



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 03:03 PM JST

PDB ID : 8XND  
Title : Crystal structure of serine hydroxymethyltransferase 1  
Authors : Fan, S.; Wei, X.; Lv, R.; Wang, C.; Tang, M.; Jin, Y.; Yang, Z.  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

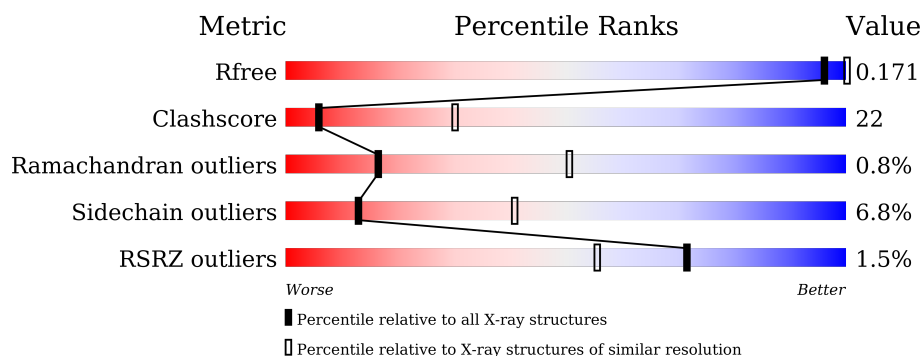
# 1 Overall quality at a glance

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))
$R_{free}$	164625	1597 (3.52-3.40)
Clashscore	180529	1041 (3.50-3.42)
Ramachandran outliers	177936	1026 (3.50-3.42)
Sidechain outliers	177891	1027 (3.50-3.42)
RSRZ outliers	164620	1596 (3.52-3.40)

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  $\geq 3$ , 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	<div> <div>0.1%</div> <div>61%</div> <div>30%</div> <div>7%</div> <div>0.1%</div> </div>
1	B	472	<div> <div>2%</div> <div>57%</div> <div>35%</div> <div>7%</div> <div>0.1%</div> </div>
1	C	472	<div> <div>0.1%</div> <div>59%</div> <div>33%</div> <div>5%</div> <div>0.1%</div> </div>
1	D	472	<div> <div>2%</div> <div>57%</div> <div>35%</div> <div>7%</div> <div>0.1%</div> </div>

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 crite-

ria:

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.

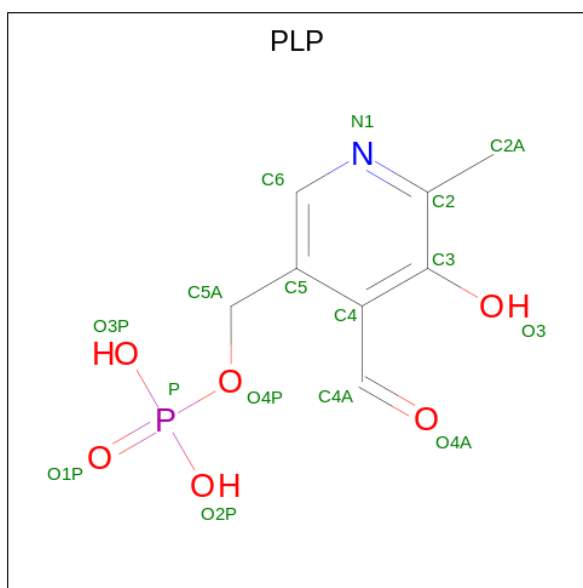
- Molecule 1 is a protein called Serine hydroxymethyltransferase, cytosolic.

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

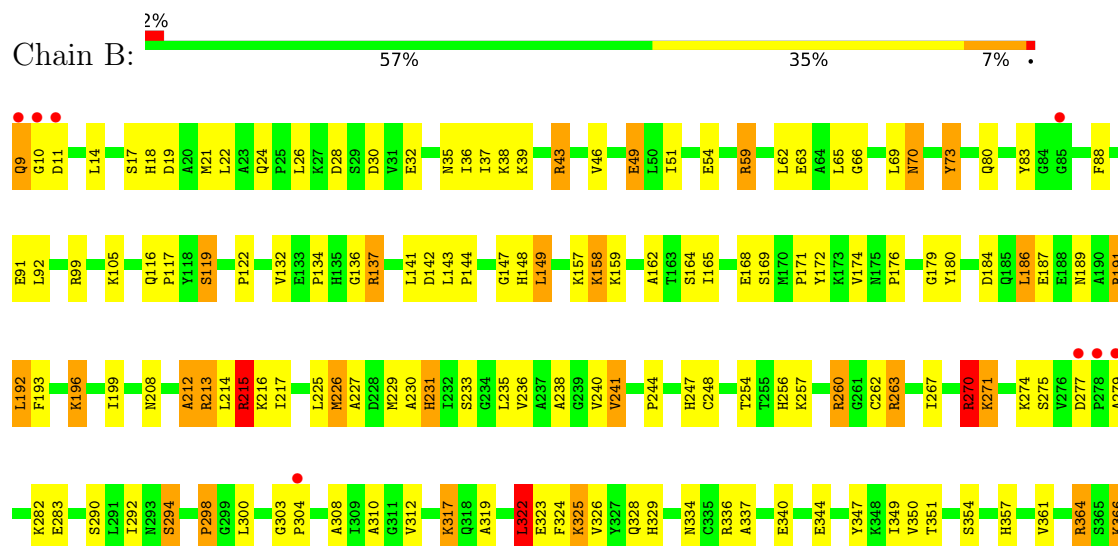
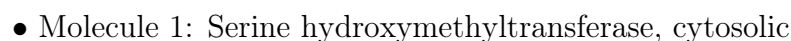
- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).

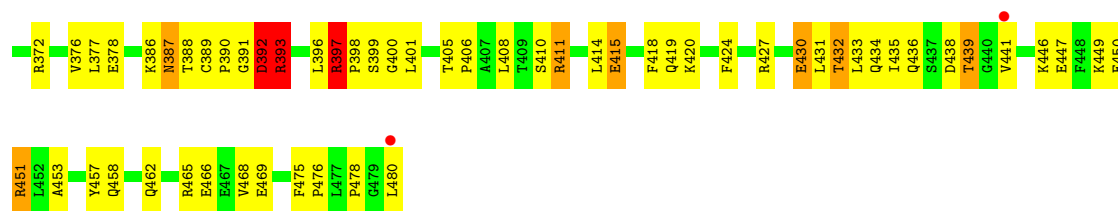


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

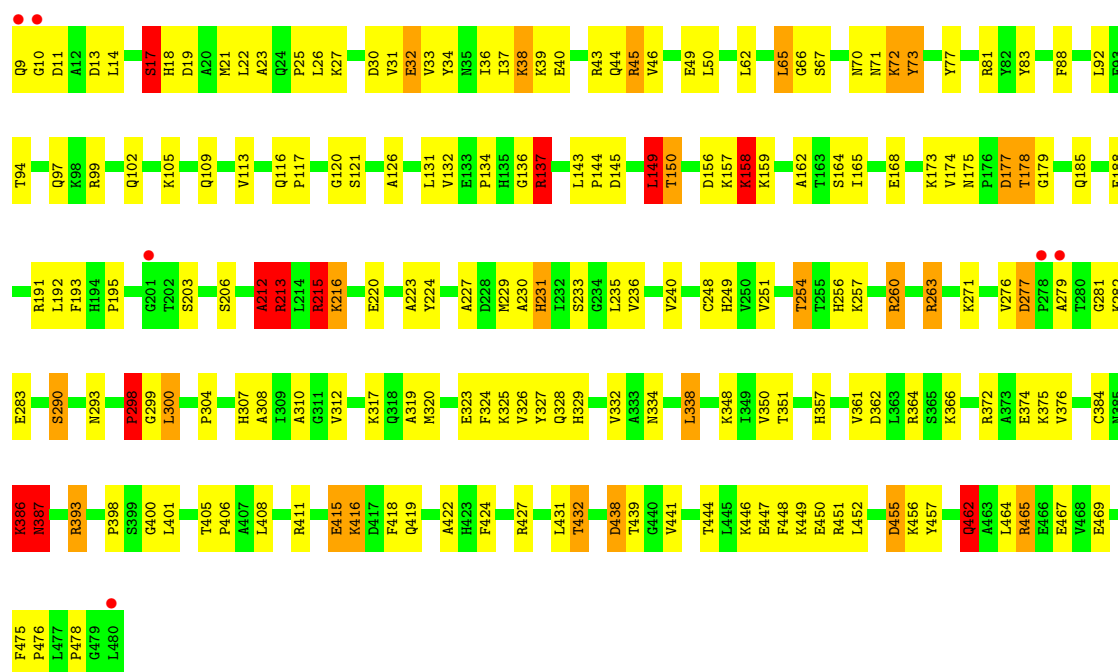


- Molecule 1: Serine hydroxymethyltransferase, cytosolic

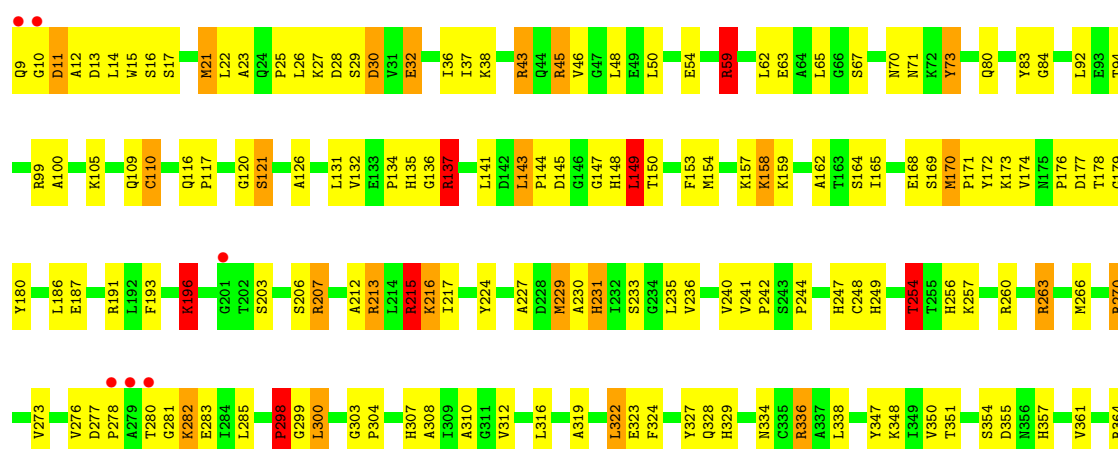


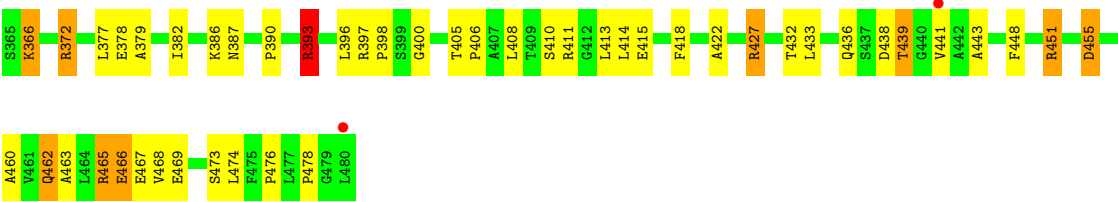


• Molecule 1: Serine hydroxymethyltransferase, cytosolic



• Molecule 1: Serine hydroxymethyltransferase, cytosolic







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.153 , 0.192 0.143 , 0.171	Depositor DCC
$R_{free}$ test set	4079 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.63	2/3705 (0.1%)	1.42	58/5012 (1.2%)
1	B	0.63	2/3705 (0.1%)	1.38	53/5012 (1.1%)
1	C	0.61	0/3705	1.38	47/5012 (0.9%)
1	D	0.65	2/3705 (0.1%)	1.42	58/5012 (1.2%)
All	All	0.63	6/14820 (0.0%)	1.40	216/20048 (1.1%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLU	CD-OE2	6.89	1.33	1.25
1	D	378	GLU	CD-OE1	6.44	1.32	1.25
1	D	32	GLU	CD-OE2	5.58	1.31	1.25
1	A	168	GLU	CD-OE1	5.29	1.31	1.25
1	B	415	GLU	CD-OE1	5.22	1.31	1.25
1	B	378	GLU	CD-OE1	5.11	1.31	1.25

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	CB-CA-C	-15.76	78.88	110.40
1	D	59	ARG	CB-CA-C	-14.04	82.32	110.40
1	D	215	ARG	NE-CZ-NH1	-13.45	113.57	120.30
1	C	188	GLU	N-CA-CB	12.48	133.06	110.60
1	D	143	LEU	CB-CG-CD2	-12.00	90.60	111.00
1	B	263	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	A	43	ARG	NE-CZ-NH2	11.21	125.90	120.30
1	B	439	THR	CA-CB-OG1	-10.67	86.60	109.00
1	D	215	ARG	CA-CB-CG	-10.56	90.16	113.40
1	B	415	GLU	N-CA-CB	10.12	128.81	110.60
1	A	137	ARG	NE-CZ-NH1	-10.02	115.29	120.30
1	D	270	ARG	CB-CG-CD	9.88	137.28	111.60
1	C	137	ARG	NE-CZ-NH1	-9.65	115.47	120.30
1	D	215	ARG	CD-NE-CZ	-9.61	110.14	123.60
1	B	427	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	D	393	ARG	CB-CA-C	9.30	129.00	110.40
1	D	466	GLU	CB-CG-CD	-9.09	89.66	114.20
1	B	196	LYS	CA-CB-CG	9.02	133.24	113.40
1	B	270	ARG	CB-CA-C	9.02	128.43	110.40
1	C	94	THR	OG1-CB-CG2	-9.01	89.28	110.00
1	C	415	GLU	N-CA-CB	8.96	126.72	110.60
1	D	94	THR	OG1-CB-CG2	-8.74	89.89	110.00
1	A	196	LYS	CA-CB-CG	8.68	132.49	113.40
1	C	158	LYS	N-CA-CB	8.64	126.15	110.60
1	A	59	ARG	N-CA-CB	8.59	126.06	110.60
1	B	226	MET	CG-SD-CE	-8.48	86.63	100.20
1	B	196	LYS	CB-CG-CD	8.47	133.62	111.60
1	D	149	LEU	CB-CG-CD2	-8.40	96.73	111.00
1	D	21	MET	CG-SD-CE	8.34	113.55	100.20
1	B	212	ALA	N-CA-CB	-8.34	98.43	110.10
1	A	191	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	A	260	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	C	43	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	B	196	LYS	CD-CE-NZ	8.24	130.66	111.70
1	B	38	LYS	CB-CG-CD	8.23	133.01	111.60
1	A	212	ALA	N-CA-CB	-8.15	98.69	110.10
1	B	157	LYS	CD-CE-NZ	8.13	130.41	111.70
1	A	216	LYS	CD-CE-NZ	8.09	130.31	111.70
1	D	43	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	C	432	THR	CA-CB-OG1	-7.99	92.23	109.00
1	B	216	LYS	CB-CA-C	7.95	126.29	110.40
1	A	414	LEU	CB-CG-CD1	-7.92	97.53	111.00
1	C	212	ALA	N-CA-CB	-7.92	99.02	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	LEU	CB-CG-CD1	-7.91	97.56	111.00
1	D	137	ARG	NE-CZ-NH2	7.85	124.22	120.30
1	C	81	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	157	LYS	CB-CG-CD	7.80	131.89	111.60
1	A	207	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	432	THR	CA-CB-OG1	-7.77	92.69	109.00
1	D	432	THR	CA-CB-OG1	-7.73	92.76	109.00
1	A	27	LYS	CB-CG-CD	7.67	131.53	111.60
1	B	270	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	215	ARG	CA-CB-CG	-7.64	96.60	113.40
1	C	427	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	216	LYS	N-CA-CB	7.57	124.22	110.60
1	D	215	ARG	NH1-CZ-NH2	7.56	127.71	119.40
1	A	348	LYS	CG-CD-CE	7.48	134.35	111.90
1	D	415	GLU	N-CA-CB	7.41	123.94	110.60
1	D	207	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	C	393	ARG	CG-CD-NE	7.36	127.26	111.80
1	A	196	LYS	CB-CG-CD	7.35	130.71	111.60
1	C	260	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	D	59	ARG	N-CA-CB	7.32	123.77	110.60
1	C	338	LEU	CB-CG-CD1	-7.28	98.63	111.00
1	D	215	ARG	CG-CD-NE	7.26	127.06	111.80
1	B	271	LYS	CG-CD-CE	7.24	133.63	111.90
1	A	414	LEU	CB-CG-CD2	7.23	123.29	111.00
1	C	439	THR	CA-CB-OG1	-7.23	93.82	109.00
1	B	393	ARG	CB-CA-C	7.22	124.84	110.40
1	B	271	LYS	CB-CG-CD	7.21	130.35	111.60
1	D	105	LYS	CD-CE-NZ	7.20	128.26	111.70
1	D	170	MET	CG-SD-CE	-7.19	88.69	100.20
1	B	414	LEU	CB-CG-CD2	7.17	123.19	111.00
1	C	298	PRO	N-CA-CB	-7.14	94.73	103.30
1	A	432	THR	CA-CB-OG1	-7.13	94.02	109.00
1	C	215	ARG	CG-CD-NE	-7.10	96.88	111.80
1	D	266	MET	CG-SD-CE	7.03	111.44	100.20
1	D	105	LYS	CG-CD-CE	6.94	132.71	111.90
1	A	263	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	225	LEU	CB-CG-CD1	-6.90	99.28	111.00
1	C	216	LYS	CG-CD-CE	6.89	132.58	111.90
1	D	378	GLU	CG-CD-OE2	-6.85	104.61	118.30
1	C	387	ASN	CB-CA-C	6.81	124.02	110.40
1	C	26	LEU	CB-CG-CD2	6.81	122.58	111.00
1	A	270	ARG	CB-CG-CD	6.79	129.25	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	PRO	N-CA-CB	-6.75	95.18	102.60
1	B	322	LEU	CB-CG-CD1	6.73	122.44	111.00
1	C	175	ASN	CB-CA-C	-6.71	96.98	110.40
1	A	154	MET	CG-SD-CE	-6.70	89.48	100.20
1	C	393	ARG	CB-CA-C	6.70	123.79	110.40
1	A	114	ASN	CB-CA-C	6.66	123.72	110.40
1	D	414	LEU	CB-CG-CD2	6.65	122.31	111.00
1	A	415	GLU	N-CA-CB	6.63	122.53	110.60
1	D	30	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	137	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	B	19	ASP	CB-CA-C	-6.58	97.24	110.40
1	B	414	LEU	CB-CG-CD1	-6.55	99.86	111.00
1	A	364	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	260	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	C	72	LYS	CD-CE-NZ	6.50	126.66	111.70
1	A	27	LYS	CG-CD-CE	6.49	131.37	111.90
1	A	213	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	D	393	ARG	CG-CD-NE	6.47	125.38	111.80
1	D	38	LYS	CD-CE-NZ	6.46	126.57	111.70
1	C	415	GLU	CG-CD-OE2	-6.42	105.47	118.30
1	C	393	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	372	ARG	CG-CD-NE	-6.40	98.35	111.80
1	D	158	LYS	CB-CG-CD	6.38	128.19	111.60
1	A	137	ARG	CB-CG-CD	6.37	128.16	111.60
1	A	427	ARG	CG-CD-NE	-6.37	98.43	111.80
1	D	196	LYS	CA-CB-CG	6.36	127.40	113.40
1	A	35	ASN	CB-CA-C	-6.32	97.76	110.40
1	D	322	LEU	CB-CG-CD2	-6.31	100.28	111.00
1	A	216	LYS	CG-CD-CE	6.29	130.76	111.90
1	A	266	MET	CG-SD-CE	6.27	110.24	100.20
1	C	188	GLU	CB-CA-C	-6.19	98.01	110.40
1	C	449	LYS	CD-CE-NZ	6.19	125.94	111.70
1	B	192	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	D	254	THR	OG1-CB-CG2	6.18	124.21	110.00
1	A	105	LYS	CB-CG-CD	6.14	127.55	111.60
1	A	59	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	397	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	14	LEU	CB-CG-CD1	6.10	121.38	111.00
1	D	135	HIS	CB-CA-C	6.09	122.58	110.40
1	C	158	LYS	CB-CG-CD	6.06	127.35	111.60
1	C	452	LEU	CB-CG-CD2	6.05	121.29	111.00
1	C	364	ARG	NE-CZ-NH1	6.01	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	254	THR	N-CA-CB	-6.01	98.88	110.30
1	A	49	GLU	CB-CG-CD	-6.01	97.98	114.20
1	D	378	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	A	158	LYS	CG-CD-CE	6.00	129.90	111.90
1	B	215	ARG	CA-CB-CG	-6.00	100.21	113.40
1	C	300	LEU	CB-CG-CD1	5.99	121.18	111.00
1	D	322	LEU	CB-CG-CD1	5.99	121.18	111.00
1	C	105	LYS	CD-CE-NZ	5.99	125.47	111.70
1	D	298	PRO	N-CA-CB	-5.98	96.03	102.60
1	A	325	LYS	CG-CD-CE	5.95	129.76	111.90
1	B	325	LYS	CD-CE-NZ	5.94	125.37	111.70
1	A	216	LYS	CA-CB-CG	5.89	126.36	113.40
1	A	82	TYR	CA-CB-CG	5.89	124.58	113.40
1	C	38	LYS	CG-CD-CE	5.88	129.54	111.90
1	A	135	HIS	CB-CA-C	5.86	122.11	110.40
1	B	196	LYS	CG-CD-CE	5.86	129.47	111.90
1	A	300	LEU	CB-CG-CD2	-5.85	101.05	111.00
1	D	263	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	C	105	LYS	CG-CD-CE	5.79	129.27	111.90
1	B	451	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	105	LYS	CB-CG-CD	5.78	126.63	111.60
1	A	81	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	340	GLU	CB-CA-C	5.74	121.87	110.40
1	B	59	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	C	150	THR	CA-CB-OG1	-5.69	97.06	109.00
1	D	216	LYS	CG-CD-CE	5.69	128.96	111.90
1	B	393	ARG	CA-CB-CG	-5.67	100.93	113.40
1	A	393	ARG	CB-CA-C	5.67	121.73	110.40
1	B	364	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	D	157	LYS	N-CA-CB	5.67	120.80	110.60
1	B	49	GLU	N-CA-CB	5.64	120.75	110.60
1	D	178	THR	OG1-CB-CG2	-5.63	97.05	110.00
1	B	378	GLU	CG-CD-OE2	-5.62	107.05	118.30
1	C	215	ARG	CB-CG-CD	5.62	126.22	111.60
1	B	427	ARG	NH1-CZ-NH2	5.61	125.58	119.40
1	D	229	MET	CG-SD-CE	-5.61	91.23	100.20
1	A	24	GLN	N-CA-CB	-5.60	100.52	110.60
1	B	449	LYS	CD-CE-NZ	5.60	124.58	111.70
1	B	377	LEU	CB-CG-CD2	-5.58	101.50	111.00
1	B	214	LEU	CB-CG-CD1	-5.54	101.57	111.00
1	D	27	LYS	CB-CG-CD	5.50	125.89	111.60
1	A	396	LEU	CB-CG-CD2	5.48	120.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105	LYS	CB-CG-CD	5.47	125.81	111.60
1	B	344	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	B	430	GLU	CB-CG-CD	5.41	128.81	114.20
1	A	433	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	B	43	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	191	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	414	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	C	455	ASP	CB-CA-C	-5.37	99.67	110.40
1	D	215	ARG	CB-CG-CD	-5.36	97.66	111.60
1	B	397	ARG	CG-CD-NE	5.35	123.03	111.80
1	C	17	SER	CB-CA-C	5.34	120.25	110.10
1	B	411	ARG	CB-CG-CD	-5.34	97.72	111.60
1	B	26	LEU	CB-CG-CD2	5.33	120.06	111.00
1	B	38	LYS	CD-CE-NZ	5.33	123.95	111.70
1	B	396	LEU	CB-CG-CD2	5.32	120.04	111.00
1	A	43	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	105	LYS	CD-CE-NZ	5.30	123.89	111.70
1	D	137	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	C	290	SER	N-CA-CB	5.28	118.43	110.50
1	D	348	LYS	CD-CE-NZ	5.28	123.85	111.70
1	C	386	LYS	CB-CG-CD	5.27	125.31	111.60
1	C	149	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	B	216	LYS	CD-CE-NZ	5.25	123.78	111.70
1	A	110	CYS	CB-CA-C	-5.25	99.91	110.40
1	D	451	ARG	CA-CB-CG	-5.24	101.87	113.40
1	D	465	ARG	CG-CD-NE	5.24	122.81	111.80
1	D	397	ARG	CB-CG-CD	5.22	125.17	111.60
1	C	325	LYS	CG-CD-CE	5.21	127.54	111.90
1	A	416	LYS	CD-CE-NZ	5.21	123.67	111.70
1	D	65	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	D	110	CYS	CB-CA-C	-5.20	99.99	110.40
1	C	464	LEU	CB-CG-CD1	-5.20	102.17	111.00
1	C	213	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	396	LEU	CB-CG-CD2	5.18	119.81	111.00
1	A	21	MET	CG-SD-CE	5.16	108.45	100.20
1	A	215	ARG	CD-NE-CZ	-5.14	116.40	123.60
1	D	300	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	D	364	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	246	GLU	CB-CA-C	5.08	120.57	110.40
1	A	298	PRO	N-CA-CB	-5.06	97.03	102.60
1	C	462	GLN	N-CA-CB	5.05	119.68	110.60
1	C	427	ARG	NH1-CZ-NH2	5.03	124.93	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	LYS	CB-CG-CD	5.01	124.64	111.60
1	D	455	ASP	CB-CA-C	5.01	120.43	110.40
1	C	254	THR	N-CA-CB	-5.01	100.78	110.30
1	B	462	GLN	N-CA-CB	5.00	119.61	110.60
1	A	229	MET	CG-SD-CE	-5.00	92.20	100.20

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	175	0
1	B	3632	0	3612	210	0
1	C	3632	0	3612	206	0
1	D	3632	0	3612	202	0
2	A	15	0	7	2	0
2	B	15	0	7	1	0
2	C	15	0	6	7	0
2	D	15	0	7	11	0
All	All	14588	0	14473	654	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 22.

All (654) 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:A:438:ASP:CB	1:A:451:ARG:HH12	1.64	1.09
1:A:350:VAL:O	1:A:351:THR:HG22	1.50	1.08
1:A:229:MET:HE2	1:A:233:SER:HA	1.31	1.07
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:B:229:MET:HE2	1:B:233:SER:HA	1.44	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
1:D:386:LYS:HD2	1:D:398:PRO:HG3	1.45	0.96
1:D:336:ARG:HH12	1:D:355:ASP:HA	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:229:MET:HE2	1:D:233:SER:HA	1.52	0.91
1:B:229:MET:CE	1:B:233:SER:HA	2.00	0.91
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:B:323:GLU:HB2	1:C:21:MET:HE1	1.57	0.86
1:D:438:ASP:HB3	1:D:451:ARG:HH12	1.38	0.86
1:B:21:MET:HE1	1:C:323:GLU:HB2	1.58	0.85
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: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
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:229:MET:CE	1:C:233:SER:HA	2.14	0.77
1:C:120:GLY:HA3	2:C:500:PLP:H5A2	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:229:MET:HE2	1:C:233:SER:HA	1.69	0.74
1:A:298:PRO:HB2	1:D:149:LEU:HD21	1.66	0.74
1:D:229:MET:CE	1:D:233:SER:HA	2.18	0.74
1:A:141:LEU:HD11	1:A:174:VAL:HG23	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:9:GLN:HG2	1:B:10:GLY:H	1.57	0.69
1:B:357:HIS:HD1	1:B:357:HIS:H	1.41	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:A:323:GLU:HB2	1:D:21:MET:HE1	1.74	0.67
1:B:158:LYS:HG2	1:B:159:LYS:N	2.09	0.67
1:A:357:HIS:HD1	1:A:357:HIS:H	1.42	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:C:357:HIS:HD1	1:C:357:HIS:H	1.44	0.65
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:229:MET:HE3	1:B:236:VAL:HB	1.84	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
1:D:256:HIS:ND1	1:D:263:ARG:HA	2.16	0.60
1:A:21:MET:HE2	1:D:323:GLU:HB2	1.84	0.60
1:D:132:VAL:HG12	1:D:136:GLY:HA3	1.82	0.60
1:A:240:VAL:HG12	1:A:332:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:323:GLU:HB2	1:D:21:MET:HE2	1.85	0.58
1:B:21:MET:HE2	1:C:323:GLU:HB2	1.84	0.58
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: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: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
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:C:231:HIS:HD2	1:C:357:HIS:NE2	2.02	0.57
1:A:229:MET:HE1	1:A:233:SER:HA	1.84	0.57
1:D:405:THR:N	1:D:406:PRO:CD	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:MET:HE3	1:C:233:SER:HA	1.86	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: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:10:GLY:O	1:D:11:ASP:C	2.43	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:C:240:VAL:CG1	1:C:332:VAL:HG21	2.35	0.56
1:A:231:HIS:HD2	1:A:357:HIS:NE2	2.04	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:B:186:LEU:HD12	1:B:186:LEU:C	2.26	0.56
1:B:260:ARG:CZ	1:C:22:LEU:HD21	2.35	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:9:GLN:O	1:A:10:GLY:C	2.44	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:B:231:HIS:HD2	1:B:357:HIS:NE2	2.04	0.55
1:A:282:LYS:HG3	1:A:283:GLU:H	1.72	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:148:HIS:HB2	2:A:500:PLP:H2A3	1.89	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:C:276:VAL:O	1:C:277:ASP:C	2.45	0.54
1:A:277:ASP:O	1:A:280:THR:N	2.41	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:30:ASP:CG	1:C:99:ARG:HH22	2.11	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:137:ARG:HB3	1:C:193:PHE:CE2	2.43	0.53
1:B:229:MET:HE1	1:B:233:SER:HA	1.86	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:154:MET:HE1	1:D:159:LYS:HE2	1.91	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: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:C:177:ASP:O	1:C:178:THR:C	2.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:14:LEU:HD21	1:D:322:LEU:HG	1.95	0.48
1:C:9:GLN:O	1:C:10:GLY:C	2.50	0.48
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:99:ARG:HH22	1:C:30:ASP:CG	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:16:SER:O	1:D:17:SER:C	2.52	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:A:32:GLU:CD	1:D:99:ARG:HH21	2.17	0.48
1:A:317:LYS:O	1:A:317:LYS:HG2	2.13	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:D:10:GLY:O	1:D:12:ALA:N	2.46	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: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
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:C:229:MET:HE1	1:C:236:VAL:HB	1.96	0.47
1:A:132:VAL:HG12	1:A:136:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:447:GLU:O	1:C:450:GLU:N	2.46	0.47
1:A:191:ARG:HD3	1:A:220:GLU:CD	2.35	0.46
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:C:444:THR:C	1:C:446:LYS:N	2.68	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: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: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:D:229:MET:HE3	1:D:236:VAL:HB	1.98	0.46
1:A:26:LEU:N	1:D:63:GLU:OE1	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:229:MET:HE3	1:A:236:VAL:HB	2.00	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:A:277:ASP:O	1:A:278:PRO:C	2.57	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:D:154:MET:HE3	1:D:159:LYS:HE2	2.00	0.43
1:C:227:ALA:HB3	1:C:251:VAL:HG22	2.01	0.43
1:A:45:ARG:HH22	1:A:473:SER:HB3	1.83	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:11:ASP:O	1:A:12:ALA:C	2.57	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: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
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:189:ASN:HA	1:B:192:LEU:HD12	2.01	0.42
1:D:473:SER:C	1:D:474:LEU:HD23	2.39	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:37:ILE:CG2	1:C:67:SER:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.86	0.42
1:B:229:MET:HE3	1:B:236:VAL:CB	2.50	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:C:444:THR:C	1:C:446:LYS:H	2.22	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: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:D:116:GLN:O	1:D:117:PRO:C	2.58	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:B:389:CYS:H	1:B:392:ASP:CG	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:SER:C	1:B:122:PRO:HD2	2.41	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:162:ALA:CB	1:D:299:GLY:O	2.68	0.41
1:C:276:VAL:HA	1:C:283:GLU:HA	2.03	0.41
1:D:11:ASP:O	1:D:12:ALA:C	2.59	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: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
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:A:65:LEU:HD13	1:D:307:HIS:CD2	2.56	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:B:180:TYR:CE1	1:B:351:THR:OG1	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASN:OD1	1:A:241:VAL:HG13	2.21	0.40
1:B:30:ASP:N	1:C:317:LYS:HZ3	2.19	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: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: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: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	48
1	B	470/472 (100%)	436 (93%)	29 (6%)	5 (1%)	12	44
1	C	470/472 (100%)	443 (94%)	22 (5%)	5 (1%)	12	44
1	D	470/472 (100%)	443 (94%)	26 (6%)	1 (0%)	44	76
All	All	1880/1888 (100%)	1761 (94%)	104 (6%)	15 (1%)	16	50

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	ASP
1	B	441	VAL

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Mol	Chain	Res	Type
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 ⓘ

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%)	15	44
1	B	385/385 (100%)	356 (92%)	29 (8%)	11	37
1	C	385/385 (100%)	358 (93%)	27 (7%)	12	40
1	D	385/385 (100%)	360 (94%)	25 (6%)	14	43
All	All	1540/1540 (100%)	1435 (93%)	105 (7%)	13	41

All (105) 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	105	LYS
1	A	114	ASN
1	A	155	THR
1	A	188	GLU

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Mol	Chain	Res	Type
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	366	LYS
1	A	393	ARG
1	A	416	LYS
1	A	438	ASP
1	A	439	THR
1	A	455	ASP
1	A	466	GLU
1	B	9	GLN
1	B	70	ASN
1	B	73	TYR
1	B	80	GLN
1	B	119	SER
1	B	134	PRO
1	B	149	LEU
1	B	158	LYS
1	B	184	ASP
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	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	433	LEU

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Mol	Chain	Res	Type
1	B	447	GLU
1	B	451	ARG
1	B	466	GLU
1	C	13	ASP
1	C	17	SER
1	C	19	ASP
1	C	32	GLU
1	C	49	GLU
1	C	50	LEU
1	C	65	LEU
1	C	73	TYR
1	C	109	GLN
1	C	134	PRO
1	C	149	LEU
1	C	158	LYS
1	C	177	ASP
1	C	185	GLN
1	C	203	SER
1	C	213	ARG
1	C	231	HIS
1	C	271	LYS
1	C	290	SER
1	C	298	PRO
1	C	366	LYS
1	C	386	LYS
1	C	387	ASN
1	C	416	LYS
1	C	438	ASP
1	C	455	ASP
1	C	462	GLN
1	D	9	GLN
1	D	28	ASP
1	D	50	LEU
1	D	73	TYR
1	D	80	GLN
1	D	109	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

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Mol	Chain	Res	Type
1	D	217	ILE
1	D	231	HIS
1	D	254	THR
1	D	282	LYS
1	D	298	PRO
1	D	366	LYS
1	D	393	ARG
1	D	427	ARG
1	D	433	LEU
1	D	439	THR
1	D	441	VAL
1	D	455	ASP
1	D	462	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	148	HIS
1	A	231	HIS
1	A	305	HIS
1	A	318	GLN
1	A	458	GLN
1	B	24	GLN
1	B	70	ASN
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	318	GLN
1	C	458	GLN
1	C	462	GLN
1	D	70	ASN
1	D	231	HIS
1	D	247	HIS
1	D	307	HIS
1	D	458	GLN
1	D	462	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	B	500	-	15,15,16	0.98	0	20,22,23	1.02	1 (5%)
2	PLP	C	500	-	15,15,16	1.10	2 (13%)	20,22,23	1.58	3 (15%)
2	PLP	A	500	-	15,15,16	0.97	1 (6%)	20,22,23	1.62	3 (15%)
2	PLP	D	500	-	15,15,16	1.06	1 (6%)	20,22,23	1.79	6 (30%)

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	B	500	-	-	5/6/6/8	0/1/1/1
2	PLP	C	500	-	-	1/6/6/8	0/1/1/1
2	PLP	A	500	-	-	1/6/6/8	0/1/1/1
2	PLP	D	500	-	-	2/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	PLP	P-O1P	2.56	1.58	1.50
2	D	500	PLP	C4A-C4	-2.32	1.46	1.51
2	A	500	PLP	C4A-C4	-2.08	1.47	1.51
2	C	500	PLP	C4A-C4	-2.05	1.47	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	PLP	O4P-C5A-C5	4.88	118.65	109.35
2	C	500	PLP	O3-C3-C2	4.09	126.42	117.49
2	C	500	PLP	O4P-C5A-C5	3.89	116.76	109.35
2	D	500	PLP	O2P-P-O4P	3.52	116.10	106.73
2	A	500	PLP	O3-C3-C2	3.51	125.14	117.49
2	D	500	PLP	O4P-C5A-C5	3.49	116.00	109.35
2	D	500	PLP	O3P-P-O4P	-3.17	98.29	106.73
2	D	500	PLP	O3-C3-C2	2.98	123.99	117.49
2	D	500	PLP	C6-C5-C4	-2.64	116.08	118.16
2	C	500	PLP	C2A-C2-C3	2.51	123.99	120.89
2	A	500	PLP	C4A-C4-C5	2.43	123.44	120.94
2	B	500	PLP	O3-C3-C2	2.23	122.34	117.49
2	D	500	PLP	O3P-P-O2P	2.05	115.48	107.64

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
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	B	500	PLP	1	0
2	C	500	PLP	7	0
2	A	500	PLP	2	0
2	D	500	PLP	11	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	472/472 (100%)	-0.57	5 (1%) 77 62	42, 90, 123, 181	0
1	B	472/472 (100%)	-0.52	10 (2%) 63 47	50, 90, 125, 174	0
1	C	472/472 (100%)	-0.61	6 (1%) 74 59	48, 89, 125, 195	0
1	D	472/472 (100%)	-0.58	8 (1%) 69 52	49, 88, 123, 179	0
All	All	1888/1888 (100%)	-0.57	29 (1%) 71 55	42, 89, 124, 195	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	GLN	8.9
1	D	10	GLY	8.2
1	C	9	GLN	5.7
1	A	9	GLN	5.2
1	B	10	GLY	5.0
1	D	9	GLN	4.8
1	A	10	GLY	4.7
1	C	10	GLY	4.7
1	D	278	PRO	4.2
1	D	441	VAL	4.0
1	B	278	PRO	3.6
1	C	278	PRO	3.3
1	B	480	LEU	3.3
1	C	201	GLY	3.2
1	A	278	PRO	3.2
1	B	304	PRO	2.8
1	D	201	GLY	2.7
1	D	279	ALA	2.6
1	D	480	LEU	2.5
1	A	201	GLY	2.5
1	B	85	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	280	THR	2.4
1	B	277	ASP	2.3
1	B	279	ALA	2.3
1	B	441	VAL	2.2
1	A	276	VAL	2.2
1	C	480	LEU	2.1
1	B	11	ASP	2.1
1	C	279	ALA	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 monosaccharides 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, 95<sup>th</sup> 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.