



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:28 PM UTC

PDB ID : 8XND / pdb_00008xnd
Title : Crystal structure of serine hydroxymethyltransferase 1
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Deposited on : 2023-12-29
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

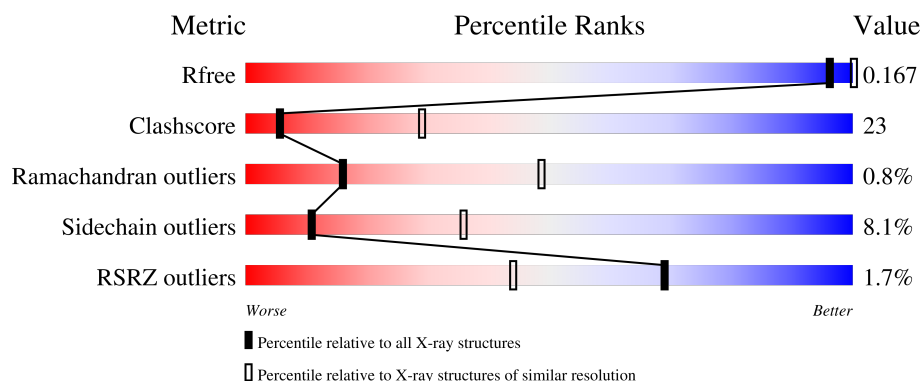
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	472	0.167 59% 33% 8% .
1	B	472	2% 57% 33% 8% .
1	C	472	0.167 56% 34% 7% .
1	D	472	2% 54% 36% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	C	500	-	-	X	-
2	PLP	D	500	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14588 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.

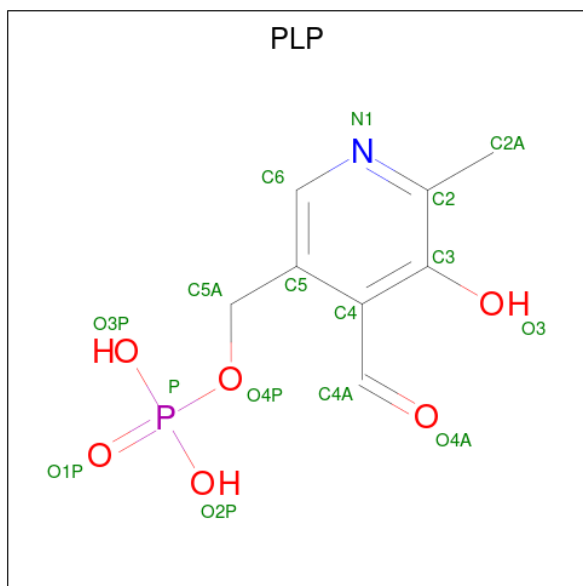
- Molecule 1 is a protein called Serine hydroxymethyltransferase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3632	2290	637	687	18			
1	B	472	Total	C	N	O	S	0	0	0
			3632	2290	637	687	18			
1	C	472	Total	C	N	O	S	0	0	0
			3632	2290	637	687	18			
1	D	472	Total	C	N	O	S	0	0	0
			3632	2290	637	687	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	-	expression tag	UNP P34896
A	10	GLY	-	expression tag	UNP P34896
A	20	ALA	LYS	conflict	UNP P34896
A	279	ALA	LYS	conflict	UNP P34896
A	442	ALA	ARG	conflict	UNP P34896
B	9	GLN	-	expression tag	UNP P34896
B	10	GLY	-	expression tag	UNP P34896
B	20	ALA	LYS	conflict	UNP P34896
B	279	ALA	LYS	conflict	UNP P34896
B	442	ALA	ARG	conflict	UNP P34896
C	9	GLN	-	expression tag	UNP P34896
C	10	GLY	-	expression tag	UNP P34896
C	20	ALA	LYS	conflict	UNP P34896
C	279	ALA	LYS	conflict	UNP P34896
C	442	ALA	ARG	conflict	UNP P34896
D	9	GLN	-	expression tag	UNP P34896
D	10	GLY	-	expression tag	UNP P34896
D	20	ALA	LYS	conflict	UNP P34896
D	279	ALA	LYS	conflict	UNP P34896
D	442	ALA	ARG	conflict	UNP P34896

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).

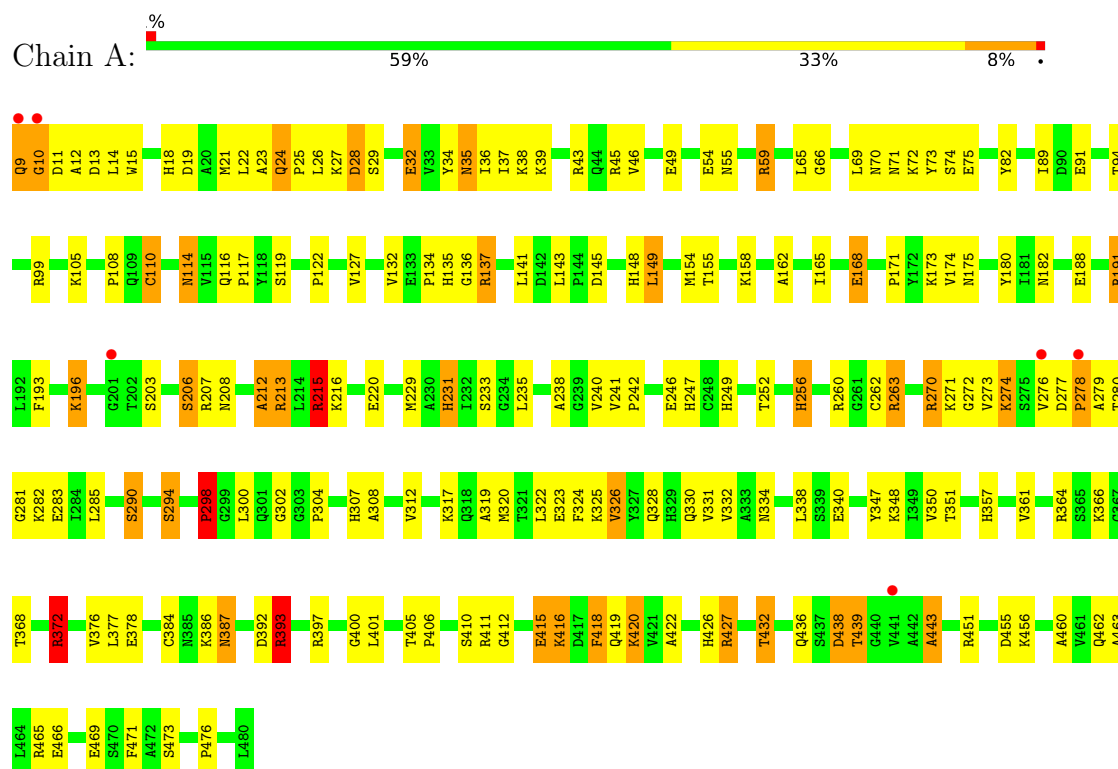


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

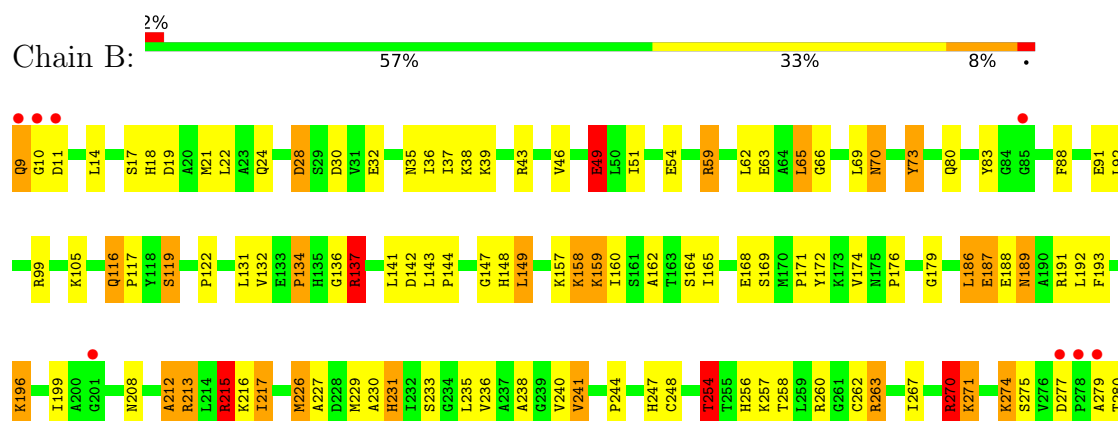
3 Residue-property plots [i](#)

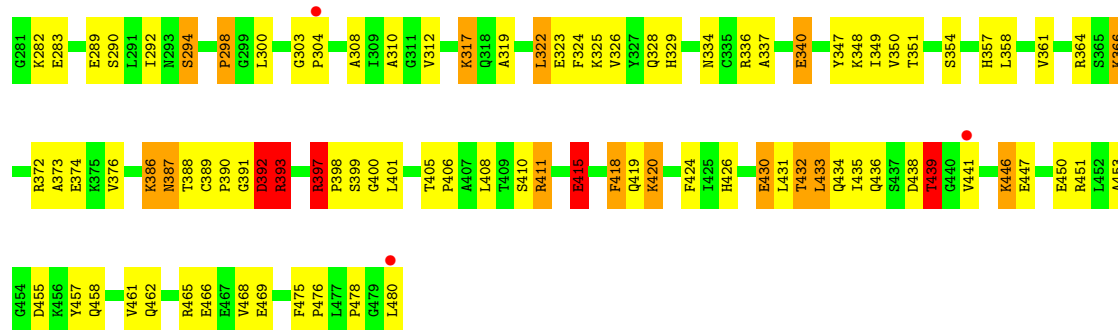
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

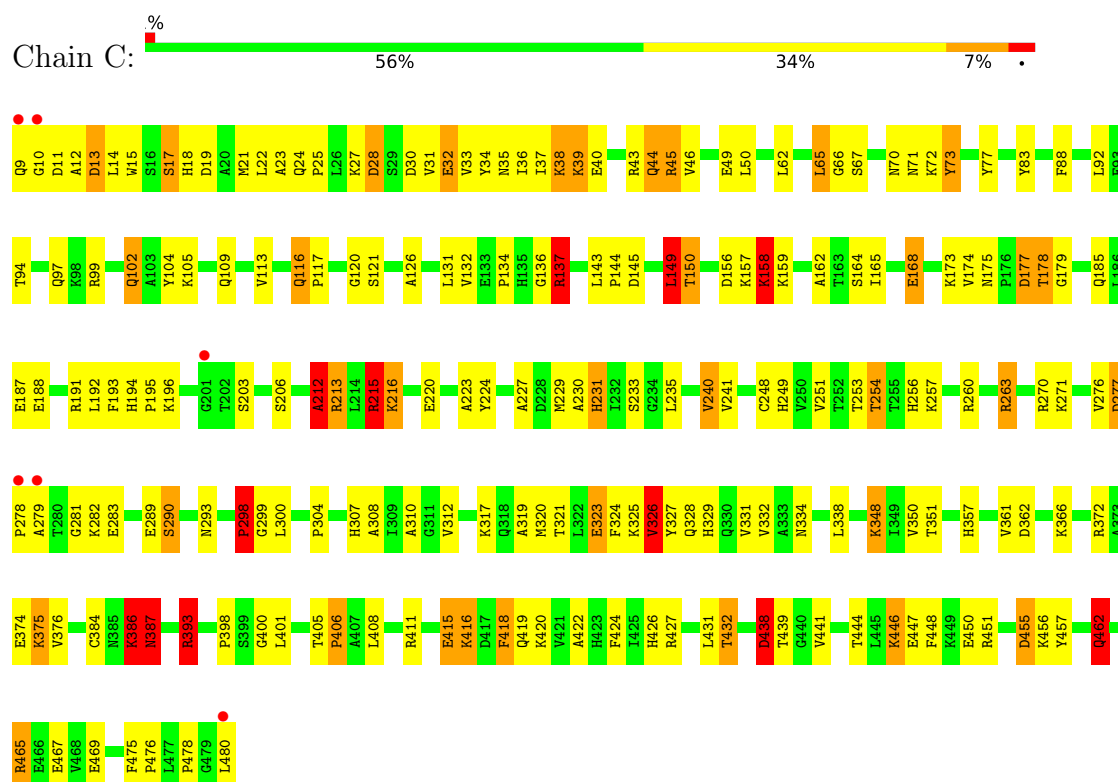


- Molecule 1: Serine hydroxymethyltransferase, cytosolic

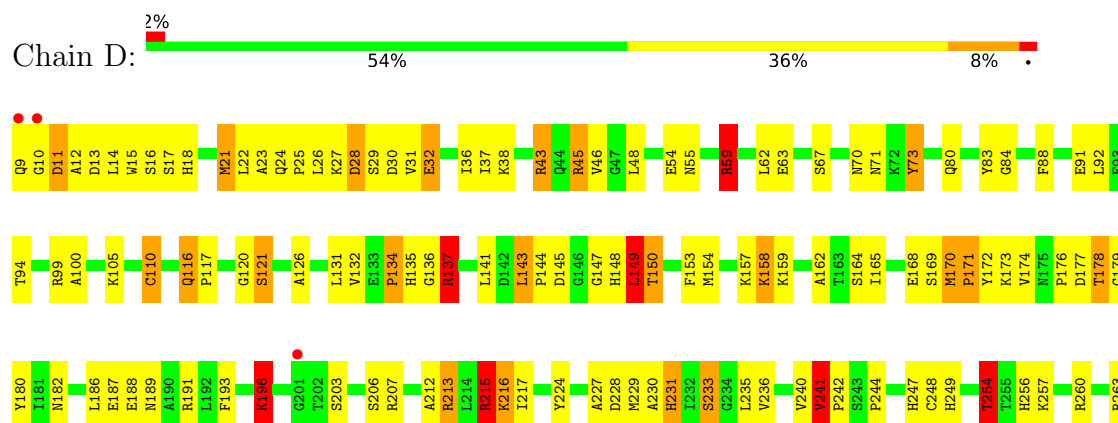


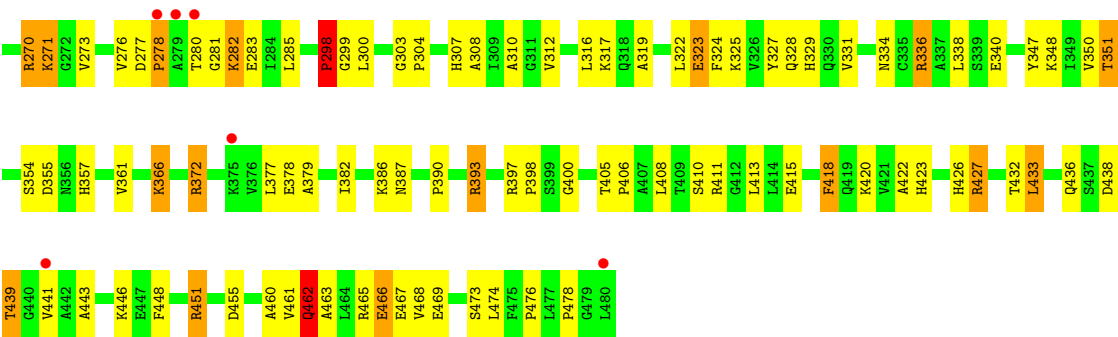


• Molecule 1: Serine hydroxymethyltransferase, cytosolic



• Molecule 1: Serine hydroxymethyltransferase, cytosolic





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	151.54Å 151.54Å 234.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.53 – 3.45 48.53 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.53-3.45) 99.9 (48.53-3.45)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.153 , 0.192 (Not available) , 0.167	Depositor DCC
R_{free} test set	4049 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.268 for -h,-k,l 0.269 for h,-h-k,-l 0.268 for -k,-h,-l	Xtriage
Reported twinning fraction	0.228 for H, K, L 0.231 for K, H, -L 0.240 for -h,-k,l 0.301 for -K, -H, -L	Depositor
Outliers	0 of 79345 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14588	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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	0.78	0/3705	1.70	65/5012 (1.3%)
1	B	0.77	1/3705 (0.0%)	1.66	61/5012 (1.2%)
1	C	0.77	0/3705	1.67	58/5012 (1.2%)
1	D	0.79	0/3705	1.71	75/5012 (1.5%)
All	All	0.78	1/14820 (0.0%)	1.69	259/20048 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
1	C	0	5
1	D	0	6
All	All	0	24

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	ARG	NE-CZ	5.68	1.39	1.33

All (259) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	CB-CA-C	-19.23	78.88	110.79
1	D	59	ARG	CB-CA-C	-17.15	82.32	110.79
1	C	188	GLU	N-CA-CB	15.47	133.06	110.16
1	B	439	THR	CA-CB-OG1	-15.34	86.60	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	466	GLU	CB-CG-CD	-13.50	89.66	112.60
1	B	415	GLU	N-CA-CB	12.72	128.81	110.12
1	D	215	ARG	CA-CB-CG	-11.97	90.16	114.10
1	C	432	THR	CA-CB-OG1	-11.58	92.23	109.60
1	C	415	GLU	N-CA-CB	11.53	126.72	110.01
1	D	270	ARG	CB-CG-CD	11.30	137.28	111.30
1	B	432	THR	CA-CB-OG1	-11.28	92.69	109.60
1	D	432	THR	CA-CB-OG1	-11.23	92.76	109.60
1	B	270	ARG	CB-CA-C	10.98	128.43	109.65
1	A	59	ARG	N-CA-CB	10.84	126.06	110.12
1	C	439	THR	CA-CB-OG1	-10.52	93.82	109.60
1	A	432	THR	CA-CB-OG1	-10.38	94.02	109.60
1	D	215	ARG	CD-NE-CZ	-10.19	110.14	124.40
1	A	348	LYS	CG-CD-CE	10.02	134.35	111.30
1	C	94	THR	OG1-CB-CG2	-10.01	89.28	109.30
1	B	271	LYS	CG-CD-CE	9.71	133.63	111.30
1	B	196	LYS	CB-CG-CD	9.70	133.62	111.30
1	D	94	THR	OG1-CB-CG2	-9.71	89.89	109.30
1	B	216	LYS	CB-CA-C	9.68	126.29	110.81
1	D	415	GLU	N-CA-CB	9.60	123.94	110.01
1	A	216	LYS	N-CA-CB	9.58	124.22	109.94
1	B	196	LYS	CA-CB-CG	9.57	133.24	114.10
1	B	430	GLU	CB-CG-CD	9.54	128.81	112.60
1	B	38	LYS	CB-CG-CD	9.44	133.01	111.30
1	D	393	ARG	CB-CA-C	9.34	129.00	110.42
1	D	105	LYS	CG-CD-CE	9.31	132.71	111.30
1	D	59	ARG	N-CA-CB	9.29	123.77	110.12
1	C	216	LYS	CG-CD-CE	9.25	132.58	111.30
1	A	196	LYS	CA-CB-CG	9.19	132.49	114.10
1	B	157	LYS	CB-CG-CD	8.95	131.89	111.30
1	A	27	LYS	CB-CG-CD	8.79	131.53	111.30
1	A	215	ARG	CA-CB-CG	-8.75	96.60	114.10
1	A	27	LYS	CG-CD-CE	8.72	131.37	111.30
1	D	182	ASN	CA-CB-CG	-8.71	103.89	112.60
1	A	415	GLU	N-CA-CB	8.64	122.53	110.01
1	A	49	GLU	CB-CG-CD	-8.60	97.98	112.60
1	A	216	LYS	CG-CD-CE	8.46	130.76	111.30
1	A	196	LYS	CB-CG-CD	8.44	130.71	111.30
1	C	158	LYS	N-CA-CB	8.43	126.15	111.39
1	C	150	THR	CA-CB-OG1	-8.36	97.06	109.60
1	A	35	ASN	CB-CA-C	-8.36	97.76	110.88
1	B	19	ASP	CA-CB-CG	8.34	120.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	LYS	CB-CG-CD	8.28	130.35	111.30
1	A	114	ASN	CB-CA-C	8.09	123.72	109.72
1	A	158	LYS	CG-CD-CE	8.09	129.90	111.30
1	A	325	LYS	CG-CD-CE	8.03	129.76	111.30
1	A	168	GLU	CB-CG-CD	7.95	126.11	112.60
1	C	38	LYS	CG-CD-CE	7.93	129.54	111.30
1	D	215	ARG	NE-CZ-NH1	-7.93	113.57	121.50
1	B	196	LYS	CG-CD-CE	7.90	129.47	111.30
1	C	105	LYS	CG-CD-CE	7.81	129.27	111.30
1	A	270	ARG	CB-CG-CD	7.80	129.25	111.30
1	D	216	LYS	CG-CD-CE	7.68	128.96	111.30
1	C	188	GLU	CB-CA-C	-7.55	98.01	110.85
1	D	254	THR	N-CA-CB	-7.51	98.88	110.29
1	D	254	THR	OG1-CB-CG2	7.46	124.21	109.30
1	A	43	ARG	NE-CZ-NH2	7.45	125.90	119.20
1	D	158	LYS	CB-CG-CD	7.34	128.19	111.30
1	A	137	ARG	CB-CG-CD	7.33	128.16	111.30
1	B	393	ARG	CB-CA-C	7.25	124.84	110.42
1	B	19	ASP	CB-CA-C	-7.24	97.24	110.63
1	C	298	PRO	N-CA-CB	-7.16	94.73	102.60
1	B	212	ALA	N-CA-CB	-7.14	98.43	110.49
1	C	116	GLN	OE1-CD-NE2	7.14	129.74	122.60
1	D	157	LYS	N-CA-CB	7.07	120.80	110.26
1	A	105	LYS	CB-CG-CD	7.07	127.55	111.30
1	C	325	LYS	CG-CD-CE	7.06	127.54	111.30
1	A	340	GLU	CB-CA-C	7.00	121.87	110.88
1	A	212	ALA	N-CA-CB	-6.98	98.69	110.49
1	C	158	LYS	CB-CG-CD	6.98	127.35	111.30
1	B	215	ARG	CA-CB-CG	-6.95	100.21	114.10
1	C	393	ARG	CG-CD-NE	6.93	127.26	112.00
1	C	215	ARG	CG-CD-NE	-6.87	96.88	112.00
1	D	215	ARG	CG-CD-NE	6.84	127.06	112.00
1	C	387	ASN	CB-CA-C	6.84	124.02	110.42
1	A	24	GLN	N-CA-CB	-6.83	100.52	110.14
1	A	393	ARG	CB-CA-C	6.80	121.73	110.92
1	C	212	ALA	N-CA-CB	-6.79	99.02	110.49
1	B	298	PRO	N-CA-CB	-6.75	95.18	102.60
1	A	91	GLU	CB-CG-CD	6.72	124.02	112.60
1	D	143	LEU	CB-CG-CD2	-6.70	90.60	110.70
1	C	175	ASN	CB-CA-C	-6.69	96.98	110.17
1	C	455	ASP	CB-CA-C	-6.67	99.67	110.74
1	B	105	LYS	CB-CG-CD	6.67	126.63	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	LYS	CA-CB-CG	6.65	127.40	114.10
1	B	49	GLU	N-CA-CB	6.63	120.75	110.21
1	B	134	PRO	N-CA-CB	-6.63	97.41	103.31
1	C	393	ARG	CB-CA-C	6.60	123.79	109.99
1	D	31	VAL	N-CA-CB	-6.60	100.69	110.58
1	B	393	ARG	CA-CB-CG	-6.59	100.93	114.10
1	A	82	TYR	N-CA-C	-6.58	104.97	114.12
1	B	226	MET	CG-SD-CE	-6.49	86.63	100.90
1	C	215	ARG	CB-CG-CD	6.49	126.22	111.30
1	D	215	ARG	NH1-CZ-NH2	6.47	127.71	119.30
1	B	131	LEU	CA-C-N	-6.46	116.40	122.66
1	B	131	LEU	C-N-CA	-6.46	116.40	122.66
1	D	158	LYS	CG-CD-CE	6.46	126.15	111.30
1	C	462	GLN	N-CA-CB	6.43	119.68	110.16
1	D	150	THR	CA-CB-OG1	-6.42	99.97	109.60
1	C	24	GLN	CB-CA-C	6.40	118.67	109.26
1	D	135	HIS	CB-CA-C	6.40	122.58	110.35
1	B	462	GLN	N-CA-CB	6.38	119.61	110.16
1	A	426	HIS	CA-CB-CG	-6.35	107.45	113.80
1	D	188	GLU	CB-CG-CD	6.35	123.39	112.60
1	D	27	LYS	CB-CG-CD	6.34	125.89	111.30
1	D	149	LEU	N-CA-CB	6.34	119.38	109.94
1	C	278	PRO	N-CA-C	-6.31	105.13	113.65
1	D	105	LYS	CB-CG-CD	6.31	125.81	111.30
1	D	420	LYS	N-CA-C	-6.23	104.59	111.82
1	B	426	HIS	CA-CB-CG	-6.22	107.58	113.80
1	A	137	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	A	372	ARG	CG-CD-NE	-6.20	98.35	112.00
1	A	427	ARG	CG-CD-NE	-6.17	98.43	112.00
1	A	135	HIS	CB-CA-C	6.16	122.11	110.35
1	C	420	LYS	N-CA-C	-6.13	104.70	111.82
1	A	216	LYS	CA-CB-CG	6.13	126.36	114.10
1	D	178	THR	OG1-CB-CG2	-6.12	97.05	109.30
1	D	451	ARG	CA-CB-CG	-6.12	101.87	114.10
1	C	386	LYS	CB-CG-CD	6.09	125.31	111.30
1	D	351	THR	CA-CB-OG1	-6.08	100.48	109.60
1	D	393	ARG	CG-CD-NE	6.08	125.38	112.00
1	B	254	THR	N-CA-CB	-6.04	101.27	110.45
1	D	397	ARG	CB-CG-CD	6.03	125.17	111.30
1	C	137	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	D	446	LYS	CB-CA-C	6.01	120.27	110.95
1	D	378	GLU	CG-CD-OE2	-6.00	104.61	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	GLN	CG-CD-NE2	-5.98	107.43	116.40
1	D	298	PRO	N-CA-CB	-5.98	96.03	102.60
1	D	418	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	82	TYR	CA-CB-CG	5.94	124.58	113.90
1	D	215	ARG	CB-CG-CD	-5.93	97.66	111.30
1	B	420	LYS	N-CA-C	-5.92	104.95	111.82
1	B	411	ARG	CB-CG-CD	-5.90	97.72	111.30
1	D	116	GLN	CG-CD-NE2	-5.89	107.56	116.40
1	C	426	HIS	CA-CB-CG	-5.89	107.91	113.80
1	A	256	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	A	420	LYS	N-CA-C	-5.87	105.01	111.82
1	C	418	PHE	CA-CB-CG	-5.87	107.93	113.80
1	B	196	LYS	CD-CE-NZ	5.86	130.66	111.90
1	C	254	THR	N-CA-CB	-5.83	100.78	110.23
1	C	43	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	D	455	ASP	CB-CA-C	5.81	120.43	110.79
1	C	19	ASP	CA-CB-CG	5.80	118.40	112.60
1	D	216	LYS	CB-CG-CD	5.80	124.64	111.30
1	A	110	CYS	CB-CA-C	-5.80	99.91	109.99
1	B	38	LYS	CG-CD-CE	5.79	124.61	111.30
1	B	157	LYS	CD-CE-NZ	5.78	130.41	111.90
1	A	216	LYS	CD-CE-NZ	5.75	130.31	111.90
1	B	189	ASN	OD1-CG-ND2	5.75	128.35	122.60
1	B	289	GLU	CA-C-N	-5.75	112.12	120.29
1	B	289	GLU	C-N-CA	-5.75	112.12	120.29
1	C	326	VAL	N-CA-CB	5.75	117.93	110.57
1	D	21	MET	CG-SD-CE	5.75	113.55	100.90
1	C	196	LYS	N-CA-C	-5.74	105.38	112.90
1	D	241	VAL	N-CA-CB	-5.74	103.18	111.21
1	A	215	ARG	CD-NE-CZ	-5.71	116.40	124.40
1	D	88	PHE	N-CA-CB	5.71	118.70	110.20
1	D	43	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	D	38	LYS	CG-CD-CE	5.70	124.41	111.30
1	D	317	LYS	N-CA-CB	5.70	118.27	110.01
1	A	196	LYS	CG-CD-CE	5.69	124.39	111.30
1	D	110	CYS	CB-CA-C	-5.69	99.99	109.55
1	B	418	PHE	CA-CB-CG	-5.67	108.13	113.80
1	C	168	GLU	CB-CG-CD	5.66	122.22	112.60
1	B	455	ASP	CB-CA-C	5.64	120.16	110.79
1	C	415	GLU	CG-CD-OE2	-5.62	105.47	118.40
1	D	271	LYS	CB-CG-CD	5.59	124.15	111.30
1	C	290	SER	N-CA-CB	5.58	118.43	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	418	PHE	CA-CB-CG	-5.56	108.24	113.80
1	D	170	MET	CG-SD-CE	-5.55	88.69	100.90
1	C	387	ASN	CA-CB-CG	5.54	118.14	112.60
1	D	433	LEU	N-CA-CB	-5.53	101.99	110.12
1	A	216	LYS	CB-CG-CD	5.50	123.95	111.30
1	B	340	GLU	CB-CA-C	5.49	119.50	110.88
1	A	24	GLN	CB-CA-C	5.48	117.32	109.26
1	C	38	LYS	N-CA-CB	5.48	117.95	110.01
1	D	462	GLN	N-CA-CB	5.47	118.16	110.12
1	B	258	THR	OG1-CB-CG2	5.46	120.23	109.30
1	D	340	GLU	CB-CA-C	5.46	119.46	110.88
1	B	216	LYS	CG-CD-CE	5.46	123.85	111.30
1	A	28	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	137	ARG	CD-NE-CZ	-5.45	116.77	124.40
1	D	32	GLU	CB-CG-CD	-5.45	103.33	112.60
1	C	187	GLU	O-C-N	5.45	127.75	122.09
1	D	426	HIS	CA-CB-CG	-5.45	108.36	113.80
1	D	423	HIS	CA-CB-CG	5.42	119.22	113.80
1	C	438	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	253	THR	CA-CB-OG1	-5.38	101.54	109.60
1	A	191	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	C	216	LYS	CB-CG-CD	5.35	123.61	111.30
1	B	187	GLU	O-C-N	5.35	127.65	122.09
1	C	270	ARG	CB-CG-CD	5.34	123.59	111.30
1	B	188	GLU	CB-CG-CD	5.34	121.68	112.60
1	D	323	GLU	CB-CA-C	-5.34	102.50	110.88
1	A	274	LYS	N-CA-C	-5.33	104.37	111.24
1	B	348	LYS	N-CA-CB	5.33	118.95	110.16
1	D	38	LYS	CB-CG-CD	5.32	123.53	111.30
1	A	19	ASP	N-CA-C	-5.30	105.62	111.71
1	B	116	GLN	OE1-CD-NE2	5.29	127.89	122.60
1	D	134	PRO	N-CA-CB	-5.29	98.43	103.19
1	A	416	LYS	CB-CG-CD	5.25	123.39	111.30
1	D	28	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	274	LYS	N-CA-C	-5.24	105.63	112.23
1	A	416	LYS	N-CA-CB	5.23	117.81	110.12
1	D	348	LYS	CG-CD-CE	5.23	123.33	111.30
1	A	94	THR	OG1-CB-CG2	-5.23	98.84	109.30
1	D	24	GLN	N-CA-CB	-5.22	101.76	110.02
1	C	44	GLN	N-CA-CB	5.21	117.79	110.12
1	D	189	ASN	CA-CB-CG	-5.21	107.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	LEU	N-CA-CB	-5.21	102.45	110.16
1	A	368	THR	OG1-CB-CG2	-5.19	98.92	109.30
1	A	154	MET	CG-SD-CE	-5.19	89.48	100.90
1	C	35	ASN	N-CA-CB	5.19	117.53	110.01
1	B	446	LYS	CB-CG-CD	5.18	123.21	111.30
1	C	289	GLU	CA-C-N	-5.18	112.94	120.29
1	C	289	GLU	C-N-CA	-5.18	112.94	120.29
1	B	59	ARG	CB-CA-C	-5.17	102.20	110.79
1	A	462	GLN	N-CA-CB	5.17	117.72	110.12
1	A	149	LEU	N-CA-CB	5.17	117.65	109.94
1	A	206	SER	CA-CB-OG	5.15	121.40	111.10
1	A	278	PRO	N-CA-C	-5.15	106.34	113.81
1	C	28	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	348	LYS	CG-CD-CE	5.14	123.13	111.30
1	B	160	ILE	CB-CA-C	-5.13	105.17	111.94
1	C	194	HIS	CB-CG-CD2	5.13	137.87	131.20
1	A	171	PRO	N-CA-C	5.12	120.23	111.68
1	D	233	SER	CB-CA-C	-5.12	102.79	110.92
1	C	216	LYS	CB-CA-C	5.11	118.99	110.81
1	D	105	LYS	CD-CE-NZ	5.11	128.26	111.90
1	D	171	PRO	N-CA-C	5.11	120.21	111.68
1	A	175	ASN	CB-CA-C	-5.09	101.42	109.82
1	C	39	LYS	CA-CB-CG	5.08	124.27	114.10
1	A	75	GLU	CA-C-N	-5.08	113.99	122.62
1	A	75	GLU	C-N-CA	-5.08	113.99	122.62
1	A	182	ASN	N-CA-CB	-5.07	103.72	110.57
1	B	159	LYS	CG-CD-CE	5.07	122.96	111.30
1	B	386	LYS	CB-CG-CD	5.07	122.96	111.30
1	A	298	PRO	N-CA-CB	-5.06	97.03	102.60
1	A	246	GLU	CB-CA-C	5.06	120.57	109.99
1	D	38	LYS	CB-CA-C	5.05	118.81	110.88
1	C	446	LYS	CB-CA-C	5.04	118.77	110.95
1	D	88	PHE	CA-CB-CG	-5.04	108.76	113.80
1	D	91	GLU	N-CA-CB	5.04	117.31	110.01
1	B	263	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	A	377	LEU	N-CA-C	-5.03	105.88	111.36
1	C	149	LEU	N-CA-CB	5.03	117.43	109.94
1	D	278	PRO	N-CA-C	-5.02	106.53	113.81
1	B	411	ARG	CA-C-N	-5.02	117.46	123.08
1	B	411	ARG	C-N-CA	-5.02	117.46	123.08
1	B	196	LYS	N-CA-C	-5.02	105.91	112.23
1	B	397	ARG	CG-CD-NE	5.01	123.03	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	ILE	CB-CA-C	-5.01	105.56	111.97
1	D	228	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	446	LYS	CB-CA-C	5.01	118.67	110.96

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ARG	Sidechain
1	A	263	ARG	Sidechain
1	A	372	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	397	ARG	Sidechain
1	A	427	ARG	Sidechain
1	A	465	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	215	ARG	Sidechain
1	B	372	ARG	Sidechain
1	B	393	ARG	Sidechain
1	B	397	ARG	Sidechain
1	B	465	ARG	Sidechain
1	C	137	ARG	Sidechain
1	C	215	ARG	Sidechain
1	C	263	ARG	Sidechain
1	C	45	ARG	Sidechain
1	C	465	ARG	Sidechain
1	D	137	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	336	ARG	Sidechain
1	D	372	ARG	Sidechain
1	D	45	ARG	Sidechain
1	D	59	ARG	Sidechain

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	3632	0	3610	182	0
1	B	3632	0	3612	217	0
1	C	3632	0	3612	213	0
1	D	3632	0	3612	210	0
2	A	15	0	7	1	0
2	B	15	0	7	2	0
2	C	15	0	6	7	0
2	D	15	0	7	11	0
All	All	14588	0	14473	679	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 23.

All (679) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:LYS:NZ	2:D:500:PLP:C4A	1.80	1.42
1:C:257:LYS:HE3	2:C:500:PLP:C4A	1.61	1.31
1:D:439:THR:HG23	1:D:443:ALA:CB	1.66	1.23
1:D:257:LYS:HZ1	2:D:500:PLP:C4A	1.45	1.19
1:D:439:THR:CG2	1:D:443:ALA:HB3	1.73	1.18
1:C:350:VAL:O	1:C:351:THR:HG22	1.40	1.18
1:B:350:VAL:O	1:B:351:THR:HG22	1.46	1.16
1:D:350:VAL:O	1:D:351:THR:HG22	1.47	1.14
1:A:438:ASP:HB3	1:A:451:ARG:HH12	1.12	1.12
1:C:229:MET:HE2	1:C:233:SER:HA	1.29	1.12
1:A:438:ASP:CB	1:A:451:ARG:HH12	1.64	1.09
1:B:229:MET:HE2	1:B:233:SER:HA	1.12	1.09
1:A:350:VAL:O	1:A:351:THR:HG22	1.50	1.08
1:D:229:MET:HE2	1:D:233:SER:HA	1.36	1.06
1:A:229:MET:HE2	1:A:233:SER:HA	1.05	1.05
1:A:34:TYR:CE2	1:A:38:LYS:HD3	1.92	1.04
1:D:257:LYS:HZ2	2:D:500:PLP:C4A	1.67	1.02
1:B:59:ARG:NH1	1:C:25:PRO:HA	1.74	1.02
1:B:21:MET:CE	1:C:323:GLU:HB2	1.90	1.01
1:B:317:LYS:NZ	1:C:30:ASP:HA	1.76	1.00
1:A:229:MET:CE	1:A:233:SER:HA	1.92	0.99
1:C:257:LYS:CE	2:C:500:PLP:C4A	2.40	0.99
1:C:386:LYS:O	1:C:387:ASN:HB3	1.63	0.97
1:D:257:LYS:CE	2:D:500:PLP:C4A	2.42	0.97
1:D:439:THR:HG23	1:D:443:ALA:HB3	0.99	0.97
1:B:317:LYS:HZ3	1:C:30:ASP:CA	1.77	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:LYS:HD2	1:D:398:PRO:HG3	1.45	0.96
1:A:229:MET:HE2	1:A:233:SER:CA	1.97	0.95
1:D:336:ARG:HH12	1:D:355:ASP:HA	1.32	0.94
1:C:386:LYS:HD2	1:C:398:PRO:HG3	1.50	0.93
1:A:173:LYS:HD2	1:C:192:LEU:HD21	1.51	0.93
1:B:386:LYS:HD2	1:B:398:PRO:HG3	1.51	0.92
1:A:372:ARG:HH12	1:A:439:THR:HG21	1.34	0.92
1:A:66:GLY:O	1:D:62:LEU:HB3	1.70	0.91
1:B:229:MET:CE	1:B:233:SER:HA	2.00	0.91
1:C:231:HIS:HD2	1:C:357:HIS:HE2	1.20	0.90
1:A:168:GLU:HG3	1:C:168:GLU:HG3	1.52	0.89
1:B:386:LYS:O	1:B:387:ASN:HB2	1.72	0.89
1:C:145:ASP:HB3	1:C:174:VAL:HG23	1.54	0.89
1:A:298:PRO:HB2	1:D:149:LEU:CD2	2.03	0.88
1:A:231:HIS:HD2	1:A:357:HIS:HE2	1.21	0.88
1:B:323:GLU:HB2	1:C:21:MET:HE1	1.54	0.87
1:B:21:MET:HE1	1:C:323:GLU:HB2	1.56	0.86
1:D:438:ASP:HB3	1:D:451:ARG:HH12	1.38	0.86
1:B:231:HIS:HD2	1:B:357:HIS:HE2	1.22	0.86
1:A:34:TYR:CE2	1:A:38:LYS:CD	2.62	0.83
1:B:54:GLU:OE1	1:C:71:ASN:O	1.97	0.83
1:A:438:ASP:CB	1:A:451:ARG:NH1	2.41	0.83
1:A:386:LYS:O	1:A:387:ASN:HB2	1.78	0.82
1:C:323:GLU:N	1:C:323:GLU:OE1	2.11	0.82
1:B:438:ASP:OD2	1:B:457:TYR:OH	1.96	0.82
1:B:59:ARG:NH1	1:C:25:PRO:CA	2.43	0.82
1:D:336:ARG:NH1	1:D:355:ASP:HA	1.93	0.82
1:B:323:GLU:OE1	1:B:323:GLU:N	2.13	0.81
1:C:350:VAL:O	1:C:351:THR:CG2	2.27	0.80
1:D:215:ARG:HH12	1:D:249:HIS:CE1	1.99	0.80
1:A:260:ARG:NH2	1:D:22:LEU:HD21	1.97	0.80
1:A:323:GLU:HB2	1:D:21:MET:CE	2.12	0.80
1:B:229:MET:HE2	1:B:233:SER:CA	2.06	0.80
1:B:282:LYS:HG3	1:B:283:GLU:H	1.46	0.80
1:B:14:LEU:CD2	1:C:326:VAL:HG21	2.12	0.79
1:B:213:ARG:HH11	1:B:213:ARG:CG	1.95	0.79
1:B:290:SER:O	1:B:294:SER:OG	1.99	0.79
1:D:141:LEU:HD11	1:D:174:VAL:HG23	1.65	0.79
1:B:14:LEU:HD21	1:C:326:VAL:HG21	1.65	0.78
1:B:22:LEU:HD13	1:C:478:PRO:CG	2.14	0.78
1:B:22:LEU:HB3	1:C:478:PRO:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:NH1	1:C:30:ASP:OD2	2.16	0.78
1:A:143:LEU:HD21	1:A:149:LEU:CD1	2.15	0.77
1:B:323:GLU:HB2	1:C:21:MET:CE	2.13	0.77
1:D:213:ARG:HG3	1:D:213:ARG:HH11	1.47	0.77
1:C:120:GLY:HA3	2:C:500:PLP:H5A2	1.64	0.77
1:B:300:LEU:HD23	1:C:162:ALA:CB	2.15	0.77
1:A:191:ARG:HD3	1:A:220:GLU:OE2	1.84	0.77
1:A:143:LEU:HD21	1:A:149:LEU:HD11	1.67	0.76
1:B:54:GLU:OE2	1:C:73:TYR:N	2.17	0.76
1:A:276:VAL:O	1:A:278:PRO:HD3	1.86	0.75
1:C:213:ARG:CG	1:C:213:ARG:HH11	1.99	0.75
1:B:149:LEU:H	1:B:149:LEU:HD12	1.51	0.75
1:D:159:LYS:HD3	1:D:164:SER:O	1.87	0.75
1:D:257:LYS:HE3	2:D:500:PLP:C4A	2.17	0.74
1:A:148:HIS:CD2	1:A:149:LEU:H	2.04	0.74
1:A:298:PRO:HB2	1:D:149:LEU:HD21	1.66	0.74
1:A:141:LEU:HD11	1:A:174:VAL:HG23	1.69	0.74
1:A:323:GLU:HB2	1:D:21:MET:HE2	1.69	0.74
1:A:149:LEU:CD2	1:D:298:PRO:HB2	2.18	0.74
1:A:384:CYS:SG	1:A:401:LEU:HD22	2.28	0.74
1:A:317:LYS:HZ2	1:D:30:ASP:H	1.36	0.73
1:B:88:PHE:CE1	1:C:39:LYS:HD3	2.24	0.73
1:B:317:LYS:NZ	1:C:30:ASP:CA	2.43	0.73
1:C:438:ASP:HB3	1:C:451:ARG:NH1	2.03	0.73
1:B:186:LEU:O	1:B:186:LEU:HD12	1.88	0.73
1:C:27:LYS:O	1:C:31:VAL:HG22	1.88	0.73
1:B:263:ARG:NH2	1:C:73:TYR:CD1	2.56	0.73
1:B:300:LEU:HD23	1:C:162:ALA:HB2	1.71	0.72
1:B:141:LEU:HD11	1:B:174:VAL:HG23	1.71	0.72
1:B:350:VAL:O	1:B:351:THR:CG2	2.32	0.72
1:D:277:ASP:O	1:D:281:GLY:N	2.22	0.72
1:C:229:MET:CE	1:C:233:SER:HA	2.14	0.72
1:D:215:ARG:NH1	1:D:249:HIS:CE1	2.56	0.72
1:D:438:ASP:CB	1:D:451:ARG:HH12	2.02	0.72
1:D:215:ARG:O	1:D:215:ARG:HG2	1.90	0.72
1:A:438:ASP:HB3	1:A:451:ARG:NH1	1.97	0.71
1:B:168:GLU:HG3	1:D:168:GLU:HG3	1.71	0.71
1:A:376:VAL:HG21	1:A:432:THR:OG1	1.91	0.71
1:B:59:ARG:HH12	1:C:25:PRO:CB	2.03	0.71
1:C:376:VAL:HG21	1:C:432:THR:OG1	1.91	0.71
1:B:149:LEU:HD23	1:C:298:PRO:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:HB3	1:A:174:VAL:HG23	1.72	0.70
1:D:408:LEU:HD13	1:D:413:LEU:HD22	1.73	0.70
1:C:386:LYS:CD	1:C:398:PRO:HG3	2.21	0.70
1:C:131:LEU:HB3	1:C:224:TYR:CE2	2.26	0.70
1:A:317:LYS:HZ2	1:D:30:ASP:N	1.90	0.70
1:A:148:HIS:CD2	1:A:149:LEU:N	2.60	0.69
1:A:215:ARG:HD2	1:A:247:HIS:O	1.91	0.69
1:C:149:LEU:HD12	1:C:149:LEU:H	1.57	0.69
1:A:145:ASP:HB3	1:A:174:VAL:CG2	2.22	0.69
1:C:230:ALA:HA	1:C:254:THR:HG22	1.75	0.69
1:A:149:LEU:HD23	1:D:298:PRO:HB2	1.75	0.69
1:A:350:VAL:O	1:A:351:THR:CG2	2.37	0.69
1:A:372:ARG:NH1	1:A:439:THR:HG21	2.07	0.69
1:D:229:MET:CE	1:D:233:SER:HA	2.18	0.69
1:B:9:GLN:HG2	1:B:10:GLY:H	1.57	0.69
1:A:70:ASN:HD21	1:D:263:ARG:H	1.42	0.68
1:A:412:GLY:HA2	1:D:15:TRP:HE1	1.58	0.68
1:B:162:ALA:CB	1:C:300:LEU:HD23	2.23	0.68
1:C:374:GLU:OE1	1:C:386:LYS:HG2	1.92	0.68
1:D:350:VAL:O	1:D:351:THR:CG2	2.34	0.68
1:B:158:LYS:HG2	1:B:159:LYS:N	2.09	0.67
1:A:71:ASN:O	1:D:54:GLU:OE1	2.12	0.67
1:B:376:VAL:HG21	1:B:432:THR:OG1	1.95	0.67
1:C:230:ALA:CA	1:C:254:THR:HG22	2.25	0.67
1:C:257:LYS:NZ	2:C:500:PLP:C4A	2.57	0.67
1:D:474:LEU:N	1:D:474:LEU:HD23	2.10	0.67
1:C:120:GLY:HA3	2:C:500:PLP:C5A	2.25	0.66
1:A:438:ASP:HB2	1:A:451:ARG:NH1	2.09	0.66
1:B:424:PHE:HD2	1:B:468:VAL:HG22	1.61	0.66
1:D:70:ASN:HD22	1:D:307:HIS:CE1	2.14	0.66
1:A:317:LYS:HD2	1:D:30:ASP:HB2	1.77	0.66
1:B:256:HIS:ND1	1:B:263:ARG:HA	2.11	0.66
1:A:70:ASN:HD22	1:A:307:HIS:CE1	2.14	0.65
1:C:149:LEU:H	1:C:149:LEU:CD1	2.09	0.65
1:A:302:GLY:HA3	2:D:500:PLP:O1P	1.97	0.65
1:A:277:ASP:O	1:A:281:GLY:N	2.28	0.65
1:D:336:ARG:NH1	1:D:354:SER:O	2.27	0.65
1:A:206:SER:HB2	1:A:351:THR:HG21	1.77	0.65
1:B:424:PHE:CD2	1:B:468:VAL:HG22	2.32	0.65
1:A:213:ARG:CG	1:A:213:ARG:HH11	2.09	0.64
1:A:317:LYS:NZ	1:D:30:ASP:H	1.93	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASP:OD2	1:C:99:ARG:NH1	2.25	0.64
1:B:215:ARG:O	1:B:215:ARG:HG3	1.95	0.64
1:C:70:ASN:HD22	1:C:307:HIS:CE1	2.15	0.64
1:B:323:GLU:HB3	1:C:18:HIS:HB2	1.78	0.64
1:D:143:LEU:HD21	1:D:149:LEU:CD1	2.27	0.64
1:C:116:GLN:N	1:C:117:PRO:CD	2.61	0.64
1:A:347:TYR:CD1	1:A:366:LYS:HD3	2.33	0.64
1:B:59:ARG:HH12	1:C:25:PRO:HB3	1.61	0.63
1:B:69:LEU:HD11	1:C:37:ILE:HG12	1.81	0.63
1:B:260:ARG:NH2	1:C:22:LEU:HD21	2.14	0.63
1:C:215:ARG:HH12	1:C:249:HIS:HE2	1.47	0.63
1:D:213:ARG:HH11	1:D:213:ARG:CG	2.11	0.63
1:D:273:VAL:HG13	1:D:283:GLU:HB2	1.79	0.63
1:B:337:ALA:CB	1:B:415:GLU:HB3	2.28	0.62
1:D:357:HIS:HD1	1:D:357:HIS:H	1.46	0.62
1:B:386:LYS:CD	1:B:398:PRO:HG3	2.26	0.62
1:C:73:TYR:HD2	1:C:83:TYR:CE2	2.17	0.62
1:B:213:ARG:HH11	1:B:213:ARG:HG3	1.63	0.62
1:A:21:MET:CE	1:D:323:GLU:HB2	2.30	0.62
1:B:59:ARG:HG3	1:B:480:LEU:H	1.64	0.62
1:B:116:GLN:N	1:B:117:PRO:CD	2.62	0.62
1:D:276:VAL:O	1:D:278:PRO:HD3	2.00	0.62
1:A:116:GLN:N	1:A:117:PRO:CD	2.63	0.62
1:A:420:LYS:HD3	1:A:471:PHE:CE1	2.35	0.62
1:A:148:HIS:HD2	1:A:149:LEU:H	1.48	0.62
1:D:116:GLN:N	1:D:117:PRO:CD	2.62	0.62
1:D:273:VAL:HA	1:D:285:LEU:HD23	1.80	0.62
1:D:465:ARG:NH1	1:D:469:GLU:OE2	2.30	0.62
1:D:143:LEU:CD2	1:D:149:LEU:CD1	2.77	0.61
1:A:415:GLU:O	1:A:419:GLN:HG3	1.99	0.61
1:A:439:THR:HG23	1:A:443:ALA:HB3	1.82	0.61
1:C:104:TYR:CE1	1:C:229:MET:HE1	2.36	0.61
1:D:212:ALA:HB2	1:D:247:HIS:CE1	2.35	0.61
1:B:317:LYS:HZ3	1:C:30:ASP:N	1.97	0.61
1:C:145:ASP:HB3	1:C:174:VAL:CG2	2.27	0.61
1:D:10:GLY:O	1:D:11:ASP:C	2.43	0.61
1:C:215:ARG:NH1	1:C:249:HIS:NE2	2.49	0.61
1:C:73:TYR:HD2	1:C:83:TYR:HE2	1.49	0.60
1:B:186:LEU:HD12	1:B:186:LEU:C	2.26	0.60
1:B:415:GLU:O	1:B:419:GLN:HG3	2.01	0.60
1:C:438:ASP:OD2	1:C:456:LYS:HE3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:HIS:ND1	1:D:263:ARG:HA	2.16	0.60
1:D:132:VAL:HG12	1:D:136:GLY:HA3	1.82	0.60
1:A:9:GLN:O	1:A:10:GLY:C	2.44	0.60
1:A:240:VAL:HG12	1:A:332:VAL:HG21	1.82	0.60
1:A:256:HIS:ND1	1:A:263:ARG:HA	2.17	0.60
1:D:408:LEU:HD13	1:D:413:LEU:CD2	2.32	0.60
1:C:213:ARG:HH11	1:C:213:ARG:HG3	1.65	0.59
1:A:59:ARG:HH21	1:D:25:PRO:HG3	1.67	0.59
1:A:213:ARG:HH11	1:A:213:ARG:HG3	1.65	0.59
1:A:108:PRO:O	1:A:271:LYS:NZ	2.35	0.59
1:D:92:LEU:HD11	1:D:310:ALA:HA	1.83	0.59
1:D:143:LEU:HD21	1:D:149:LEU:HD13	1.82	0.59
1:D:282:LYS:HG3	1:D:283:GLU:H	1.67	0.59
1:A:15:TRP:CZ3	1:D:327:TYR:HA	2.37	0.59
1:B:22:LEU:HD21	1:C:260:ARG:CZ	2.32	0.59
1:B:317:LYS:HZ3	1:C:30:ASP:CB	2.15	0.58
1:B:24:GLN:HE21	1:B:28:ASP:HB2	1.67	0.58
1:C:276:VAL:O	1:C:277:ASP:C	2.45	0.58
1:B:30:ASP:CG	1:C:99:ARG:HH22	2.11	0.58
1:B:215:ARG:HH21	1:B:270:ARG:HH12	1.50	0.58
1:A:110:CYS:O	1:A:270:ARG:HG3	2.03	0.58
1:A:263:ARG:H	1:D:70:ASN:HD21	1.52	0.58
1:B:149:LEU:HD12	1:B:149:LEU:N	2.19	0.58
1:B:263:ARG:H	1:C:70:ASN:HD21	1.50	0.58
1:D:176:PRO:HA	1:D:390:PRO:HB3	1.85	0.58
1:B:158:LYS:HG2	1:B:159:LYS:H	1.68	0.58
1:C:121:SER:HB3	1:C:150:THR:HG21	1.85	0.58
1:C:206:SER:HB2	1:C:351:THR:HG21	1.85	0.58
1:B:17:SER:OG	1:C:323:GLU:HG3	2.04	0.58
1:C:372:ARG:HB3	1:C:448:PHE:CZ	2.39	0.58
1:B:66:GLY:O	1:C:62:LEU:HB3	2.04	0.57
1:B:149:LEU:H	1:B:149:LEU:CD1	2.16	0.57
1:B:282:LYS:CG	1:B:283:GLU:H	2.14	0.57
1:D:154:MET:HE3	1:D:159:LYS:HE2	1.86	0.57
1:C:191:ARG:HD3	1:C:220:GLU:OE2	2.05	0.57
1:C:405:THR:N	1:C:406:PRO:HD3	2.19	0.57
1:D:254:THR:HG21	1:D:257:LYS:HD2	1.85	0.57
1:C:159:LYS:HD3	1:C:164:SER:O	2.05	0.57
1:D:154:MET:CE	1:D:159:LYS:HE2	2.35	0.57
1:C:73:TYR:CD2	1:C:83:TYR:CE2	2.92	0.57
1:D:206:SER:HB2	1:D:351:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:PLP:C4A	2:D:500:PLP:O4P	2.53	0.57
1:B:22:LEU:CD1	1:C:478:PRO:HG3	2.35	0.57
1:D:405:THR:N	1:D:406:PRO:CD	2.68	0.57
1:A:168:GLU:HG3	1:C:168:GLU:CG	2.31	0.57
1:A:300:LEU:HD23	1:D:162:ALA:CB	2.34	0.57
1:B:162:ALA:HB2	1:C:300:LEU:HD23	1.86	0.57
1:B:326:VAL:HG21	1:C:14:LEU:HD23	1.87	0.57
1:B:405:THR:N	1:B:406:PRO:CD	2.68	0.57
1:C:230:ALA:HB1	1:C:254:THR:CG2	2.35	0.57
1:A:420:LYS:HD3	1:A:471:PHE:CZ	2.40	0.56
1:B:172:TYR:CD2	1:B:186:LEU:HD22	2.40	0.56
1:C:231:HIS:CD2	1:C:357:HIS:HE2	2.11	0.56
1:D:411:ARG:O	1:D:476:PRO:HD2	2.05	0.56
1:C:405:THR:N	1:C:406:PRO:CD	2.68	0.56
1:A:231:HIS:CD2	1:A:357:HIS:HE2	2.13	0.56
1:D:231:HIS:HD2	1:D:357:HIS:NE2	2.03	0.56
1:A:143:LEU:CD2	1:A:149:LEU:HD12	2.35	0.56
1:C:215:ARG:NH1	1:C:249:HIS:HE2	2.03	0.56
1:D:213:ARG:HA	1:D:216:LYS:HD2	1.88	0.56
1:C:132:VAL:HG12	1:C:136:GLY:HA3	1.88	0.56
1:B:231:HIS:CD2	1:B:357:HIS:HE2	2.13	0.56
1:C:240:VAL:CG1	1:C:332:VAL:HG21	2.35	0.56
1:A:405:THR:N	1:A:406:PRO:CD	2.69	0.56
1:B:22:LEU:HD13	1:C:478:PRO:HG3	1.87	0.56
1:A:21:MET:HE2	1:D:323:GLU:HB2	1.88	0.56
1:B:260:ARG:CZ	1:C:22:LEU:HD21	2.35	0.56
1:C:177:ASP:O	1:C:178:THR:C	2.49	0.56
1:D:462:GLN:HG3	1:D:466:GLU:OE2	2.06	0.56
1:A:412:GLY:HA2	1:D:15:TRP:NE1	2.20	0.55
1:B:431:LEU:O	1:B:435:ILE:HG13	2.07	0.55
1:D:282:LYS:HE2	1:D:282:LYS:HA	1.88	0.55
1:B:137:ARG:NH2	1:D:168:GLU:OE1	2.37	0.55
1:C:45:ARG:HG2	1:C:45:ARG:NH2	2.21	0.55
1:B:169:SER:O	1:D:137:ARG:NH1	2.38	0.55
1:B:176:PRO:HA	1:B:390:PRO:HB3	1.88	0.55
1:B:236:VAL:HG11	1:B:244:PRO:HD2	1.87	0.55
1:C:405:THR:H	1:C:406:PRO:HD3	1.72	0.55
1:C:213:ARG:CG	1:C:213:ARG:NH1	2.68	0.55
1:A:412:GLY:CA	1:D:15:TRP:HE1	2.18	0.55
1:B:215:ARG:HD3	1:B:247:HIS:O	2.06	0.55
1:A:282:LYS:HG3	1:A:283:GLU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:LYS:NZ	1:C:30:ASP:N	2.55	0.55
1:B:405:THR:N	1:B:406:PRO:HD3	2.22	0.55
1:D:460:ALA:O	1:D:463:ALA:HB3	2.06	0.55
1:A:260:ARG:HH21	1:D:22:LEU:HD21	1.71	0.55
1:C:34:TYR:CE2	1:C:38:LYS:HD3	2.41	0.55
1:D:212:ALA:O	1:D:216:LYS:HG3	2.07	0.55
1:A:15:TRP:HZ3	1:D:327:TYR:HA	1.71	0.54
1:C:384:CYS:SG	1:C:401:LEU:HD22	2.47	0.54
1:D:131:LEU:HB3	1:D:224:TYR:CE2	2.42	0.54
1:A:405:THR:N	1:A:406:PRO:HD3	2.22	0.54
1:A:59:ARG:HD3	1:D:25:PRO:HA	1.88	0.54
1:C:456:LYS:HD3	1:C:457:TYR:CD2	2.43	0.54
1:A:277:ASP:HB3	1:A:280:THR:OG1	2.07	0.54
1:C:149:LEU:HD12	1:C:149:LEU:N	2.23	0.54
1:A:143:LEU:HD21	1:A:149:LEU:HD12	1.88	0.54
1:A:238:ALA:HB3	1:A:240:VAL:HG23	1.89	0.54
1:B:326:VAL:HG21	1:C:14:LEU:CD2	2.38	0.54
1:C:235:LEU:HD23	1:C:328:GLN:OE1	2.07	0.54
1:D:48:LEU:HD12	1:D:468:VAL:HG13	1.89	0.54
1:B:22:LEU:HD21	1:C:260:ARG:NH2	2.23	0.54
1:B:411:ARG:O	1:B:476:PRO:HD2	2.08	0.54
1:A:277:ASP:O	1:A:280:THR:N	2.41	0.54
1:C:229:MET:HE2	1:C:233:SER:CA	2.20	0.54
1:A:272:GLY:O	1:A:285:LEU:HD22	2.07	0.53
1:A:323:GLU:CB	1:D:21:MET:CE	2.84	0.53
1:B:59:ARG:HH11	1:C:25:PRO:HA	1.64	0.53
1:B:317:LYS:HZ3	1:C:30:ASP:HA	1.40	0.53
1:C:121:SER:CB	1:C:150:THR:HG21	2.38	0.53
1:A:141:LEU:HD11	1:A:174:VAL:CG2	2.38	0.53
1:A:411:ARG:O	1:A:476:PRO:HD2	2.09	0.53
1:C:9:GLN:O	1:C:10:GLY:C	2.50	0.53
1:C:137:ARG:HB3	1:C:193:PHE:CE2	2.43	0.53
1:B:99:ARG:HH22	1:C:30:ASP:CG	2.17	0.53
1:D:143:LEU:HD22	1:D:149:LEU:HD12	1.89	0.53
1:B:322:LEU:HD12	1:B:326:VAL:HG23	1.91	0.53
1:C:277:ASP:O	1:C:281:GLY:N	2.41	0.53
1:B:405:THR:H	1:B:406:PRO:HD3	1.74	0.53
1:D:16:SER:O	1:D:17:SER:C	2.52	0.53
1:A:22:LEU:HB3	1:D:478:PRO:HB3	1.91	0.52
1:D:308:ALA:O	1:D:312:VAL:HG23	2.08	0.52
1:A:32:GLU:CD	1:D:99:ARG:HH21	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ALA:O	1:C:216:LYS:HG3	2.09	0.52
1:C:456:LYS:HD3	1:C:457:TYR:CE2	2.45	0.52
1:B:14:LEU:HD21	1:C:326:VAL:CG2	2.37	0.52
1:D:213:ARG:CG	1:D:213:ARG:NH1	2.71	0.52
1:D:439:THR:O	1:D:443:ALA:HB2	2.09	0.52
1:B:308:ALA:O	1:B:312:VAL:HG23	2.09	0.52
1:B:430:GLU:O	1:B:434:GLN:HG3	2.08	0.52
1:B:213:ARG:O	1:B:217:ILE:HG13	2.09	0.52
1:B:92:LEU:HD11	1:B:310:ALA:HA	1.92	0.52
1:A:127:VAL:HG21	1:A:252:THR:CG2	2.40	0.52
1:B:18:HIS:HB2	1:C:323:GLU:HB3	1.92	0.52
1:B:215:ARG:HH21	1:B:270:ARG:NH1	2.07	0.52
1:C:92:LEU:HD11	1:C:310:ALA:HA	1.92	0.52
1:C:411:ARG:O	1:C:476:PRO:HD2	2.09	0.52
1:B:18:HIS:CD2	1:C:327:TYR:HB2	2.44	0.51
1:D:427:ARG:NH2	1:D:467:GLU:OE1	2.41	0.51
1:A:191:ARG:HD3	1:A:220:GLU:CD	2.35	0.51
1:B:137:ARG:NH1	1:D:169:SER:O	2.36	0.51
1:D:121:SER:HB3	1:D:150:THR:HG21	1.92	0.51
1:A:330:GLN:HG2	1:D:15:TRP:CH2	2.44	0.51
1:B:347:TYR:CE1	1:B:366:LYS:HG2	2.46	0.51
1:C:40:GLU:HG3	1:C:44:GLN:HE21	1.75	0.51
1:D:162:ALA:HA	1:D:165:ILE:HD12	1.93	0.51
1:B:282:LYS:HE2	1:B:283:GLU:HG2	1.93	0.51
1:A:72:LYS:HD3	1:D:43:ARG:NH2	2.26	0.51
1:B:17:SER:OG	1:C:323:GLU:CG	2.59	0.51
1:B:137:ARG:HB3	1:B:193:PHE:CE2	2.46	0.51
1:B:435:ILE:HG12	1:B:457:TYR:CE1	2.45	0.51
1:D:45:ARG:HG2	1:D:45:ARG:NH2	2.25	0.51
1:C:240:VAL:HG22	1:C:329:HIS:CE1	2.46	0.51
1:C:338:LEU:HD12	1:C:422:ALA:HB2	1.92	0.51
1:B:254:THR:HG21	1:B:257:LYS:HD2	1.91	0.51
1:D:462:GLN:HG3	1:D:462:GLN:O	2.09	0.51
1:C:230:ALA:CB	1:C:254:THR:HG22	2.41	0.51
1:B:99:ARG:NH2	1:C:30:ASP:OD2	2.44	0.50
1:C:308:ALA:O	1:C:312:VAL:HG23	2.11	0.50
1:A:35:ASN:HB3	1:A:39:LYS:HE3	1.93	0.50
1:C:424:PHE:HE1	1:C:467:GLU:OE2	1.94	0.50
1:A:308:ALA:O	1:A:312:VAL:HG23	2.11	0.50
1:A:405:THR:H	1:A:406:PRO:HD3	1.75	0.50
1:B:162:ALA:CB	1:C:299:GLY:O	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:ASP:HB3	1:C:451:ARG:HH11	1.73	0.50
1:D:137:ARG:HB3	1:D:193:PHE:CE2	2.46	0.50
1:B:478:PRO:HB3	1:C:22:LEU:HB3	1.93	0.50
1:D:347:TYR:CE1	1:D:366:LYS:HG2	2.47	0.50
1:D:405:THR:H	1:D:406:PRO:HD3	1.77	0.50
1:A:326:VAL:HG21	1:D:14:LEU:CD2	2.42	0.50
1:B:229:MET:HE1	1:B:236:VAL:HB	1.92	0.50
1:D:338:LEU:HD12	1:D:422:ALA:HB2	1.94	0.50
1:D:277:ASP:HB3	1:D:280:THR:OG1	2.12	0.50
1:D:405:THR:N	1:D:406:PRO:HD3	2.26	0.50
1:B:337:ALA:HB2	1:B:415:GLU:HB3	1.93	0.50
1:B:9:GLN:HG2	1:B:10:GLY:N	2.24	0.49
1:B:142:ASP:HA	1:B:171:PRO:HB3	1.93	0.49
1:B:436:GLN:HA	1:B:439:THR:HB	1.93	0.49
1:A:180:TYR:CE2	1:A:207:ARG:HG3	2.47	0.49
1:A:326:VAL:HG21	1:D:14:LEU:HD21	1.94	0.49
1:B:168:GLU:HG3	1:D:168:GLU:CG	2.41	0.49
1:B:435:ILE:HG12	1:B:457:TYR:CD1	2.46	0.49
1:B:132:VAL:HG12	1:B:136:GLY:HA3	1.93	0.49
1:A:240:VAL:HG21	1:A:328:GLN:HB3	1.93	0.49
1:A:334:ASN:HB3	1:A:418:PHE:CD2	2.47	0.49
1:C:14:LEU:O	1:C:17:SER:N	2.46	0.49
1:C:158:LYS:CG	1:C:159:LYS:N	2.76	0.49
1:A:23:ALA:O	1:D:59:ARG:HG3	2.12	0.49
1:A:54:GLU:OE1	1:D:71:ASN:O	2.31	0.49
1:B:149:LEU:CD2	1:C:298:PRO:HB2	2.41	0.49
1:C:162:ALA:HA	1:C:165:ILE:HD12	1.93	0.49
1:D:229:MET:HE1	1:D:236:VAL:HB	1.95	0.49
1:D:116:GLN:OE1	1:D:304:PRO:HG3	2.13	0.49
1:A:273:VAL:HA	1:A:285:LEU:HD23	1.95	0.49
1:A:298:PRO:HB2	1:D:149:LEU:HD23	1.89	0.49
1:A:235:LEU:HD23	1:A:328:GLN:OE1	2.12	0.49
1:A:436:GLN:HA	1:A:439:THR:HB	1.94	0.49
1:C:116:GLN:OE1	1:C:304:PRO:HG3	2.13	0.49
1:C:126:ALA:HA	1:C:300:LEU:CD1	2.42	0.49
1:D:277:ASP:O	1:D:280:THR:N	2.46	0.49
1:C:447:GLU:O	1:C:450:GLU:HB2	2.14	0.48
1:B:59:ARG:CG	1:B:480:LEU:H	2.26	0.48
1:B:162:ALA:HB2	1:C:299:GLY:O	2.13	0.48
1:C:444:THR:C	1:C:446:LYS:N	2.68	0.48
1:A:14:LEU:HD21	1:D:322:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:HH22	1:C:72:LYS:HD3	1.77	0.48
1:B:386:LYS:O	1:B:387:ASN:CB	2.51	0.48
1:B:99:ARG:CZ	1:C:30:ASP:OD2	2.61	0.48
1:B:391:GLY:O	1:B:392:ASP:O	2.32	0.48
1:C:256:HIS:ND1	1:C:263:ARG:HA	2.28	0.48
1:A:137:ARG:HB3	1:A:193:PHE:CE2	2.49	0.48
1:A:277:ASP:O	1:A:278:PRO:C	2.57	0.48
1:B:116:GLN:OE1	1:B:304:PRO:HG3	2.13	0.48
1:D:334:ASN:HB3	1:D:418:PHE:CD2	2.49	0.48
1:A:338:LEU:HD12	1:A:422:ALA:HB2	1.94	0.48
1:B:235:LEU:HD23	1:B:328:GLN:OE1	2.14	0.48
1:B:336:ARG:NH1	1:B:354:SER:O	2.47	0.48
1:D:227:ALA:HB2	1:D:248:CYS:SG	2.54	0.48
1:A:364:ARG:NH1	1:A:392:ASP:OD1	2.47	0.48
1:B:208:ASN:OD1	1:B:241:VAL:HG22	2.14	0.48
1:B:364:ARG:HG3	1:B:399:SER:HB3	1.94	0.48
1:C:158:LYS:CG	1:C:159:LYS:H	2.27	0.48
1:B:21:MET:CE	1:C:323:GLU:CB	2.78	0.47
2:B:500:PLP:O4P	2:B:500:PLP:C4A	2.62	0.47
1:A:11:ASP:O	1:A:12:ALA:C	2.57	0.47
1:A:323:GLU:HB2	1:D:21:MET:HE1	1.91	0.47
1:B:389:CYS:H	1:B:392:ASP:CG	2.22	0.47
1:C:215:ARG:NH1	1:C:249:HIS:CE1	2.82	0.47
1:C:334:ASN:HB3	1:C:418:PHE:CD2	2.49	0.47
1:C:348:LYS:HB3	1:C:362:ASP:HB3	1.96	0.47
1:A:116:GLN:N	1:A:117:PRO:HD3	2.29	0.47
1:B:388:THR:HB	1:B:392:ASP:HB2	1.96	0.47
1:D:241:VAL:HG13	1:D:242:PRO:HD2	1.96	0.47
1:B:143:LEU:HD12	1:B:147:GLY:O	2.14	0.47
1:D:10:GLY:O	1:D:12:ALA:N	2.46	0.47
1:C:77:TYR:OH	1:C:293:ASN:O	2.18	0.47
1:C:416:LYS:H	1:C:416:LYS:HG2	1.34	0.47
1:D:439:THR:CG2	1:D:443:ALA:CB	2.56	0.47
1:B:240:VAL:HG22	1:B:329:HIS:CD2	2.49	0.47
1:D:120:GLY:N	2:D:500:PLP:O3P	2.48	0.47
1:D:148:HIS:ND1	2:D:500:PLP:C6	2.78	0.47
1:A:162:ALA:HA	1:A:165:ILE:HD12	1.97	0.47
1:B:35:ASN:HB3	1:B:39:LYS:HE3	1.97	0.47
1:C:213:ARG:HA	1:C:216:LYS:HD2	1.96	0.47
1:C:230:ALA:HB1	1:C:254:THR:HG22	1.96	0.47
1:D:26:LEU:O	1:D:29:SER:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:HD22	1:D:149:LEU:CD1	2.45	0.47
1:D:386:LYS:O	1:D:387:ASN:HB2	2.15	0.47
1:D:473:SER:C	1:D:474:LEU:HD23	2.39	0.47
1:A:132:VAL:HG12	1:A:136:GLY:HA3	1.97	0.47
1:A:149:LEU:N	1:A:149:LEU:HD12	2.30	0.47
1:B:54:GLU:OE2	1:C:72:LYS:HD2	2.14	0.47
1:B:159:LYS:HD3	1:B:164:SER:O	2.14	0.47
1:C:32:GLU:H	1:C:32:GLU:HG3	1.54	0.47
1:C:444:THR:C	1:C:446:LYS:H	2.22	0.47
1:C:447:GLU:O	1:C:450:GLU:N	2.46	0.47
1:D:116:GLN:O	1:D:117:PRO:C	2.58	0.47
1:B:22:LEU:HD13	1:C:478:PRO:HG2	1.91	0.46
1:D:436:GLN:HA	1:D:439:THR:HB	1.97	0.46
1:D:235:LEU:HD23	1:D:328:GLN:OE1	2.15	0.46
1:B:116:GLN:N	1:B:117:PRO:HD3	2.30	0.46
1:A:213:ARG:CG	1:A:213:ARG:NH1	2.73	0.46
1:A:215:ARG:NH1	1:A:249:HIS:CE1	2.83	0.46
1:B:11:ASP:O	1:B:14:LEU:N	2.46	0.46
1:B:179:GLY:HA2	1:B:390:PRO:HG2	1.97	0.46
1:D:73:TYR:HB3	1:D:83:TYR:CD2	2.51	0.46
1:D:158:LYS:HG2	1:D:159:LYS:N	2.31	0.46
1:B:14:LEU:HD23	1:C:326:VAL:HG21	1.96	0.46
1:B:453:ALA:HA	1:B:458:GLN:OE1	2.15	0.46
1:D:45:ARG:HG2	1:D:45:ARG:HH21	1.80	0.46
1:D:377:LEU:HD22	1:D:382:ILE:HG21	1.98	0.46
1:A:59:ARG:HD2	1:D:23:ALA:O	2.16	0.46
1:A:116:GLN:OE1	1:A:304:PRO:HG3	2.16	0.46
1:A:290:SER:O	1:A:294:SER:OG	2.31	0.46
1:B:119:SER:C	1:B:122:PRO:HD2	2.41	0.46
1:C:102:GLN:HB3	1:C:320:MET:SD	2.55	0.46
1:C:177:ASP:O	1:C:179:GLY:N	2.49	0.46
1:A:220:GLU:O	1:A:220:GLU:HG2	2.15	0.46
1:A:317:LYS:O	1:A:317:LYS:HG2	2.13	0.46
1:C:121:SER:HB3	1:C:150:THR:CG2	2.45	0.46
1:D:170:MET:HG3	1:D:171:PRO:HD2	1.97	0.46
1:D:196:LYS:NZ	1:D:196:LYS:HA	2.31	0.46
1:A:26:LEU:N	1:D:63:GLU:OE1	2.37	0.46
1:D:11:ASP:O	1:D:12:ALA:C	2.59	0.46
1:B:142:ASP:HB2	1:B:171:PRO:HB2	1.97	0.46
1:C:424:PHE:CE1	1:C:467:GLU:OE2	2.69	0.46
1:D:120:GLY:HA3	2:D:500:PLP:H5A2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:THR:O	1:D:254:THR:CG2	2.63	0.46
1:B:73:TYR:HB3	1:B:83:TYR:CD2	2.52	0.45
1:B:238:ALA:HB1	1:B:325:LYS:HA	1.97	0.45
1:D:236:VAL:HG11	1:D:244:PRO:HD2	1.98	0.45
1:D:254:THR:O	1:D:254:THR:HG23	2.15	0.45
1:D:319:ALA:HA	1:D:324:PHE:CG	2.50	0.45
1:A:262:CYS:HA	1:D:70:ASN:OD1	2.16	0.45
1:A:319:ALA:HA	1:A:324:PHE:CG	2.50	0.45
1:C:415:GLU:O	1:C:419:GLN:HG3	2.17	0.45
1:D:180:TYR:CE2	1:D:207:ARG:HG3	2.50	0.45
1:D:393:ARG:HD3	1:D:393:ARG:HA	1.77	0.45
1:A:99:ARG:NH1	1:D:30:ASP:OD2	2.33	0.45
1:B:137:ARG:HA	1:B:168:GLU:O	2.17	0.45
1:C:375:LYS:HA	1:C:375:LYS:HD3	1.71	0.45
1:A:34:TYR:CZ	1:A:38:LYS:HD2	2.52	0.45
1:D:379:ALA:O	1:D:465:ARG:HD3	2.16	0.45
1:B:187:GLU:HG2	1:B:191:ARG:NH2	2.32	0.45
1:B:334:ASN:HB3	1:B:418:PHE:CD2	2.52	0.45
1:D:451:ARG:HD3	1:D:451:ARG:HA	1.74	0.45
1:B:215:ARG:NE	1:B:247:HIS:O	2.50	0.45
1:C:137:ARG:HA	1:C:168:GLU:O	2.17	0.45
1:C:319:ALA:HA	1:C:324:PHE:CG	2.52	0.45
1:C:462:GLN:HE21	1:C:465:ARG:NH2	2.15	0.45
1:D:11:ASP:O	1:D:14:LEU:N	2.50	0.45
1:D:143:LEU:N	1:D:144:PRO:HD2	2.31	0.45
1:A:37:ILE:CG2	1:D:67:SER:HB2	2.47	0.45
1:A:323:GLU:CB	1:D:21:MET:HE2	2.44	0.45
1:B:21:MET:HE2	1:C:323:GLU:HB2	1.89	0.45
1:A:22:LEU:HD21	1:D:260:ARG:NH2	2.31	0.45
1:B:132:VAL:CG1	1:B:136:GLY:HA3	2.47	0.45
1:B:148:HIS:CD2	1:B:149:LEU:H	2.35	0.45
1:B:420:LYS:HE2	1:B:424:PHE:CZ	2.52	0.45
1:D:137:ARG:HA	1:D:168:GLU:O	2.15	0.45
1:B:9:GLN:O	1:B:10:GLY:C	2.60	0.44
1:C:277:ASP:OD1	1:C:279:ALA:HB3	2.18	0.44
1:D:121:SER:HB3	1:D:150:THR:CG2	2.47	0.44
1:B:213:ARG:CG	1:B:213:ARG:NH1	2.66	0.44
1:D:12:ALA:O	1:D:13:ASP:C	2.60	0.44
1:A:378:GLU:OE2	1:D:84:GLY:CA	2.66	0.44
1:B:73:TYR:CE1	1:B:303:GLY:HA3	2.52	0.44
1:C:227:ALA:HB2	1:C:248:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HG23	1:D:67:SER:HB2	1.99	0.44
1:A:415:GLU:OE1	1:A:415:GLU:N	2.48	0.44
1:B:213:ARG:HH11	1:B:213:ARG:HG2	1.78	0.44
1:B:274:LYS:O	1:B:275:SER:HB3	2.18	0.44
1:B:446:LYS:O	1:B:450:GLU:N	2.43	0.44
1:B:91:GLU:HB2	1:C:36:ILE:HD13	1.98	0.44
1:B:319:ALA:HA	1:B:324:PHE:CG	2.52	0.44
1:C:30:ASP:OD1	1:C:33:VAL:HG23	2.18	0.44
1:C:116:GLN:O	1:C:117:PRO:C	2.61	0.44
1:D:230:ALA:HA	1:D:254:THR:HG22	2.00	0.44
1:B:277:ASP:OD2	1:B:279:ALA:HB3	2.18	0.44
1:B:408:LEU:O	1:B:411:ARG:HB2	2.18	0.44
1:C:30:ASP:CG	1:C:33:VAL:HG23	2.43	0.44
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.76	0.44
1:C:156:ASP:OD1	1:C:157:LYS:HG2	2.18	0.44
1:C:431:LEU:HD23	1:C:431:LEU:HA	1.90	0.44
1:D:174:VAL:HG13	1:D:180:TYR:C	2.43	0.44
1:B:282:LYS:CG	1:B:283:GLU:N	2.81	0.43
1:A:137:ARG:HA	1:A:168:GLU:O	2.18	0.43
1:A:320:MET:HE3	1:A:320:MET:HB2	1.81	0.43
1:D:177:ASP:O	1:D:178:THR:C	2.60	0.43
1:A:34:TYR:CZ	1:A:38:LYS:CD	3.02	0.43
1:D:116:GLN:N	1:D:117:PRO:HD2	2.32	0.43
1:D:126:ALA:HA	1:D:300:LEU:CD1	2.49	0.43
1:D:187:GLU:HG2	1:D:191:ARG:NH2	2.33	0.43
1:B:282:LYS:HG3	1:B:283:GLU:N	2.22	0.43
1:C:462:GLN:NE2	1:C:465:ARG:NH2	2.66	0.43
1:C:227:ALA:HB3	1:C:251:VAL:HG22	2.01	0.43
1:D:16:SER:C	1:D:18:HIS:N	2.73	0.43
1:A:45:ARG:HH22	1:A:473:SER:HB3	1.83	0.43
1:B:99:ARG:HH21	1:C:32:GLU:CD	2.26	0.43
1:D:145:ASP:OD2	1:D:173:LYS:HB3	2.19	0.43
1:A:69:LEU:HD11	1:D:37:ILE:HG12	2.01	0.43
1:A:34:TYR:HE2	1:A:38:LYS:CD	2.28	0.43
1:B:59:ARG:HD3	1:C:23:ALA:O	2.19	0.43
1:C:132:VAL:CG1	1:C:136:GLY:HA3	2.47	0.43
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.77	0.43
1:B:59:ARG:HE	1:B:59:ARG:HB3	1.28	0.43
1:D:55:ASN:CG	1:D:260:ARG:HG2	2.44	0.43
1:B:162:ALA:HA	1:B:165:ILE:HD12	2.01	0.42
1:C:149:LEU:CD1	1:C:149:LEU:N	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:CD2	1:A:149:LEU:CD1	2.88	0.42
1:A:162:ALA:CB	1:D:300:LEU:HD23	2.49	0.42
1:A:361:VAL:O	1:A:400:GLY:HA2	2.19	0.42
1:A:451:ARG:HA	1:A:451:ARG:HD3	1.80	0.42
1:C:11:ASP:O	1:C:14:LEU:N	2.51	0.42
1:C:257:LYS:HZ2	2:C:500:PLP:C4A	2.32	0.42
1:C:451:ARG:HA	1:C:451:ARG:HD3	1.77	0.42
1:A:260:ARG:HD3	1:A:410:SER:OG	2.19	0.42
1:B:49:GLU:OE2	1:B:51:ILE:HD12	2.18	0.42
1:B:227:ALA:HB2	1:B:248:CYS:SG	2.59	0.42
1:B:168:GLU:HG3	1:D:168:GLU:CD	2.44	0.42
1:B:189:ASN:HA	1:B:192:LEU:HD12	2.01	0.42
1:C:12:ALA:O	1:C:13:ASP:C	2.62	0.42
1:A:116:GLN:O	1:A:117:PRO:C	2.61	0.42
1:A:272:GLY:C	1:A:285:LEU:HD22	2.44	0.42
1:A:273:VAL:HA	1:A:285:LEU:CD2	2.50	0.42
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.82	0.42
1:B:30:ASP:N	1:C:317:LYS:HZ3	2.18	0.42
1:B:37:ILE:CG2	1:C:67:SER:HB2	2.49	0.42
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.86	0.42
1:C:14:LEU:O	1:C:15:TRP:C	2.62	0.42
1:D:149:LEU:HD11	1:D:153:PHE:CD2	2.55	0.42
1:D:240:VAL:HG22	1:D:329:HIS:CE1	2.54	0.42
1:A:55:ASN:ND2	1:A:260:ARG:HG2	2.35	0.42
1:A:460:ALA:O	1:A:463:ALA:HB3	2.20	0.42
2:A:500:PLP:O3P	1:D:303:GLY:N	2.47	0.42
1:B:257:LYS:HZ1	2:B:500:PLP:C4	2.33	0.42
1:D:408:LEU:O	1:D:411:ARG:HB2	2.20	0.42
1:A:149:LEU:HD21	1:D:298:PRO:HB2	2.00	0.42
1:B:46:VAL:O	1:B:469:GLU:HA	2.20	0.42
1:C:143:LEU:N	1:C:144:PRO:HD2	2.34	0.42
1:C:361:VAL:O	1:C:400:GLY:HA2	2.19	0.42
1:B:446:LYS:HE2	1:B:450:GLU:OE2	2.20	0.42
1:D:32:GLU:O	1:D:36:ILE:HG13	2.20	0.42
1:D:110:CYS:O	1:D:270:ARG:HG3	2.19	0.42
1:A:24:GLN:HA	1:A:25:PRO:HD3	1.90	0.42
1:C:195:PRO:O	1:C:223:ALA:HB2	2.20	0.42
1:C:408:LEU:O	1:C:411:ARG:HB2	2.19	0.42
1:D:257:LYS:HZ2	2:D:500:PLP:C3	2.33	0.42
1:D:361:VAL:O	1:D:400:GLY:HA2	2.20	0.42
1:A:12:ALA:O	1:A:13:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:O	1:A:174:VAL:HG21	2.20	0.41
1:A:215:ARG:NH1	1:A:249:HIS:NE2	2.67	0.41
1:B:267:ILE:HG21	1:B:292:ILE:HG21	2.01	0.41
1:B:431:LEU:HD23	1:B:431:LEU:HA	1.89	0.41
1:C:73:TYR:CD2	1:C:83:TYR:HE2	2.33	0.41
1:C:46:VAL:O	1:C:469:GLU:HA	2.19	0.41
1:D:408:LEU:HD22	1:D:413:LEU:HD13	2.01	0.41
1:A:25:PRO:HA	1:D:59:ARG:HD3	2.02	0.41
1:A:32:GLU:OE2	1:D:99:ARG:NH2	2.49	0.41
1:B:43:ARG:HB2	1:C:88:PHE:HE2	1.85	0.41
1:C:145:ASP:OD2	1:C:173:LYS:HB3	2.20	0.41
1:D:46:VAL:O	1:D:469:GLU:HA	2.20	0.41
1:D:177:ASP:O	1:D:179:GLY:N	2.53	0.41
1:A:32:GLU:O	1:A:36:ILE:HG13	2.20	0.41
1:A:46:VAL:O	1:A:469:GLU:HA	2.19	0.41
1:B:30:ASP:HB2	1:C:317:LYS:HD3	2.02	0.41
1:B:32:GLU:O	1:B:36:ILE:HG13	2.20	0.41
1:B:59:ARG:CG	1:B:480:LEU:N	2.83	0.41
1:B:230:ALA:HA	1:B:254:THR:HG22	2.03	0.41
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.86	0.41
1:C:158:LYS:HG2	1:C:159:LYS:N	2.36	0.41
1:D:172:TYR:HB3	1:D:186:LEU:HD13	2.03	0.41
1:B:260:ARG:HD3	1:B:410:SER:OG	2.20	0.41
1:C:393:ARG:HA	1:C:393:ARG:HD3	1.52	0.41
1:A:119:SER:C	1:A:122:PRO:HD2	2.45	0.41
1:A:162:ALA:CB	1:D:299:GLY:O	2.68	0.41
1:B:229:MET:CE	1:B:236:VAL:HB	2.50	0.41
1:C:276:VAL:HA	1:C:283:GLU:HA	2.03	0.41
1:D:229:MET:HB2	1:D:229:MET:HE3	1.81	0.41
1:A:26:LEU:O	1:A:29:SER:O	2.39	0.41
1:A:168:GLU:CG	1:C:168:GLU:HG3	2.38	0.41
1:A:241:VAL:HG13	1:A:242:PRO:HD2	2.03	0.41
1:B:11:ASP:O	1:B:14:LEU:HB3	2.20	0.41
1:B:361:VAL:O	1:B:400:GLY:HA2	2.21	0.41
1:B:373:ALA:O	1:B:374:GLU:C	2.64	0.41
1:D:100:ALA:HA	1:D:316:LEU:HD22	2.02	0.41
1:A:59:ARG:NH2	1:D:25:PRO:HG3	2.33	0.41
1:A:317:LYS:HZ1	1:D:30:ASP:HA	1.85	0.41
1:B:143:LEU:N	1:B:144:PRO:HD2	2.36	0.41
1:B:303:GLY:N	2:C:500:PLP:O3P	2.51	0.41
1:B:317:LYS:NZ	1:C:30:ASP:H	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ASP:OD1	1:D:13:ASP:HB2	2.20	0.41
1:D:143:LEU:HD12	1:D:147:GLY:O	2.21	0.41
1:A:11:ASP:O	1:A:14:LEU:N	2.54	0.41
1:B:168:GLU:CG	1:D:168:GLU:HG3	2.46	0.41
1:B:280:THR:C	1:B:282:LYS:H	2.28	0.41
1:A:65:LEU:HD13	1:D:307:HIS:CD2	2.56	0.40
1:A:277:ASP:C	1:A:279:ALA:N	2.78	0.40
1:B:62:LEU:HB3	1:C:66:GLY:O	2.21	0.40
1:B:215:ARG:CD	1:B:247:HIS:O	2.67	0.40
1:B:323:GLU:CB	1:C:21:MET:CE	2.93	0.40
1:B:475:PHE:HB3	1:B:476:PRO:HD2	2.03	0.40
1:D:372:ARG:NH1	1:D:448:PHE:HB2	2.36	0.40
1:D:438:ASP:CB	1:D:451:ARG:NH1	2.78	0.40
1:B:70:ASN:O	1:C:263:ARG:NE	2.54	0.40
1:C:475:PHE:HB3	1:C:476:PRO:HD2	2.03	0.40
1:D:260:ARG:HD3	1:D:410:SER:OG	2.21	0.40
1:A:18:HIS:HB2	1:D:323:GLU:HB3	2.02	0.40
1:A:277:ASP:OD1	1:A:280:THR:HG23	2.21	0.40
1:A:317:LYS:HZ2	1:D:30:ASP:CA	2.34	0.40
1:A:317:LYS:NZ	1:D:30:ASP:N	2.59	0.40
1:A:393:ARG:HD3	1:A:393:ARG:HA	1.88	0.40
1:C:277:ASP:CG	1:C:279:ALA:HB3	2.45	0.40
1:A:208:ASN:OD1	1:A:241:VAL:HG13	2.21	0.40
1:B:59:ARG:O	1:B:63:GLU:HG3	2.21	0.40
1:B:240:VAL:HG22	1:B:329:HIS:CE1	2.57	0.40
1:B:262:CYS:HA	1:C:70:ASN:OD1	2.21	0.40
1:B:358:LEU:HD12	1:B:358:LEU:C	2.47	0.40
1:C:97:GLN:HG2	1:C:113:VAL:HG13	2.02	0.40
1:C:282:LYS:HG3	1:C:283:GLU:H	1.87	0.40
1:C:438:ASP:HB3	1:C:451:ARG:HH12	1.79	0.40
1:D:154:MET:HE3	1:D:159:LYS:HG2	2.03	0.40
1:D:366:LYS:HA	1:D:366:LYS:HD2	1.95	0.40
1:A:74:SER:CB	1:A:89:ILE:HG21	2.51	0.40
1:A:455:ASP:O	1:A:456:LYS:C	2.64	0.40
1:B:21:MET:HE1	1:C:321:THR:OG1	2.22	0.40
1:B:199:ILE:HA	1:B:226:MET:O	2.22	0.40
1:B:240:VAL:HG22	1:B:329:HIS:NE2	2.36	0.40
1:B:349:ILE:CD1	1:B:361:VAL:HG22	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/472 (100%)	439 (93%)	27 (6%)	4 (1%)	14	46
1	B	470/472 (100%)	436 (93%)	29 (6%)	5 (1%)	11	42
1	C	470/472 (100%)	443 (94%)	22 (5%)	5 (1%)	11	42
1	D	470/472 (100%)	443 (94%)	26 (6%)	1 (0%)	43	74
All	All	1880/1888 (100%)	1761 (94%)	104 (6%)	15 (1%)	16	49

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	ASP
1	B	441	VAL
1	C	441	VAL
1	D	11	ASP
1	A	10	GLY
1	A	387	ASN
1	B	387	ASN
1	B	393	ARG
1	C	178	THR
1	C	387	ASN
1	A	212	ALA
1	A	443	ALA
1	B	212	ALA
1	C	212	ALA
1	C	277	ASP

5.3.2 Protein sidechains [i](#)

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	385/385 (100%)	361 (94%)	24 (6%)	16	44
1	B	385/385 (100%)	349 (91%)	36 (9%)	8	31
1	C	385/385 (100%)	347 (90%)	38 (10%)	7	30
1	D	385/385 (100%)	359 (93%)	26 (7%)	14	41
All	All	1540/1540 (100%)	1416 (92%)	124 (8%)	11	36

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	28	ASP
1	A	32	GLU
1	A	73	TYR
1	A	114	ASN
1	A	134	PRO
1	A	155	THR
1	A	188	GLU
1	A	196	LYS
1	A	203	SER
1	A	213	ARG
1	A	231	HIS
1	A	274	LYS
1	A	290	SER
1	A	294	SER
1	A	298	PRO
1	A	322	LEU
1	A	326	VAL
1	A	331	VAL
1	A	393	ARG
1	A	416	LYS
1	A	438	ASP
1	A	439	THR
1	A	466	GLU
1	B	9	GLN
1	B	28	ASP
1	B	49	GLU
1	B	65	LEU
1	B	70	ASN
1	B	73	TYR
1	B	80	GLN

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Mol	Chain	Res	Type
1	B	119	SER
1	B	134	PRO
1	B	137	ARG
1	B	149	LEU
1	B	158	LYS
1	B	186	LEU
1	B	196	LYS
1	B	213	ARG
1	B	215	ARG
1	B	231	HIS
1	B	241	VAL
1	B	254	THR
1	B	270	ARG
1	B	271	LYS
1	B	294	SER
1	B	298	PRO
1	B	317	LYS
1	B	322	LEU
1	B	340	GLU
1	B	366	LYS
1	B	392	ASP
1	B	397	ARG
1	B	415	GLU
1	B	433	LEU
1	B	439	THR
1	B	447	GLU
1	B	451	ARG
1	B	461	VAL
1	B	466	GLU
1	C	13	ASP
1	C	17	SER
1	C	28	ASP
1	C	32	GLU
1	C	49	GLU
1	C	50	LEU
1	C	65	LEU
1	C	73	TYR
1	C	102	GLN
1	C	109	GLN
1	C	134	PRO
1	C	149	LEU
1	C	158	LYS

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Mol	Chain	Res	Type
1	C	177	ASP
1	C	185	GLN
1	C	203	SER
1	C	213	ARG
1	C	231	HIS
1	C	240	VAL
1	C	241	VAL
1	C	271	LYS
1	C	290	SER
1	C	298	PRO
1	C	323	GLU
1	C	326	VAL
1	C	331	VAL
1	C	366	LYS
1	C	375	LYS
1	C	386	LYS
1	C	387	ASN
1	C	393	ARG
1	C	406	PRO
1	C	416	LYS
1	C	427	ARG
1	C	438	ASP
1	C	455	ASP
1	C	462	GLN
1	C	480	LEU
1	D	9	GLN
1	D	28	ASP
1	D	73	TYR
1	D	80	GLN
1	D	121	SER
1	D	134	PRO
1	D	149	LEU
1	D	196	LYS
1	D	203	SER
1	D	213	ARG
1	D	217	ILE
1	D	231	HIS
1	D	241	VAL
1	D	254	THR
1	D	271	LYS
1	D	282	LYS
1	D	298	PRO

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Mol	Chain	Res	Type
1	D	325	LYS
1	D	331	VAL
1	D	366	LYS
1	D	427	ARG
1	D	433	LEU
1	D	439	THR
1	D	441	VAL
1	D	461	VAL
1	D	462	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	70	ASN
1	A	231	HIS
1	A	305	HIS
1	A	318	GLN
1	A	329	HIS
1	A	387	ASN
1	A	423	HIS
1	B	24	GLN
1	B	42	ASN
1	B	70	ASN
1	B	148	HIS
1	B	231	HIS
1	B	305	HIS
1	B	318	GLN
1	B	423	HIS
1	C	44	GLN
1	C	70	ASN
1	C	231	HIS
1	C	307	HIS
1	C	318	GLN
1	C	423	HIS
1	C	434	GLN
1	C	458	GLN
1	C	462	GLN
1	D	70	ASN
1	D	185	GLN
1	D	208	ASN
1	D	231	HIS

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Mol	Chain	Res	Type
1	D	247	HIS
1	D	307	HIS

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLP	A	500	-	15,15,16	0.99	1 (6%)	21,22,23	1.61	3 (14%)
2	PLP	D	500	-	15,15,16	1.09	1 (6%)	21,22,23	1.78	7 (33%)
2	PLP	B	500	-	15,15,16	0.99	1 (6%)	21,22,23	1.02	1 (4%)
2	PLP	C	500	-	15,15,16	1.13	2 (13%)	21,22,23	1.58	3 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	500	-	-	1/6/6/8	0/1/1/1
2	PLP	D	500	-	-	2/6/6/8	0/1/1/1
2	PLP	B	500	-	-	5/6/6/8	0/1/1/1
2	PLP	C	500	-	-	1/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	PLP	P-O1P	2.68	1.58	1.50
2	D	500	PLP	C4A-C4	-2.40	1.46	1.51
2	A	500	PLP	C4A-C4	-2.15	1.47	1.51
2	C	500	PLP	C4A-C4	-2.13	1.47	1.51
2	B	500	PLP	C4A-C4	-2.00	1.47	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	PLP	O4P-C5A-C5	4.96	118.65	109.36
2	C	500	PLP	O3-C3-C2	4.26	126.42	117.58
2	C	500	PLP	O4P-C5A-C5	3.95	116.76	109.36
2	A	500	PLP	O3-C3-C2	3.65	125.14	117.58
2	D	500	PLP	O2P-P-O4P	3.62	116.10	106.67
2	D	500	PLP	O4P-C5A-C5	3.55	116.00	109.36
2	D	500	PLP	O3P-P-O4P	-3.21	98.29	106.67
2	D	500	PLP	O3-C3-C2	3.09	123.99	117.58
2	C	500	PLP	C2A-C2-C3	2.73	123.99	120.80
2	D	500	PLP	C6-C5-C4	-2.46	116.08	118.10
2	A	500	PLP	C4A-C4-C5	2.42	123.44	120.94
2	B	500	PLP	O3-C3-C2	2.30	122.34	117.58
2	D	500	PLP	C2A-C2-C3	2.16	123.33	120.80
2	D	500	PLP	O3P-P-O2P	2.05	115.48	107.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	PLP	C4-C5-C5A-O4P
2	B	500	PLP	C6-C5-C5A-O4P
2	B	500	PLP	C5A-O4P-P-O2P
2	B	500	PLP	C5A-O4P-P-O3P
2	D	500	PLP	C4-C5-C5A-O4P
2	D	500	PLP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
2	B	500	PLP	C5A-O4P-P-O1P
2	A	500	PLP	C5A-O4P-P-O1P
2	C	500	PLP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PLP	1	0
2	D	500	PLP	11	0
2	B	500	PLP	2	0
2	C	500	PLP	7	0

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	472/472 (100%)	-0.43	6 (1%) 75 51	42, 90, 123, 181	0
1	B	472/472 (100%)	-0.38	11 (2%) 61 38	50, 90, 125, 174	0
1	C	472/472 (100%)	-0.47	6 (1%) 75 51	48, 89, 125, 195	0
1	D	472/472 (100%)	-0.44	9 (1%) 66 42	49, 88, 123, 179	0
All	All	1888/1888 (100%)	-0.43	32 (1%) 69 44	42, 89, 124, 195	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	GLN	9.0
1	D	10	GLY	8.4
1	C	9	GLN	5.8
1	A	9	GLN	5.4
1	B	10	GLY	5.2
1	D	9	GLN	4.9
1	A	10	GLY	4.9
1	C	10	GLY	4.8
1	D	278	PRO	4.4
1	D	441	VAL	4.2
1	B	278	PRO	3.8
1	C	278	PRO	3.5
1	B	480	LEU	3.4
1	C	201	GLY	3.4
1	A	278	PRO	3.4
1	B	304	PRO	3.0
1	D	201	GLY	2.9
1	D	279	ALA	2.7
1	D	480	LEU	2.7
1	A	201	GLY	2.6
1	B	85	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	280	THR	2.6
1	B	277	ASP	2.5
1	B	279	ALA	2.4
1	B	441	VAL	2.4
1	A	276	VAL	2.3
1	C	480	LEU	2.3
1	B	11	ASP	2.3
1	C	279	ALA	2.2
1	B	201	GLY	2.1
1	A	441	VAL	2.1
1	D	375	LYS	2.1

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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	A	500	15/16	0.99	0.06	69,83,118,120	0
2	PLP	B	500	15/16	0.99	0.05	74,84,103,123	0
2	PLP	C	500	15/16	0.99	0.04	49,65,95,97	0
2	PLP	D	500	15/16	0.99	0.04	62,70,93,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.