C-N-CA	5.03	127.02	120.28
1	I	491	TYR	CA-C-N	5.03	127.33	120.54
1	I	491	TYR	C-N-CA	5.03	127.33	120.54
1	D	554	GLN	N-CA-C	-5.02	107.13	113.20
1	C	367	THR	CA-CB-OG1	-5.01	102.08	109.60
1	L	214	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3454	0	3446	50	0
1	B	3454	0	3442	45	0
1	C	3486	0	3468	56	0
1	D	3429	0	3413	83	0
1	E	3460	0	3443	56	0
1	F	3467	0	3449	70	0
1	G	3460	0	3442	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3431	0	3418	65	0
1	I	3456	0	3438	53	0
1	J	3461	0	3446	59	0
1	K	3419	0	3406	97	0
1	L	3463	0	3446	60	0
2	A	32	0	0	2	0
2	B	24	0	0	0	0
2	C	35	0	0	2	0
2	D	12	0	0	0	0
2	E	30	0	0	0	0
2	F	18	0	0	5	0
2	G	15	0	0	1	0
2	H	6	0	0	0	0
2	I	24	0	0	1	0
2	J	26	0	0	1	0
2	K	14	0	0	1	0
2	L	20	0	0	0	0
All	All	41696	0	41257	705	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 9.

All (705) 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:I:497:MET:HG3	1:I:568:LEU:HD21	1.11	1.10
1:H:452:ASN:HD22	1:H:527:THR:HG22	1.10	1.08
1:G:249:ARG:HB3	1:G:306:TYR:HE1	1.16	1.05
1:A:526:MET:HG3	1:A:539:MET:HE1	1.08	1.04
1:B:560:SER:OG	1:B:563:GLU:HB2	1.60	1.01
1:I:497:MET:CG	1:I:568:LEU:HD21	1.92	0.98
1:G:251:MET:HE3	1:G:308:PRO:HG3	1.45	0.97
1:A:526:MET:HG3	1:A:539:MET:CE	1.95	0.97
1:G:186:SER:HB3	1:G:193:ARG:HH11	1.28	0.96
1:G:186:SER:HB3	1:G:193:ARG:NH1	1.83	0.93
1:K:253:LEU:HD23	1:K:254:ASP:N	1.85	0.92
1:G:249:ARG:HB3	1:G:306:TYR:CE1	2.06	0.91
1:G:589:GLU:HG2	1:H:127:ARG:HG3	1.52	0.91
1:D:578:ARG:O	1:D:581:VAL:HG12	1.71	0.90
1:D:230:TYR:CE2	1:D:419:GLN:HB3	2.07	0.89
1:K:578:ARG:O	1:K:581:VAL:HG12	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:MET:HE2	1:D:366:SER:HB2	1.55	0.88
1:D:369:HIS:CD2	1:D:376:ARG:HA	2.10	0.86
1:G:251:MET:HG3	1:G:283:PHE:O	1.76	0.85
1:D:463:ARG:HG3	1:D:463:ARG:HH11	1.38	0.85
1:F:449:MET:CE	1:F:524:PRO:HG3	2.07	0.85
1:A:526:MET:CG	1:A:539:MET:HE1	2.01	0.84
1:I:497:MET:HG3	1:I:568:LEU:CD2	2.04	0.84
1:D:539:MET:O	1:D:543:LEU:HD13	1.79	0.83
1:I:498:CYS:O	1:I:581:VAL:HG21	1.78	0.82
1:G:251:MET:HE1	1:G:303:ALA:HA	1.59	0.82
1:L:168:PHE:CD1	1:L:590:MET:HE1	2.14	0.81
1:F:449:MET:HE2	1:F:524:PRO:HG3	1.63	0.81
1:H:436:GLN:O	1:H:439:THR:HG22	1.82	0.80
1:G:369:HIS:CD2	1:G:376:ARG:HA	2.17	0.80
1:H:452:ASN:ND2	1:H:527:THR:HG22	1.93	0.80
1:L:232:CYS:HB2	1:L:367:THR:HG22	1.64	0.79
1:H:497:MET:HG3	1:H:568:LEU:HG	1.63	0.79
1:K:449:MET:HE3	1:K:524:PRO:HB3	1.66	0.78
1:C:387:LYS:NZ	1:C:401:SER:HB3	1.98	0.77
1:D:498:CYS:O	1:D:581:VAL:HG11	1.84	0.76
1:G:128:ALA:HA	1:G:131:ARG:HG2	1.67	0.76
1:L:498:CYS:O	1:L:581:VAL:HG11	1.85	0.76
1:G:251:MET:CE	1:G:308:PRO:HG3	2.16	0.75
1:A:438:ALA:O	1:I:352:LYS:HE3	1.86	0.75
1:H:557:HIS:HB3	1:H:564:PHE:HD1	1.51	0.75
1:K:180[B]:HIS:NE2	1:L:592:ALA:O	2.21	0.73
1:H:557:HIS:HB3	1:H:564:PHE:CD1	2.22	0.73
1:F:305:ASP:HB3	1:G:283:PHE:HZ	1.53	0.73
1:F:459:ALA:O	1:F:463:ARG:HG2	1.89	0.73
1:F:464:LYS:HG3	1:F:464:LYS:O	1.89	0.73
1:C:592:ALA:O	1:D:180[B]:HIS:NE2	2.22	0.72
1:E:369:HIS:CD2	1:E:376:ARG:HA	2.23	0.72
1:F:572:LYS:O	1:F:576:GLU:HG3	1.89	0.72
1:A:160:ILE:HG23	1:A:539:MET:CE	2.19	0.72
1:K:317:SER:HB2	1:K:476:LEU:HD21	1.72	0.72
1:G:249:ARG:HD3	1:G:306:TYR:CE1	2.25	0.71
1:L:578:ARG:O	1:L:581:VAL:HG12	1.90	0.71
1:K:166:GLU:HA	1:L:185:TYR:CE2	2.27	0.70
1:E:497:MET:HA	1:E:497:MET:HE2	1.72	0.70
1:K:501:THR:HG22	1:L:196:THR:HG22	1.72	0.70
1:D:463:ARG:HG3	1:D:463:ARG:NH1	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:PHE:HB2	1:G:306:TYR:CE2	2.25	0.70
1:E:184:LYS:HG2	1:E:201:ILE:CD1	2.22	0.70
1:F:498:CYS:O	1:F:581:VAL:HG11	1.93	0.69
1:E:526:MET:HG3	1:E:539:MET:HE1	1.74	0.69
1:H:369:HIS:CD2	1:H:376:ARG:HA	2.27	0.69
1:D:342:MET:HE2	1:D:366:SER:CB	2.22	0.69
1:F:578:ARG:O	1:F:581:VAL:HG12	1.94	0.68
1:F:184:LYS:HG2	1:F:201:ILE:HD13	1.75	0.67
1:H:498:CYS:HA	1:H:578:ARG:HG3	1.76	0.67
1:H:288:ASN:HB3	1:H:291:THR:HG22	1.77	0.67
1:B:369:HIS:CD2	1:B:376:ARG:HA	2.30	0.66
1:G:369:HIS:HD2	1:G:377:GLY:H	1.44	0.66
1:H:439:THR:HG23	1:H:442:TYR:H	1.59	0.66
1:F:184:LYS:HG2	1:F:201:ILE:CD1	2.25	0.66
1:L:560:SER:HB3	1:L:563:GLU:HG2	1.77	0.66
1:F:291:THR:HG22	1:F:293:TYR:HD2	1.61	0.66
1:C:288:ASN:CG	1:C:291:THR:HG22	2.20	0.66
1:E:149:MET:O	1:F:180[A]:HIS:NE2	2.28	0.66
1:E:387:LYS:HZ2	1:E:401:SER:HB3	1.61	0.66
1:H:526:MET:HG3	1:H:539:MET:HE1	1.78	0.66
1:A:523:THR:N	1:A:524:PRO:HD3	2.11	0.66
1:C:387:LYS:HZ3	1:C:401:SER:HB3	1.61	0.66
1:I:463:ARG:HD2	1:I:544:ILE:HD11	1.78	0.66
1:A:160:ILE:HG23	1:A:539:MET:HE2	1.76	0.65
1:F:526:MET:HG3	1:F:539:MET:HE1	1.78	0.65
1:G:574:ILE:HD12	1:G:578:ARG:HH12	1.62	0.65
1:F:123:LEU:HD11	2:F:608:HOH:O	1.96	0.65
1:D:283:PHE:HB2	1:D:306:TYR:CZ	2.32	0.65
1:K:342:MET:HE3	1:K:364:VAL:CG1	2.27	0.65
1:C:526:MET:HG3	1:C:539:MET:HE1	1.78	0.65
1:K:317:SER:HB2	1:K:476:LEU:CD2	2.28	0.64
1:K:164:ALA:CB	1:K:476:LEU:HD13	2.26	0.64
1:J:228:GLN:N	1:J:229:PRO:CD	2.60	0.64
1:J:307:ARG:NH1	1:J:334:CYS:HA	2.13	0.64
1:E:387:LYS:NZ	1:E:401:SER:HB3	2.12	0.64
1:D:291:THR:HG23	1:D:293:TYR:H	1.62	0.64
1:B:185:TYR:CE1	1:B:187:GLU:HG3	2.32	0.64
1:E:586:LEU:HD12	1:J:586:LEU:HD12	1.79	0.64
1:D:342:MET:O	1:D:342:MET:HG2	1.99	0.63
1:I:497:MET:HE2	1:I:568:LEU:CD2	2.28	0.63
1:I:464:LYS:HG2	1:I:464:LYS:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:342:MET:HE3	1:K:364:VAL:HG12	1.79	0.63
1:J:342:MET:HE3	1:J:366:SER:HB2	1.80	0.62
1:A:160:ILE:CG2	1:A:539:MET:HE2	2.29	0.62
1:K:496:GLU:CG	1:L:196:THR:HG23	2.29	0.62
1:L:511:ASN:OD1	1:L:513:THR:HG22	2.00	0.62
1:D:288:ASN:HB3	1:D:291:THR:HG22	1.82	0.62
1:E:283:PHE:CE1	1:H:305:ASP:OD1	2.52	0.62
1:J:232:CYS:HB2	1:J:367:THR:HG22	1.81	0.62
1:C:291:THR:HG23	1:C:293:TYR:H	1.63	0.62
1:H:497:MET:HG3	1:H:568:LEU:CG	2.29	0.62
1:C:514:ILE:N	1:C:514:ILE:HD12	2.15	0.62
1:D:369:HIS:HD2	1:D:377:GLY:H	1.48	0.62
1:C:288:ASN:HB3	1:C:291:THR:HG22	1.82	0.61
1:D:526:MET:HG3	1:D:539:MET:HE1	1.83	0.61
1:F:538:THR:HG22	1:F:542:PHE:CE1	2.35	0.61
1:D:228:GLN:N	1:D:229:PRO:CD	2.64	0.61
1:I:578:ARG:O	1:I:581:VAL:HG22	2.01	0.61
1:J:526:MET:HG3	1:J:539:MET:HE1	1.83	0.61
1:C:228:GLN:N	1:C:229:PRO:CD	2.64	0.61
1:L:466:ARG:HH11	1:L:466:ARG:HG3	1.66	0.61
1:A:523:THR:N	1:A:524:PRO:CD	2.64	0.60
1:J:124:GLU:OE2	1:J:127:ARG:HD3	2.01	0.60
1:I:589:GLU:HG2	1:J:127:ARG:HG3	1.82	0.60
1:C:433:ALA:O	1:C:437:VAL:HG23	2.02	0.60
1:H:288:ASN:CG	1:H:291:THR:HG22	2.26	0.60
1:F:127:ARG:HD3	2:F:608:HOH:O	2.00	0.60
1:B:228:GLN:N	1:B:229:PRO:CD	2.65	0.60
1:K:288:ASN:HB3	1:K:291:THR:HG22	1.82	0.60
1:K:526:MET:HG3	1:K:539:MET:HE1	1.82	0.60
1:K:476:LEU:HD12	1:K:521:ILE:O	2.01	0.60
1:K:164:ALA:HB2	1:K:476:LEU:HD13	1.83	0.59
1:D:523:THR:N	1:D:524:PRO:HD3	2.17	0.59
1:G:523:THR:N	1:G:524:PRO:HD3	2.17	0.59
1:K:463:ARG:NH1	1:K:541:ASP:OD1	2.35	0.59
1:K:291:THR:HG23	1:K:293:TYR:H	1.68	0.59
1:K:454:GLN:HA	1:K:454:GLN:OE1	2.03	0.59
1:K:522:GLY:C	1:K:524:PRO:HD2	2.28	0.59
1:G:191:GLY:N	1:G:202:ASP:OD2	2.36	0.59
1:K:589:GLU:OE2	1:L:127:ARG:HG2	2.03	0.59
1:B:490:VAL:HG11	1:B:554:GLN:NE2	2.18	0.59
1:K:169:VAL:HB	1:K:173:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:523:THR:N	1:K:524:PRO:HD2	2.17	0.58
1:K:476:LEU:HD11	1:K:520:ARG:CG	2.33	0.58
1:B:570:THR:O	1:B:570:THR:HG22	2.04	0.58
1:A:502:LEU:HD21	1:A:521:ILE:HG12	1.84	0.58
1:C:288:ASN:CB	1:C:291:THR:HG22	2.33	0.58
1:G:283:PHE:CB	1:G:306:TYR:CE2	2.86	0.58
1:H:452:ASN:HD22	1:H:527:THR:CG2	2.01	0.58
1:G:499:HIS:NE2	1:G:578:ARG:HD2	2.18	0.58
1:I:523:THR:N	1:I:524:PRO:HD3	2.18	0.58
1:J:502:LEU:CD2	1:J:521:ILE:HG12	2.33	0.58
1:K:319:PRO:HG3	1:K:478:LEU:HD13	1.85	0.58
1:L:162:LEU:HB2	1:L:502:LEU:CD2	2.33	0.58
1:L:228:GLN:N	1:L:229:PRO:CD	2.66	0.58
1:F:305:ASP:HB3	1:G:283:PHE:CZ	2.35	0.58
1:G:589:GLU:HG2	1:H:127:ARG:CG	2.29	0.58
1:G:523:THR:N	1:G:524:PRO:CD	2.66	0.58
1:H:449:MET:HA	1:H:527:THR:HG21	1.85	0.58
1:L:526:MET:HG3	1:L:539:MET:HE1	1.84	0.58
1:G:228:GLN:N	1:G:229:PRO:CD	2.67	0.58
1:I:568:LEU:C	1:I:568:LEU:HD23	2.29	0.58
1:J:218:LEU:HD11	1:J:358:PHE:CE2	2.39	0.58
1:D:124:GLU:OE1	1:D:124:GLU:HA	2.04	0.57
1:B:185:TYR:HE1	1:B:187:GLU:CG	2.17	0.57
1:L:245:LEU:O	1:L:248:GLU:HG3	2.03	0.57
1:L:523:THR:N	1:L:524:PRO:CD	2.68	0.57
1:H:288:ASN:CB	1:H:291:THR:HG22	2.34	0.57
1:H:288:ASN:HB3	1:H:291:THR:CG2	2.34	0.57
1:E:227:VAL:HG23	1:E:427:ILE:CD1	2.35	0.57
1:C:497:MET:HG3	1:C:568:LEU:HD11	1.87	0.57
1:F:562:LYS:HA	1:F:565:VAL:HG22	1.87	0.57
1:L:523:THR:N	1:L:524:PRO:HD3	2.20	0.57
1:C:376:ARG:NH1	1:D:185:TYR:CD1	2.72	0.57
1:G:211:ARG:NH1	1:H:142:ASP:OD2	2.34	0.57
1:K:253:LEU:HD23	1:K:254:ASP:H	1.66	0.57
1:D:523:THR:N	1:D:524:PRO:CD	2.68	0.56
1:E:180[B]:HIS:NE2	1:F:592:ALA:O	2.26	0.56
1:J:306:TYR:HD1	1:K:306:TYR:HE1	1.50	0.56
1:L:463:ARG:HD2	1:L:544:ILE:HG13	1.87	0.56
1:L:466:ARG:HH11	1:L:466:ARG:CG	2.17	0.56
1:E:228:GLN:N	1:E:229:PRO:CD	2.68	0.56
1:F:228:GLN:N	1:F:229:PRO:CD	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:VAL:HG22	1:D:293:TYR:C	2.31	0.56
1:A:369:HIS:CD2	1:A:376:ARG:HA	2.40	0.56
1:B:523:THR:N	1:B:524:PRO:HD3	2.21	0.56
1:A:523:THR:H	1:A:524:PRO:HD3	1.70	0.56
1:E:490:VAL:HG11	1:E:554:GLN:NE2	2.21	0.56
1:K:288:ASN:CG	1:K:291:THR:HG22	2.30	0.56
1:K:369:HIS:O	1:L:185:TYR:OH	2.24	0.56
1:L:560:SER:HB3	1:L:563:GLU:CG	2.34	0.56
1:C:523:THR:N	1:C:524:PRO:HD3	2.21	0.56
1:C:562:LYS:HB2	2:C:628:HOH:O	2.06	0.56
1:K:228:GLN:N	1:K:229:PRO:CD	2.69	0.56
1:A:487:THR:OG1	1:A:490:VAL:HG12	2.06	0.56
1:B:502:LEU:HD13	1:B:519:VAL:HG13	1.88	0.56
1:G:402:THR:HG23	1:G:403:HIS:ND1	2.21	0.56
1:D:283:PHE:CD2	1:D:306:TYR:CD1	2.94	0.56
1:C:149:MET:O	1:D:180[A]:HIS:NE2	2.38	0.56
1:H:557:HIS:CB	1:H:564:PHE:CD1	2.87	0.56
1:I:228:GLN:N	1:I:229:PRO:CD	2.69	0.56
1:D:565:VAL:HA	1:D:568:LEU:HD12	1.88	0.55
1:F:307:ARG:NH2	1:F:334:CYS:HA	2.21	0.55
1:H:523:THR:N	1:H:524:PRO:HD3	2.21	0.55
1:J:251:MET:HE1	1:J:302:LYS:HB3	1.89	0.55
1:J:342:MET:CE	1:J:366:SER:HB2	2.36	0.55
1:E:475:HIS:CE1	1:E:476:LEU:HD23	2.41	0.55
1:J:307:ARG:HH12	1:J:334:CYS:HA	1.72	0.55
1:L:463:ARG:NH1	1:L:541:ASP:OD1	2.38	0.55
1:D:328:ARG:HD2	1:D:360:HIS:O	2.06	0.55
1:C:511:ASN:OD1	1:C:513:THR:HG23	2.07	0.55
1:I:366:SER:OG	1:I:367:THR:N	2.38	0.55
1:C:387:LYS:HZ1	1:C:401:SER:HB3	1.70	0.55
1:I:180[B]:HIS:NE2	1:J:149:MET:O	2.37	0.55
1:J:228:GLN:N	1:J:229:PRO:HD3	2.22	0.55
1:C:497:MET:HG3	1:C:568:LEU:CD1	2.36	0.55
1:I:463:ARG:CD	1:I:544:ILE:CD1	2.85	0.55
1:E:342:MET:HE2	1:E:366:SER:HB2	1.89	0.55
1:G:361:CYS:O	1:G:383:ARG:NH2	2.39	0.55
1:F:249:ARG:CD	1:F:283:PHE:HZ	2.19	0.55
1:L:369:HIS:CD2	1:L:376:ARG:HA	2.41	0.55
1:H:500:ILE:HG22	1:H:502:LEU:HD13	1.88	0.55
1:B:343:ALA:HA	1:B:367:THR:HG22	1.88	0.54
1:L:369:HIS:HD2	1:L:377:GLY:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:N	1:B:524:PRO:CD	2.70	0.54
1:I:523:THR:N	1:I:524:PRO:CD	2.70	0.54
1:L:466:ARG:HG3	1:L:466:ARG:NH1	2.22	0.54
1:H:442:TYR:O	1:H:445:TYR:HB3	2.08	0.54
1:E:592:ALA:O	1:F:180[B]:HIS:NE2	2.40	0.54
1:K:228:GLN:N	1:K:229:PRO:HD3	2.23	0.54
1:E:184:LYS:HG2	1:E:201:ILE:HD13	1.88	0.54
1:G:153:LYS:HE2	1:G:593:SER:HB3	1.89	0.54
1:J:523:THR:N	1:J:524:PRO:HD3	2.22	0.54
1:F:523:THR:N	1:F:524:PRO:CD	2.71	0.54
1:H:557:HIS:HB2	1:H:564:PHE:CE1	2.43	0.54
1:I:502:LEU:HD12	1:I:503:ASN:N	2.23	0.54
1:A:291:THR:HG22	1:A:293:TYR:HD1	1.72	0.54
1:F:127:ARG:CD	2:F:608:HOH:O	2.55	0.54
1:C:502:LEU:HD13	1:C:519:VAL:HG21	1.88	0.54
1:E:195:TYR:HE1	1:F:503:ASN:ND2	2.06	0.54
1:A:228:GLN:N	1:A:229:PRO:CD	2.71	0.54
1:D:288:ASN:CG	1:D:291:THR:HG22	2.32	0.54
1:D:463:ARG:HD2	1:D:544:ILE:HG13	1.90	0.54
1:K:180[B]:HIS:CE1	1:L:592:ALA:O	2.61	0.54
1:C:288:ASN:HB3	1:C:291:THR:CG2	2.38	0.53
1:B:502:LEU:HD13	1:B:519:VAL:CG1	2.38	0.53
1:E:369:HIS:HD2	1:E:377:GLY:H	1.55	0.53
1:J:523:THR:N	1:J:524:PRO:CD	2.71	0.53
1:K:185:TYR:CE2	1:K:187:GLU:HG3	2.43	0.53
1:D:369:HIS:HD2	1:D:376:ARG:HA	1.66	0.53
1:L:158:ARG:HD3	1:L:582:GLU:OE2	2.07	0.53
1:D:287:VAL:HG21	1:D:292:GLY:O	2.08	0.53
1:B:154:GLN:O	1:B:158:ARG:HG3	2.09	0.53
1:D:366:SER:OG	1:D:367:THR:N	2.40	0.53
1:H:228:GLN:N	1:H:229:PRO:CD	2.72	0.53
1:K:322:TRP:HB2	1:K:324:PHE:CZ	2.43	0.53
1:K:523:THR:N	1:K:524:PRO:CD	2.72	0.53
1:I:343:ALA:HA	1:I:367:THR:HG22	1.90	0.53
1:G:190:PRO:HB2	1:G:202:ASP:OD1	2.09	0.53
1:G:131:ARG:NH1	1:H:589:GLU:OE1	2.41	0.53
1:D:566:LYS:O	1:D:570:THR:HG22	2.08	0.53
1:K:498:CYS:O	1:K:581:VAL:HG11	2.09	0.53
1:K:288:ASN:CB	1:K:291:THR:HG22	2.39	0.52
1:D:287:VAL:HG22	1:D:293:TYR:O	2.09	0.52
1:D:369:HIS:HB3	1:D:375:PRO:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:560:SER:O	1:I:564:PHE:HB2	2.10	0.52
1:K:288:ASN:HB3	1:K:291:THR:CG2	2.40	0.52
1:L:162:LEU:HB2	1:L:502:LEU:HD23	1.89	0.52
1:E:523:THR:N	1:E:524:PRO:HD3	2.25	0.52
1:A:154:GLN:O	1:A:158:ARG:HG3	2.09	0.52
1:J:158:ARG:HB3	1:J:582:GLU:HG3	1.92	0.52
1:E:138:ILE:HG22	1:F:175:GLU:OE2	2.09	0.52
1:K:287:VAL:HG21	1:K:292:GLY:O	2.09	0.52
1:D:459:ALA:O	1:D:463:ARG:NH1	2.43	0.52
1:K:496:GLU:HG3	1:L:196:THR:HG23	1.91	0.52
1:F:523:THR:N	1:F:524:PRO:HD3	2.25	0.52
1:A:288:ASN:OD1	1:A:288:ASN:C	2.53	0.52
1:B:184:LYS:HG2	1:B:201:ILE:CD1	2.40	0.52
1:B:185:TYR:CE1	1:B:187:GLU:CG	2.92	0.52
1:D:433:ALA:O	1:D:437:VAL:HG23	2.10	0.52
1:C:369:HIS:CD2	1:C:376:ARG:HA	2.45	0.52
1:D:288:ASN:HB3	1:D:291:THR:CG2	2.40	0.52
1:D:288:ASN:CB	1:D:291:THR:HG22	2.40	0.52
1:K:367:THR:OG1	1:K:369:HIS:CD2	2.63	0.52
1:L:283:PHE:CE2	1:L:302:LYS:HE3	2.45	0.52
1:L:459:ALA:HB1	1:L:463:ARG:HH21	1.75	0.52
1:D:230:TYR:CZ	1:D:419:GLN:HB3	2.44	0.51
1:G:433:ALA:O	1:G:437:VAL:HG23	2.10	0.51
1:H:369:HIS:HD2	1:H:377:GLY:H	1.58	0.51
1:E:154:GLN:O	1:E:158:ARG:HG3	2.10	0.51
1:G:162:LEU:HB2	1:G:502:LEU:HD23	1.92	0.51
1:G:342:MET:HE2	1:G:366:SER:HB2	1.91	0.51
1:H:514:ILE:O	1:H:514:ILE:HG13	2.11	0.51
1:G:592:ALA:O	1:H:180[A]:HIS:NE2	2.43	0.51
1:H:523:THR:N	1:H:524:PRO:CD	2.73	0.51
1:J:482:THR:HG23	1:J:517:GLY:HA3	1.92	0.51
1:K:342:MET:CE	1:K:364:VAL:HG11	2.40	0.51
1:K:497:MET:SD	1:K:568:LEU:HD21	2.50	0.51
1:E:211:ARG:NH1	1:F:142:ASP:OD2	2.37	0.51
1:B:502:LEU:C	1:B:502:LEU:HD12	2.36	0.51
1:C:482:THR:N	1:C:483:PRO:CD	2.74	0.51
1:K:294:ILE:CG2	1:K:296:TYR:CE2	2.93	0.51
1:F:249:ARG:HB3	1:F:283:PHE:CE1	2.45	0.51
1:F:283:PHE:CG	1:F:306:TYR:CD2	2.99	0.51
1:F:514:ILE:HG13	1:F:514:ILE:O	2.10	0.51
1:H:343:ALA:HA	1:H:367:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:433:ALA:O	1:J:437:VAL:HG23	2.11	0.51
1:C:446:ILE:O	1:C:449:MET:HB3	2.11	0.50
1:G:482:THR:HG23	1:G:517:GLY:HA3	1.93	0.50
1:I:283:PHE:CE1	1:L:305:ASP:HB3	2.46	0.50
1:B:366:SER:OG	1:B:367:THR:N	2.40	0.50
1:H:184:LYS:HG2	1:H:201:ILE:CD1	2.41	0.50
1:J:283:PHE:HZ	1:K:305:ASP:HB3	1.75	0.50
1:A:291:THR:HG22	1:A:293:TYR:CD1	2.47	0.50
1:F:468:VAL:CG2	1:F:507:ILE:HD11	2.41	0.50
1:F:525:ALA:O	1:F:528:THR:HB	2.11	0.50
1:I:154:GLN:O	1:I:158:ARG:HG3	2.11	0.50
1:J:459:ALA:HB1	1:J:463:ARG:HH12	1.77	0.50
1:K:442:TYR:O	1:K:445:TYR:HB3	2.11	0.50
1:A:343:ALA:HA	1:A:367:THR:HG22	1.92	0.50
1:D:244:LEU:CD1	1:D:244:LEU:N	2.74	0.50
1:E:127:ARG:HE	1:F:589:GLU:HG2	1.76	0.50
1:E:186:SER:HB2	1:E:424:ASN:HD21	1.77	0.50
1:C:523:THR:N	1:C:524:PRO:CD	2.75	0.49
1:F:287:VAL:CG1	1:F:292:GLY:C	2.85	0.49
1:G:190:PRO:HA	1:G:193:ARG:HE	1.77	0.49
1:B:283:PHE:CZ	1:C:305:ASP:OD2	2.65	0.49
1:G:158:ARG:HB3	1:G:582:GLU:HG3	1.94	0.49
1:K:557:HIS:O	1:K:564:PHE:HD1	1.95	0.49
1:F:557:HIS:HB2	1:F:564:PHE:CE1	2.48	0.49
1:K:476:LEU:HD11	1:K:520:ARG:HG3	1.95	0.49
1:L:230:TYR:CE2	1:L:419:GLN:HB3	2.48	0.49
1:A:305:ASP:OD2	1:D:283:PHE:CZ	2.66	0.49
1:E:480:ASP:HB2	1:E:507:ILE:HD11	1.94	0.49
1:F:120:SER:HA	1:F:123:LEU:HB3	1.93	0.49
1:F:158:ARG:HB3	1:F:582:GLU:HG3	1.95	0.49
1:H:367:THR:OG1	1:H:369:HIS:NE2	2.46	0.49
1:J:482:THR:N	1:J:483:PRO:CD	2.75	0.49
1:D:206:ASN:O	1:D:210:GLU:HG3	2.11	0.49
1:E:127:ARG:HG3	1:F:589:GLU:HG2	1.95	0.49
1:F:273:ILE:HG13	1:F:274:SER:H	1.76	0.49
1:G:123:LEU:C	1:G:123:LEU:HD23	2.37	0.49
1:I:574:ILE:HG13	1:I:575:ALA:N	2.26	0.49
1:B:228:GLN:N	1:B:229:PRO:HD3	2.28	0.49
1:D:158:ARG:HB3	1:D:582:GLU:HG3	1.94	0.49
1:D:185:TYR:CE2	1:D:187:GLU:HG3	2.48	0.49
1:F:251:MET:HE1	1:F:302:LYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:207:LEU:O	1:I:211:ARG:HG3	2.13	0.49
1:K:449:MET:CE	1:K:524:PRO:HB3	2.41	0.49
1:C:123:LEU:C	1:C:123:LEU:HD23	2.37	0.49
1:E:228:GLN:N	1:E:229:PRO:HD3	2.28	0.49
1:A:291:THR:CG2	1:A:293:TYR:HB2	2.43	0.48
1:B:514:ILE:HG13	1:B:514:ILE:O	2.13	0.48
1:F:446:ILE:O	1:F:449:MET:HB3	2.13	0.48
1:B:413:ALA:O	1:B:417:SER:HB2	2.13	0.48
1:H:255:SER:O	1:H:256:PRO:C	2.57	0.48
1:H:366:SER:OG	1:H:367:THR:N	2.46	0.48
1:J:288:ASN:ND2	1:J:291:THR:HG23	2.28	0.48
1:C:245:LEU:O	1:C:248:GLU:HG3	2.13	0.48
1:I:463:ARG:HD3	1:I:544:ILE:HD12	1.94	0.48
1:K:343:ALA:HA	1:K:367:THR:HG22	1.96	0.48
1:K:287:VAL:HG22	1:K:293:TYR:C	2.38	0.48
1:A:291:THR:HG22	1:A:293:TYR:H	1.79	0.48
1:D:243:LEU:C	1:D:244:LEU:HD12	2.38	0.48
1:F:449:MET:HE3	1:F:524:PRO:HG3	1.92	0.48
1:I:254:ASP:HB2	1:I:284:PRO:HB2	1.95	0.48
1:J:342:MET:O	1:J:342:MET:HG2	2.13	0.48
1:D:463:ARG:NH2	1:D:541:ASP:OD1	2.42	0.48
1:F:538:THR:HG22	1:F:542:PHE:HE1	1.77	0.48
1:G:190:PRO:CB	1:G:202:ASP:OD1	2.62	0.48
1:L:253:LEU:HD23	1:L:316:SER:HB2	1.94	0.48
1:A:560:SER:OG	1:A:563:GLU:CB	2.61	0.48
1:C:228:GLN:N	1:C:229:PRO:HD3	2.29	0.48
1:H:189:MET:HG3	1:H:190:PRO:HD2	1.96	0.48
1:H:288:ASN:ND2	1:H:291:THR:HG22	2.29	0.48
1:I:463:ARG:HD2	1:I:544:ILE:CD1	2.41	0.48
1:E:180[B]:HIS:CE1	1:F:153:LYS:HE3	2.49	0.48
1:J:369:HIS:HD2	1:J:377:GLY:H	1.61	0.48
1:K:369:HIS:CG	1:K:376:ARG:HG2	2.49	0.48
1:F:290:GLN:OE1	1:F:290:GLN:N	2.47	0.47
1:G:476:LEU:O	1:G:477:LEU:HD12	2.14	0.47
1:G:482:THR:N	1:G:483:PRO:CD	2.77	0.47
1:C:211:ARG:NH1	1:D:142:ASP:OD2	2.38	0.47
1:C:291:THR:HG23	1:C:293:TYR:N	2.29	0.47
1:C:490:VAL:HG11	1:C:554:GLN:HE21	1.78	0.47
1:G:162:LEU:HB2	1:G:502:LEU:CD2	2.44	0.47
1:J:369:HIS:CD2	1:J:376:ARG:HA	2.48	0.47
1:L:433:ALA:O	1:L:437:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:LYS:HZ1	1:C:401:SER:CB	2.28	0.47
1:D:168:PHE:CE2	1:D:590:MET:HE1	2.49	0.47
1:F:283:PHE:CG	1:F:306:TYR:HD2	2.32	0.47
1:J:171:ARG:HH11	1:J:594:LEU:HD23	1.79	0.47
1:J:207:LEU:O	1:J:211:ARG:HG3	2.15	0.47
1:K:571:ASN:O	1:K:574:ILE:HG13	2.15	0.47
1:C:561:HIS:O	1:C:565:VAL:HG23	2.15	0.47
1:G:342:MET:CE	1:G:366:SER:HB2	2.45	0.47
1:J:312:ILE:HA	1:J:339:MET:O	2.14	0.47
1:K:559:LYS:HD2	1:K:559:LYS:O	2.14	0.47
1:L:328:ARG:HA	1:L:328:ARG:HD3	1.58	0.47
1:D:228:GLN:N	1:D:229:PRO:HD3	2.29	0.47
1:E:123:LEU:C	1:E:123:LEU:HD23	2.39	0.47
1:G:283:PHE:HB2	1:G:306:TYR:HE2	1.75	0.47
1:I:185:TYR:CE2	1:I:187:GLU:HG3	2.50	0.47
1:K:254:ASP:HB2	1:K:284:PRO:HB2	1.97	0.47
1:B:463:ARG:O	1:B:464:LYS:CG	2.62	0.47
1:G:490:VAL:HG11	1:G:554:GLN:NE2	2.30	0.47
1:H:446:ILE:O	1:H:449:MET:HB3	2.15	0.47
1:L:551:SER:O	1:L:554:GLN:HG3	2.15	0.47
1:E:482:THR:N	1:E:483:PRO:CD	2.78	0.47
1:G:312:ILE:HD13	1:G:339:MET:HB3	1.97	0.47
1:G:342:MET:HG2	1:G:342:MET:O	2.15	0.47
1:A:482:THR:N	1:A:483:PRO:CD	2.77	0.47
1:J:249:ARG:HB3	1:J:306:TYR:CE2	2.50	0.47
1:H:571:ASN:O	1:H:574:ILE:HG13	2.15	0.47
1:I:497:MET:SD	1:I:568:LEU:HD21	2.55	0.47
1:L:482:THR:N	1:L:483:PRO:CD	2.78	0.47
1:A:245:LEU:O	1:A:248:GLU:HG3	2.15	0.47
1:D:245:LEU:O	1:D:248:GLU:HG3	2.15	0.47
1:G:562:LYS:O	1:G:565:VAL:HG12	2.15	0.47
1:L:153:LYS:O	1:L:157:VAL:HG13	2.15	0.47
1:D:243:LEU:HB2	1:D:244:LEU:HD13	1.96	0.46
1:F:288:ASN:OD1	1:F:288:ASN:C	2.59	0.46
1:H:557:HIS:CB	1:H:564:PHE:CE1	2.99	0.46
1:J:306:TYR:CD1	1:K:306:TYR:HE1	2.30	0.46
1:L:325:ALA:O	1:L:328:ARG:HB3	2.15	0.46
1:G:153:LYS:O	1:G:157:VAL:HG12	2.16	0.46
1:C:158:ARG:HB3	1:C:582:GLU:HG3	1.98	0.46
1:E:245:LEU:O	1:E:248:GLU:HG3	2.15	0.46
1:E:288:ASN:ND2	1:E:291:THR:HG23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:ASN:ND2	1:G:291:THR:HG23	2.30	0.46
1:L:228:GLN:N	1:L:229:PRO:HD3	2.29	0.46
1:D:523:THR:H	1:D:524:PRO:HD3	1.81	0.46
1:L:345:ILE:O	1:L:346:SER:C	2.56	0.46
1:E:195:TYR:CE1	1:F:503:ASN:ND2	2.84	0.46
1:E:343:ALA:HA	1:E:367:THR:HG22	1.96	0.46
1:I:532:ILE:HD11	1:I:534:SER:OG	2.16	0.46
1:L:163:ILE:HB	1:L:166:GLU:HG3	1.97	0.46
1:I:198:ASN:HB2	2:I:616:HOH:O	2.15	0.46
1:K:163:ILE:HB	1:K:166:GLU:HG3	1.97	0.46
1:A:291:THR:HG22	1:A:293:TYR:HB2	1.97	0.46
1:B:288:ASN:ND2	1:B:291:THR:HG23	2.31	0.46
1:E:288:ASN:C	1:E:288:ASN:OD1	2.58	0.46
1:G:251:MET:CG	1:G:283:PHE:O	2.55	0.46
1:G:523:THR:H	1:G:524:PRO:HD3	1.81	0.46
1:I:502:LEU:HD12	1:I:502:LEU:C	2.40	0.46
1:A:184:LYS:HG2	1:A:201:ILE:HD13	1.98	0.46
1:A:210:GLU:HB3	2:A:609:HOH:O	2.17	0.46
1:B:185:TYR:CD1	1:B:187:GLU:HG3	2.51	0.46
1:H:482:THR:N	1:H:483:PRO:CD	2.79	0.46
1:K:317:SER:CB	1:K:476:LEU:HD21	2.42	0.46
1:L:369:HIS:CD2	1:L:377:GLY:H	2.34	0.46
1:E:295:ASP:OD1	1:E:295:ASP:C	2.56	0.45
1:K:369:HIS:CD2	1:K:376:ARG:HA	2.51	0.45
1:A:369:HIS:HD2	1:A:377:GLY:H	1.64	0.45
1:C:207:LEU:O	1:C:211:ARG:HG3	2.15	0.45
1:E:523:THR:N	1:E:524:PRO:CD	2.78	0.45
1:H:500:ILE:HG22	1:H:502:LEU:CD1	2.45	0.45
1:E:342:MET:CE	1:E:366:SER:HB2	2.47	0.45
1:F:123:LEU:C	1:F:123:LEU:HD13	2.41	0.45
1:G:127:ARG:HG3	1:H:589:GLU:HG2	1.97	0.45
1:I:133:TRP:CZ2	1:J:170:CYS:HB3	2.51	0.45
1:J:157:VAL:HG22	1:J:590:MET:HG2	1.99	0.45
1:J:468:VAL:HB	1:J:478:LEU:HB2	1.98	0.45
1:L:442:TYR:O	1:L:445:TYR:HB3	2.16	0.45
1:B:369:HIS:HD2	1:B:377:GLY:H	1.63	0.45
1:F:123:LEU:CD1	2:F:608:HOH:O	2.59	0.45
1:F:535:ASP:O	1:F:539:MET:HG3	2.16	0.45
1:H:185:TYR:CE2	1:H:187:GLU:HG3	2.51	0.45
1:K:160:ILE:HG23	1:K:539:MET:CE	2.47	0.45
1:K:290:GLN:NE2	1:K:290:GLN:HA	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:560:SER:OG	1:K:563:GLU:CB	2.65	0.45
1:L:413:ALA:O	1:L:417:SER:HB2	2.17	0.45
1:E:594:LEU:O	1:E:594:LEU:HD12	2.17	0.45
1:K:291:THR:HG23	1:K:293:TYR:N	2.30	0.45
1:E:283:PHE:CZ	1:H:305:ASP:OD1	2.70	0.45
1:F:567:SER:HB2	2:F:611:HOH:O	2.16	0.45
1:K:514:ILE:O	1:K:514:ILE:HG13	2.17	0.45
1:L:369:HIS:HB3	1:L:375:PRO:O	2.17	0.45
1:G:245:LEU:O	1:G:246:PRO:C	2.60	0.45
1:G:255:SER:O	1:G:256:PRO:C	2.60	0.45
1:L:232:CYS:HB2	1:L:367:THR:CG2	2.40	0.45
1:A:297:ASP:OD1	1:A:326:ARG:NH2	2.50	0.45
1:A:560:SER:OG	1:A:563:GLU:HB3	2.17	0.45
1:B:545:LYS:HD2	1:B:580:ARG:HH12	1.82	0.45
1:D:545:LYS:HA	1:D:548:GLN:HG2	1.99	0.45
1:E:160:ILE:HG23	1:E:539:MET:CE	2.47	0.45
1:I:482:THR:N	1:I:483:PRO:CD	2.80	0.45
1:J:463:ARG:O	1:J:464:LYS:HG2	2.17	0.45
1:J:502:LEU:HD21	1:J:521:ILE:HG12	1.99	0.45
1:A:467:LEU:HD13	1:A:477:LEU:HD22	1.99	0.44
1:C:468:VAL:HB	1:C:478:LEU:HB2	1.99	0.44
1:D:123:LEU:HD23	1:D:123:LEU:C	2.42	0.44
1:D:291:THR:HG23	1:D:293:TYR:N	2.29	0.44
1:K:476:LEU:HD11	1:K:520:ARG:HG2	1.98	0.44
1:K:501:THR:HG22	1:L:196:THR:CG2	2.45	0.44
1:A:283:PHE:CZ	1:D:305:ASP:HB3	2.53	0.44
1:C:514:ILE:HD12	1:C:514:ILE:H	1.80	0.44
1:L:160:ILE:HG23	1:L:539:MET:CE	2.48	0.44
1:A:413:ALA:O	1:A:417:SER:HB2	2.18	0.44
1:B:482:THR:N	1:B:483:PRO:CD	2.80	0.44
1:K:185:TYR:CD1	1:L:376:ARG:NH1	2.85	0.44
1:B:256:PRO:HG3	1:B:508:PHE:CE2	2.52	0.44
1:I:158:ARG:HB3	1:I:582:GLU:HG3	2.00	0.44
1:K:294:ILE:CG2	1:K:296:TYR:CZ	3.01	0.44
1:K:560:SER:OG	1:K:563:GLU:HB2	2.18	0.44
1:D:342:MET:HE3	1:D:346:SER:HB3	1.99	0.44
1:D:482:THR:HG23	1:D:517:GLY:HA3	2.00	0.44
1:F:249:ARG:HB3	1:F:283:PHE:HE1	1.82	0.44
1:K:532:ILE:HG12	1:K:533:GLU:OE1	2.18	0.44
1:B:367:THR:OG1	1:B:369:HIS:NE2	2.50	0.44
1:C:343:ALA:HA	1:C:367:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:GLU:OE2	1:D:151:LYS:HE3	2.18	0.44
1:D:369:HIS:HB3	1:D:375:PRO:C	2.42	0.44
1:F:287:VAL:HG11	1:F:292:GLY:O	2.17	0.44
1:H:413:ALA:O	1:H:417:SER:HB2	2.16	0.44
1:I:345:ILE:O	1:I:346:SER:C	2.61	0.44
1:J:254:ASP:HB2	1:J:284:PRO:HB2	1.98	0.44
1:K:496:GLU:CD	1:L:196:THR:HG23	2.42	0.44
1:K:523:THR:O	1:K:524:PRO:C	2.61	0.44
1:B:463:ARG:O	1:B:464:LYS:HG2	2.17	0.44
1:E:413:ALA:O	1:E:417:SER:HB2	2.17	0.44
1:G:120:SER:O	1:G:124:GLU:HB3	2.18	0.44
1:I:184:LYS:HG2	1:I:201:ILE:CD1	2.48	0.44
1:C:497:MET:HG3	1:C:568:LEU:HG	1.99	0.44
1:F:553:LEU:HG	1:F:564:PHE:CE2	2.53	0.44
1:K:124:GLU:OE1	1:K:124:GLU:HA	2.18	0.44
1:K:324:PHE:CE2	1:K:355:SER:HB2	2.52	0.44
1:F:537:GLU:O	1:F:540:ALA:HB3	2.18	0.43
1:G:288:ASN:C	1:G:288:ASN:OD1	2.61	0.43
1:G:371:GLY:O	1:G:442:TYR:OH	2.33	0.43
1:G:446:ILE:O	1:G:449:MET:HB3	2.18	0.43
1:H:328:ARG:O	1:H:329:GLN:C	2.61	0.43
1:K:127:ARG:NH2	2:K:603:HOH:O	2.50	0.43
1:A:163:ILE:HB	1:A:166:GLU:HG3	1.99	0.43
1:E:433:ALA:O	1:E:437:VAL:HG23	2.18	0.43
1:H:291:THR:HG23	1:H:293:TYR:N	2.33	0.43
1:H:525:ALA:O	1:H:528:THR:HB	2.18	0.43
1:J:463:ARG:O	1:J:464:LYS:CG	2.66	0.43
1:A:562:LYS:O	1:A:566:LYS:HG3	2.18	0.43
1:B:369:HIS:HB3	1:B:375:PRO:O	2.19	0.43
1:C:366:SER:OG	1:C:367:THR:N	2.52	0.43
1:G:228:GLN:N	1:G:229:PRO:HD3	2.32	0.43
1:F:147:GLU:HG2	1:F:151:LYS:HE3	2.00	0.43
1:F:449:MET:HE3	1:F:524:PRO:CB	2.48	0.43
1:G:226:ASN:HA	2:G:603:HOH:O	2.18	0.43
1:H:556:GLU:HG2	1:H:557:HIS:HD1	1.82	0.43
1:J:160:ILE:HG23	1:J:539:MET:CE	2.48	0.43
1:J:476:LEU:O	1:J:477:LEU:HD12	2.19	0.43
1:K:342:MET:O	1:K:342:MET:HG2	2.17	0.43
1:K:482:THR:N	1:K:483:PRO:CD	2.81	0.43
1:K:502:LEU:HD12	1:K:502:LEU:C	2.43	0.43
1:K:590:MET:O	1:K:591:PRO:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ALA:O	1:D:417:SER:HB2	2.18	0.43
1:D:564:PHE:O	1:D:568:LEU:HG	2.17	0.43
1:E:163:ILE:HB	1:E:166:GLU:HG3	1.99	0.43
1:G:133:TRP:CZ2	1:H:170:CYS:HB3	2.54	0.43
1:I:228:GLN:N	1:I:229:PRO:HD3	2.34	0.43
1:J:306:TYR:HD1	1:K:306:TYR:CE1	2.35	0.43
1:J:342:MET:HE2	1:J:342:MET:HB3	1.88	0.43
1:K:476:LEU:HD12	1:K:477:LEU:H	1.82	0.43
1:A:307:ARG:NE	2:A:601:HOH:O	2.42	0.43
1:D:342:MET:HE3	1:D:346:SER:CB	2.49	0.43
1:D:514:ILE:HD12	1:D:514:ILE:N	2.33	0.43
1:I:367:THR:OG1	1:I:369:HIS:CD2	2.72	0.43
1:K:556:GLU:HG3	1:K:557:HIS:CD2	2.54	0.43
1:A:553:LEU:HD23	1:A:568:LEU:HD23	2.00	0.43
1:D:482:THR:N	1:D:483:PRO:CD	2.82	0.43
1:E:366:SER:OG	1:E:367:THR:N	2.52	0.43
1:I:413:ALA:O	1:I:417:SER:HB2	2.18	0.43
1:J:342:MET:HE3	1:J:366:SER:CB	2.45	0.43
1:D:507:ILE:HG23	1:D:515:SER:OG	2.19	0.43
1:E:142:ASP:OD2	1:F:211:ARG:NH1	2.43	0.43
1:E:287:VAL:CG1	1:E:292:GLY:C	2.91	0.43
1:F:326:ARG:O	1:F:330:ILE:HG13	2.18	0.43
1:G:572:LYS:HG3	1:G:573:ASP:N	2.33	0.43
1:J:466:ARG:HG3	2:J:621:HOH:O	2.17	0.43
1:D:283:PHE:HB2	1:D:306:TYR:CE1	2.54	0.43
1:E:184:LYS:O	1:F:376:ARG:NH1	2.52	0.43
1:F:228:GLN:N	1:F:229:PRO:HD3	2.34	0.43
1:A:207:LEU:O	1:A:211:ARG:HG3	2.18	0.43
1:A:228:GLN:N	1:A:229:PRO:HD3	2.33	0.43
1:B:348:LEU:HD11	1:B:474:ASN:HB2	2.00	0.43
1:C:367:THR:OG1	1:C:369:HIS:NE2	2.52	0.43
1:F:153:LYS:O	1:F:157:VAL:HG12	2.19	0.43
1:A:306:TYR:HA	1:D:283:PHE:CE1	2.54	0.42
1:B:369:HIS:CD2	1:B:377:GLY:H	2.37	0.42
1:F:482:THR:N	1:F:483:PRO:CD	2.82	0.42
1:H:228:GLN:N	1:H:229:PRO:HD3	2.34	0.42
1:K:185:TYR:CE2	1:K:187:GLU:CG	3.02	0.42
1:C:367:THR:OG1	1:C:369:HIS:CD2	2.72	0.42
1:D:160:ILE:HG23	1:D:539:MET:CE	2.49	0.42
1:D:345:ILE:O	1:D:346:SER:C	2.63	0.42
1:K:317:SER:CB	1:K:476:LEU:CD2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:HIS:HD2	1:C:377:GLY:H	1.67	0.42
1:D:423:HIS:HB3	1:D:426:HIS:CD2	2.54	0.42
1:B:123:LEU:HD23	1:B:123:LEU:C	2.44	0.42
1:C:560:SER:HB3	2:C:628:HOH:O	2.19	0.42
1:D:160:ILE:HG23	1:D:539:MET:HE3	2.01	0.42
1:G:576:GLU:O	1:G:580:ARG:HG3	2.20	0.42
1:H:442:TYR:OH	1:H:446:ILE:HD11	2.20	0.42
1:I:170:CYS:HB3	1:J:133:TRP:CZ2	2.54	0.42
1:J:184:LYS:O	1:J:424:ASN:ND2	2.52	0.42
1:L:131:ARG:NH2	1:L:135:ASP:OD2	2.53	0.42
1:E:367:THR:OG1	1:E:369:HIS:NE2	2.53	0.42
1:G:415:PHE:CG	1:G:416:PRO:HA	2.54	0.42
1:I:369:HIS:CE1	1:I:376:ARG:NH2	2.88	0.42
1:I:482:THR:HG23	1:I:517:GLY:HA3	2.00	0.42
1:K:578:ARG:C	1:K:581:VAL:HG12	2.43	0.42
1:L:475:HIS:CE1	1:L:476:LEU:HD23	2.54	0.42
1:G:238:ALA:HA	1:G:418:LEU:CD1	2.50	0.42
1:G:490:VAL:HG11	1:G:554:GLN:HE22	1.85	0.42
1:I:562:LYS:HD3	1:I:562:LYS:HA	1.70	0.42
1:J:294:ILE:CD1	1:J:322:TRP:CH2	3.02	0.42
1:E:153:LYS:O	1:E:157:VAL:HG12	2.20	0.42
1:B:254:ASP:HB2	1:B:284:PRO:HB2	2.02	0.42
1:D:140:LEU:HD11	1:G:555:ARG:CD	2.50	0.42
1:G:343:ALA:HA	1:G:367:THR:HG22	2.01	0.42
1:K:482:THR:HG23	1:K:517:GLY:HA3	2.01	0.42
1:C:376:ARG:NH1	1:C:376:ARG:HG2	2.35	0.42
1:D:140:LEU:HD11	1:G:555:ARG:HD3	2.02	0.42
1:D:343:ALA:HA	1:D:367:THR:HG22	2.02	0.42
1:H:497:MET:O	1:H:578:ARG:HD3	2.19	0.42
1:H:556:GLU:HG2	1:H:557:HIS:ND1	2.35	0.42
1:I:123:LEU:HD23	1:I:123:LEU:C	2.43	0.42
1:L:255:SER:O	1:L:256:PRO:C	2.62	0.42
1:A:367:THR:OG1	1:A:369:HIS:NE2	2.52	0.42
1:F:160:ILE:HG23	1:F:539:MET:HE3	2.01	0.42
1:I:526:MET:HG3	1:I:539:MET:HE1	2.02	0.42
1:C:170:CYS:HB3	1:D:133:TRP:CZ2	2.55	0.41
1:C:206:ASN:O	1:C:210:GLU:HG3	2.20	0.41
1:E:167:ASN:CG	1:E:373:ARG:HG2	2.44	0.41
1:H:342:MET:CE	1:H:366:SER:HB2	2.50	0.41
1:J:209:ILE:HG23	1:J:225:VAL:CG1	2.49	0.41
1:A:433:ALA:O	1:A:437:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:VAL:HB	1:A:478:LEU:HB2	2.02	0.41
1:C:209:ILE:HG23	1:C:225:VAL:CG1	2.50	0.41
1:G:154:GLN:O	1:G:155:ARG:C	2.63	0.41
1:G:221:ASP:OD1	1:G:222:LYS:HG3	2.19	0.41
1:I:255:SER:HA	1:I:256:PRO:HD2	1.96	0.41
1:K:170:CYS:O	1:K:173:VAL:HG22	2.20	0.41
1:I:590:MET:O	1:I:591:PRO:C	2.60	0.41
1:K:433:ALA:O	1:K:437:VAL:HG23	2.21	0.41
1:B:158:ARG:HB3	1:B:582:GLU:HG3	2.01	0.41
1:C:452:ASN:HB3	1:C:536:PHE:CE2	2.55	0.41
1:D:163:ILE:HB	1:D:166:GLU:HG3	2.03	0.41
1:E:468:VAL:HB	1:E:478:LEU:HB2	2.02	0.41
1:F:366:SER:OG	1:F:367:THR:N	2.53	0.41
1:K:230:TYR:CZ	1:K:419:GLN:HB3	2.55	0.41
1:B:564:PHE:O	1:B:567:SER:OG	2.27	0.41
1:C:387:LYS:NZ	1:C:401:SER:CB	2.76	0.41
1:H:291:THR:HG23	1:H:293:TYR:H	1.84	0.41
1:A:170:CYS:HB3	1:B:133:TRP:CZ2	2.56	0.41
1:D:185:TYR:CE2	1:D:187:GLU:CG	3.03	0.41
1:I:463:ARG:CD	1:I:544:ILE:HD12	2.50	0.41
1:J:160:ILE:HG23	1:J:539:MET:HE3	2.02	0.41
1:A:160:ILE:HG23	1:A:539:MET:HE3	2.00	0.41
1:A:230:TYR:CE2	1:A:419:GLN:HB3	2.55	0.41
1:A:554:GLN:O	1:A:558:GLY:HA3	2.21	0.41
1:C:511:ASN:OD1	1:C:512:GLY:N	2.54	0.41
1:C:592:ALA:O	1:D:180[B]:HIS:CE1	2.73	0.41
1:F:287:VAL:HG13	1:F:293:TYR:C	2.46	0.41
1:G:413:ALA:O	1:G:417:SER:HB2	2.21	0.41
1:I:369:HIS:CD2	1:I:376:ARG:HA	2.56	0.41
1:G:342:MET:O	1:G:343:ALA:C	2.64	0.41
1:J:283:PHE:CZ	1:K:305:ASP:HB3	2.55	0.41
1:J:342:MET:HE2	1:J:364:VAL:HG12	2.02	0.41
1:K:581:VAL:HG13	1:K:582:GLU:N	2.35	0.41
1:L:567:SER:O	1:L:571:ASN:HB2	2.20	0.41
1:B:460:LEU:O	1:B:465:CYS:HB2	2.21	0.41
1:D:348:LEU:HD11	1:D:474:ASN:HB2	2.02	0.41
1:E:342:MET:O	1:E:342:MET:HG2	2.21	0.41
1:E:497:MET:HE2	1:E:497:MET:CA	2.45	0.41
1:F:249:ARG:CG	1:F:283:PHE:HZ	2.34	0.41
1:G:416:PRO:HG2	1:H:273:ILE:HG23	2.03	0.41
1:J:184:LYS:HG2	1:J:201:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:294:ILE:HG21	1:K:296:TYR:CZ	2.56	0.41
1:K:459:ALA:O	1:K:462:ARG:HG2	2.21	0.41
1:K:463:ARG:HD2	1:K:544:ILE:HD11	2.03	0.41
1:B:384:ARG:HD3	1:B:407:GLU:OE2	2.21	0.41
1:C:589:GLU:HB3	1:D:130:VAL:HG11	2.02	0.41
1:G:589:GLU:HG3	1:H:127:ARG:O	2.21	0.41
1:H:482:THR:HG23	1:H:517:GLY:HA3	2.03	0.41
1:I:589:GLU:HG2	1:J:127:ARG:CG	2.51	0.41
1:C:185:TYR:CE2	1:C:187:GLU:HG3	2.56	0.40
1:D:570:THR:HG23	1:D:570:THR:O	2.20	0.40
1:I:502:LEU:HD13	1:I:519:VAL:HB	2.02	0.40
1:J:230:TYR:CE2	1:J:419:GLN:HB3	2.56	0.40
1:L:288:ASN:ND2	1:L:291:THR:HG23	2.36	0.40
1:B:463:ARG:HD3	1:B:544:ILE:HG13	2.03	0.40
1:E:158:ARG:HB3	1:E:582:GLU:HG3	2.03	0.40
1:I:302:LYS:NZ	1:L:305:ASP:OD2	2.51	0.40
1:J:213:LEU:O	1:J:214:THR:C	2.65	0.40
1:A:537:GLU:O	1:A:540:ALA:HB3	2.21	0.40
1:B:294:ILE:HG13	1:B:318:TYR:CZ	2.56	0.40
1:B:490:VAL:HG11	1:B:554:GLN:HE22	1.86	0.40
1:H:342:MET:HE2	1:H:366:SER:HB2	2.04	0.40
1:H:433:ALA:O	1:H:437:VAL:HG23	2.21	0.40
1:H:486:LEU:HD23	1:H:554:GLN:OE1	2.20	0.40
1:B:245:LEU:O	1:B:248:GLU:HG3	2.22	0.40
1:D:254:ASP:HB2	1:D:284:PRO:HB2	2.03	0.40
1:J:154:GLN:O	1:J:158:ARG:HG3	2.22	0.40
1:J:574:ILE:HG13	1:J:575:ALA:N	2.37	0.40
1:K:123:LEU:O	1:K:126:ARG:HG2	2.22	0.40
1:K:376:ARG:HH21	1:L:185:TYR:HE1	1.69	0.40
1:K:413:ALA:O	1:K:417:SER:HB2	2.21	0.40
1:A:254:ASP:HB2	1:A:284:PRO:HB2	2.03	0.40
1:B:356:ASN:OD1	1:B:356:ASN:C	2.62	0.40
1:C:413:ALA:O	1:C:417:SER:HB2	2.21	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	435/479 (91%)	417 (96%)	18 (4%)	0	100	100
1	B	435/479 (91%)	418 (96%)	17 (4%)	0	100	100
1	C	441/479 (92%)	419 (95%)	22 (5%)	0	100	100
1	D	429/479 (90%)	411 (96%)	18 (4%)	0	100	100
1	E	433/479 (90%)	415 (96%)	18 (4%)	0	100	100
1	F	437/479 (91%)	417 (95%)	20 (5%)	0	100	100
1	G	436/479 (91%)	418 (96%)	18 (4%)	0	100	100
1	H	431/479 (90%)	410 (95%)	21 (5%)	0	100	100
1	I	435/479 (91%)	418 (96%)	17 (4%)	0	100	100
1	J	436/479 (91%)	419 (96%)	17 (4%)	0	100	100
1	K	430/479 (90%)	410 (95%)	20 (5%)	0	100	100
1	L	438/479 (91%)	409 (93%)	29 (7%)	0	100	100
All	All	5216/5748 (91%)	4981 (96%)	235 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	366/396 (92%)	363 (99%)	3 (1%)	73	83
1	B	367/396 (93%)	361 (98%)	6 (2%)	55	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	371/396 (94%)	364 (98%)	7 (2%)	50	68
1	D	364/396 (92%)	357 (98%)	7 (2%)	50	68
1	E	368/396 (93%)	358 (97%)	10 (3%)	39	61
1	F	369/396 (93%)	350 (95%)	19 (5%)	21	39
1	G	368/396 (93%)	361 (98%)	7 (2%)	50	68
1	H	365/396 (92%)	356 (98%)	9 (2%)	42	63
1	I	367/396 (93%)	365 (100%)	2 (0%)	81	88
1	J	368/396 (93%)	359 (98%)	9 (2%)	43	63
1	K	363/396 (92%)	351 (97%)	12 (3%)	33	55
1	L	368/396 (93%)	359 (98%)	9 (2%)	43	63
All	All	4404/4752 (93%)	4304 (98%)	100 (2%)	44	65

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	250	ILE
1	A	505	THR
1	B	201	ILE
1	B	250	ILE
1	B	317	SER
1	B	505	THR
1	B	545	LYS
1	B	560	SER
1	C	151	LYS
1	C	250	ILE
1	C	355	SER
1	C	502	LEU
1	C	505	THR
1	C	510	ASP
1	C	514	ILE
1	D	157	VAL
1	D	201	ILE
1	D	286	LYS
1	D	287	VAL
1	D	384	ARG
1	D	463	ARG
1	D	510	ASP

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Mol	Chain	Res	Type
1	E	121	ASN
1	E	127	ARG
1	E	201	ILE
1	E	222	LYS
1	E	384	ARG
1	E	399	ASP
1	E	408	GLU
1	E	493	LYS
1	E	505	THR
1	E	551	SER
1	F	121	ASN
1	F	157	VAL
1	F	163	ILE
1	F	184	LYS
1	F	189	MET
1	F	201	ILE
1	F	283	PHE
1	F	317	SER
1	F	355	SER
1	F	367	THR
1	F	384	ARG
1	F	505	THR
1	F	514	ILE
1	F	521	ILE
1	F	553	LEU
1	F	557	HIS
1	F	564	PHE
1	F	568	LEU
1	F	572	LYS
1	G	121	ASN
1	G	157	VAL
1	G	171	ARG
1	G	189	MET
1	G	312	ILE
1	G	451	LYS
1	G	464	LYS
1	H	189	MET
1	H	199	GLN
1	H	250	ILE
1	H	309	LYS
1	H	384	ARG
1	H	544	ILE

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Mol	Chain	Res	Type
1	H	567	SER
1	H	568	LEU
1	H	586	LEU
1	I	201	ILE
1	I	384	ARG
1	J	201	ILE
1	J	250	ILE
1	J	273	ILE
1	J	328	ARG
1	J	493	LYS
1	J	514	ILE
1	J	534	SER
1	J	568	LEU
1	J	576	GLU
1	K	157	VAL
1	K	287	VAL
1	K	290	GLN
1	K	317	SER
1	K	321	ASP
1	K	345	ILE
1	K	355	SER
1	K	384	ARG
1	K	463	ARG
1	K	500	ILE
1	K	544	ILE
1	K	551	SER
1	L	157	VAL
1	L	187	GLU
1	L	219	GLU
1	L	328	ARG
1	L	384	ARG
1	L	419	GLN
1	L	466	ARG
1	L	580	ARG
1	L	587	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	ASN
1	A	548	GLN
1	A	557	HIS

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Mol	Chain	Res	Type
1	B	290	GLN
1	B	360	HIS
1	C	360	HIS
1	C	369	HIS
1	C	424	ASN
1	C	554	GLN
1	D	360	HIS
1	D	369	HIS
1	D	448	GLN
1	E	198	ASN
1	E	424	ASN
1	E	554	GLN
1	E	587	GLN
1	F	447	GLN
1	F	454	GLN
1	F	475	HIS
1	F	503	ASN
1	G	360	HIS
1	G	369	HIS
1	G	557	HIS
1	H	423	HIS
1	H	424	ASN
1	H	448	GLN
1	H	452	ASN
1	H	454	GLN
1	H	579	ASN
1	I	199	GLN
1	I	360	HIS
1	J	360	HIS
1	J	423	HIS
1	J	424	ASN
1	J	447	GLN
1	J	554	GLN
1	K	136	GLN
1	K	290	GLN
1	K	360	HIS
1	K	423	HIS
1	K	424	ASN
1	K	557	HIS
1	L	360	HIS
1	L	369	HIS
1	L	424	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	443/479 (92%)	-0.17	8 (1%) 67 64	43, 56, 97, 147	0
1	B	443/479 (92%)	0.01	9 (2%) 65 62	39, 70, 125, 174	0
1	C	447/479 (93%)	-0.17	10 (2%) 62 59	42, 56, 124, 183	0
1	D	438/479 (91%)	0.08	7 (1%) 70 68	26, 79, 135, 179	1 (0%)
1	E	442/479 (92%)	0.01	12 (2%) 56 53	40, 64, 122, 195	1 (0%)
1	F	444/479 (92%)	0.21	8 (1%) 67 64	25, 89, 151, 209	1 (0%)
1	G	444/479 (92%)	0.41	16 (3%) 46 44	53, 97, 142, 178	0
1	H	438/479 (91%)	0.54	32 (7%) 21 21	31, 94, 180, 219	1 (0%)
1	I	442/479 (92%)	-0.04	6 (1%) 73 72	25, 64, 143, 193	1 (0%)
1	J	444/479 (92%)	-0.12	3 (0%) 84 84	41, 66, 107, 134	0
1	K	437/479 (91%)	0.41	20 (4%) 37 36	29, 106, 156, 199	1 (0%)
1	L	443/479 (92%)	0.12	11 (2%) 58 55	46, 75, 139, 182	1 (0%)
All	All	5305/5748 (92%)	0.11	142 (2%) 56 53	25, 74, 146, 219	7 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	568	LEU	5.5
1	C	594	LEU	4.8
1	A	594	LEU	4.7
1	E	564	PHE	4.6
1	G	512	GLY	4.2
1	E	594	LEU	4.1
1	J	594	LEU	4.0
1	L	594	LEU	4.0
1	K	122	ALA	3.8
1	H	162	LEU	3.7
1	K	514	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	512	GLY	3.5
1	H	519	VAL	3.5
1	H	442	TYR	3.5
1	G	194	TYR	3.4
1	D	306	TYR	3.4
1	A	516	PRO	3.4
1	F	594	LEU	3.4
1	F	340	CYS	3.3
1	C	123	LEU	3.3
1	K	476	LEU	3.2
1	K	507	ILE	3.1
1	H	565	VAL	3.0
1	B	514	ILE	3.0
1	L	185	TYR	2.9
1	A	509	GLY	2.9
1	I	516	PRO	2.9
1	L	256	PRO	2.9
1	B	512	GLY	2.9
1	J	256	PRO	2.8
1	A	194	TYR	2.8
1	H	569	CYS	2.8
1	E	508	PHE	2.8
1	E	256	PRO	2.8
1	H	160	ILE	2.8
1	F	306	TYR	2.8
1	F	514	ILE	2.8
1	L	123	LEU	2.7
1	E	516	PRO	2.7
1	A	123	LEU	2.7
1	H	479	TRP	2.7
1	A	513	THR	2.7
1	H	542	PHE	2.7
1	D	516	PRO	2.7
1	H	561	HIS	2.6
1	F	314	GLY	2.6
1	H	459	ALA	2.6
1	K	304	LEU	2.6
1	A	256	PRO	2.6
1	D	514	ILE	2.6
1	H	502	LEU	2.6
1	K	123	LEU	2.6
1	H	460	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	565	VAL	2.5
1	E	514	ILE	2.5
1	K	285	TYR	2.5
1	A	512	GLY	2.5
1	F	516	PRO	2.5
1	K	315	GLY	2.5
1	I	565	VAL	2.5
1	H	500	ILE	2.5
1	C	516	PRO	2.5
1	D	256	PRO	2.5
1	K	536	PHE	2.5
1	H	221	ASP	2.4
1	E	194	TYR	2.4
1	G	508	PHE	2.4
1	G	305	ASP	2.4
1	L	221	ASP	2.4
1	B	256	PRO	2.4
1	G	196	THR	2.4
1	K	467	LEU	2.4
1	C	180	HIS	2.4
1	K	340	CYS	2.4
1	C	512	GLY	2.4
1	H	477	LEU	2.4
1	H	505	THR	2.4
1	K	255	SER	2.4
1	H	218	LEU	2.3
1	I	502	LEU	2.3
1	L	513	THR	2.3
1	H	506	ALA	2.3
1	H	521	ILE	2.3
1	C	400	THR	2.3
1	K	322	TRP	2.3
1	I	553	LEU	2.3
1	L	564	PHE	2.3
1	G	400	THR	2.3
1	H	593	SER	2.3
1	E	568	LEU	2.3
1	H	372	LEU	2.3
1	D	283	PHE	2.3
1	B	271	LYS	2.2
1	K	314	GLY	2.2
1	L	508	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	200	TYR	2.2
1	G	516	PRO	2.2
1	B	270	GLY	2.2
1	B	565	VAL	2.2
1	F	479	TRP	2.2
1	D	402	THR	2.2
1	D	503	ASN	2.2
1	K	516	PRO	2.2
1	G	302	LYS	2.2
1	G	485	GLY	2.2
1	C	271	LYS	2.2
1	H	478	LEU	2.2
1	L	371	GLY	2.2
1	C	514	ILE	2.2
1	H	294	ILE	2.2
1	K	402	THR	2.1
1	F	256	PRO	2.1
1	L	194	TYR	2.1
1	H	123	LEU	2.1
1	K	477	LEU	2.1
1	G	188	GLY	2.1
1	E	186	SER	2.1
1	H	560	SER	2.1
1	K	164	ALA	2.1
1	K	479	TRP	2.1
1	G	199	GLN	2.1
1	H	490	VAL	2.1
1	H	212	ALA	2.1
1	E	554	GLN	2.1
1	C	561	HIS	2.1
1	G	191	GLY	2.1
1	G	217	GLY	2.1
1	H	125	SER	2.1
1	H	518	GLY	2.1
1	E	185	TYR	2.1
1	I	521	ILE	2.1
1	G	468	VAL	2.1
1	E	125	SER	2.0
1	C	256	PRO	2.0
1	H	467	LEU	2.0
1	I	568	LEU	2.0
1	B	561	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	163	ILE	2.0
1	K	189	MET	2.0
1	B	516	PRO	2.0
1	G	514	ILE	2.0
1	B	494	VAL	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.