



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1LDB  
Title : STRUCTURE DETERMINATION AND REFINEMENT OF BACILLUS  
STEAROTHERMOPHILUS LACTATE DEHYDROGENASE  
Authors : Piontek, K.; Rossmann, M.G.  
Deposited on : 1989-03-27  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

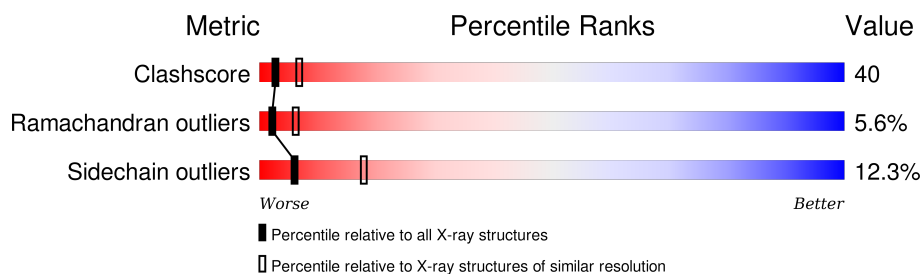
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
1	C	317	
1	D	317	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9119 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 APO-L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	B	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	C	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	D	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

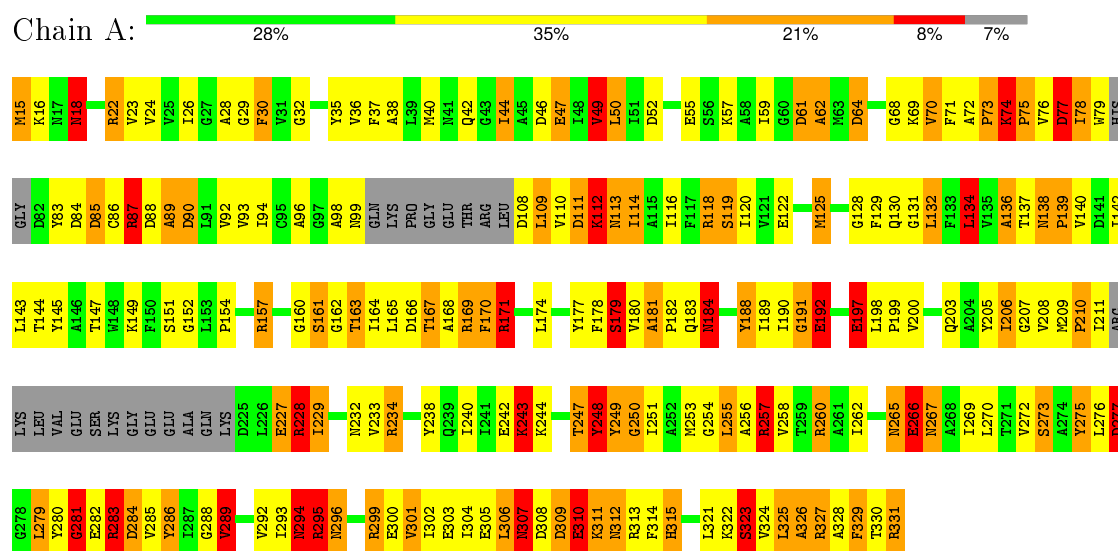
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

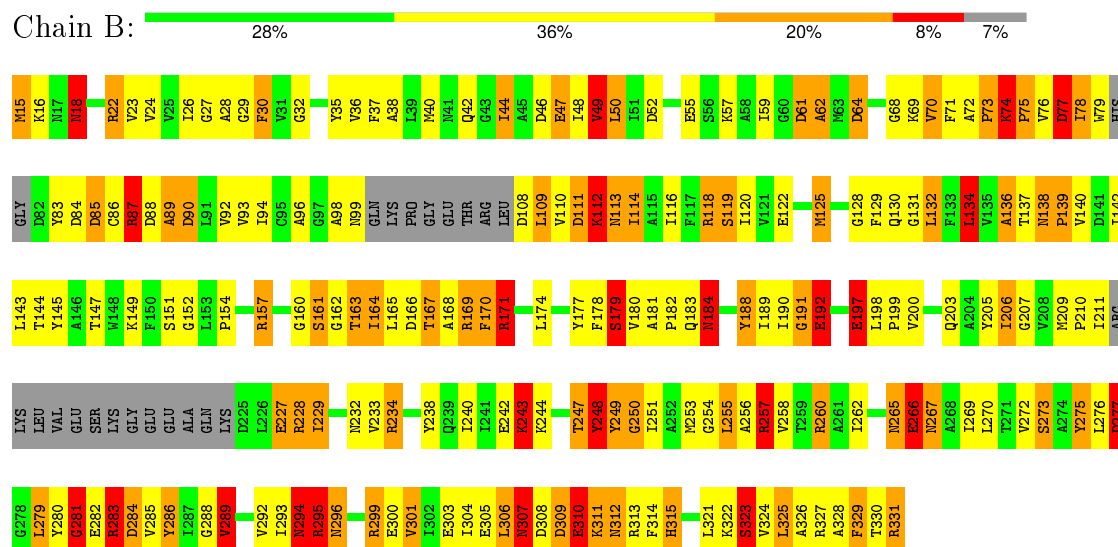
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: APO-L-LACTATE DEHYDROGENASE

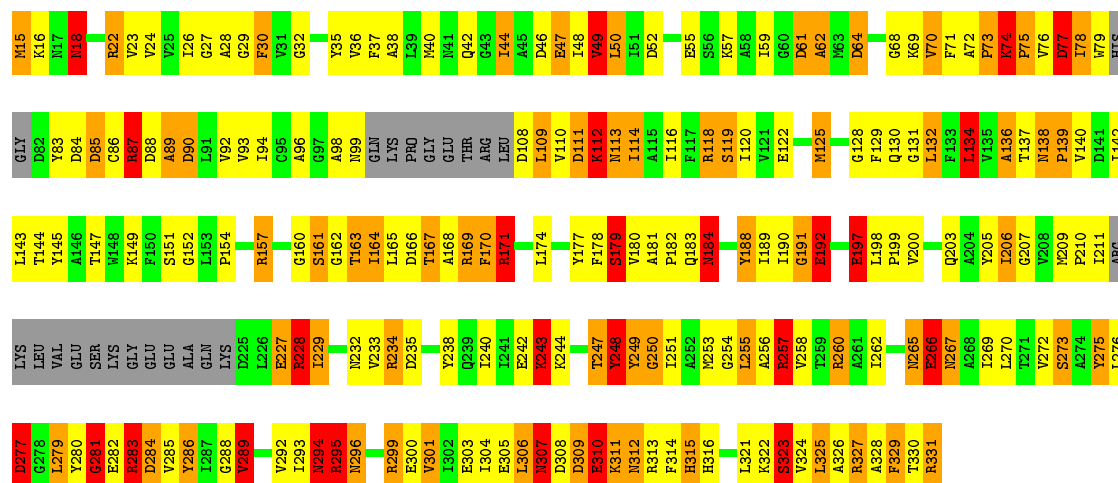


#### • Molecule 1: APO-L-LACTATE DEHYDROGENASE




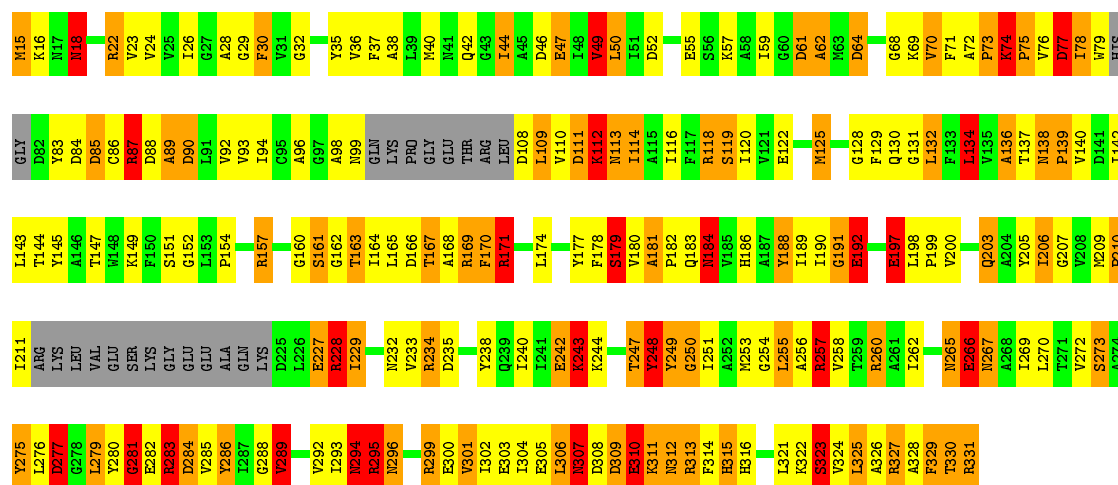
• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain C: 



• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain D: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.90 Å 86.90 Å 357.30 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.286 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.56	15/2320 (0.6%)	2.69	140/3146 (4.5%)
1	B	1.56	15/2320 (0.6%)	2.69	140/3146 (4.5%)
1	C	1.56	15/2320 (0.6%)	2.69	140/3146 (4.5%)
1	D	1.56	15/2320 (0.6%)	2.69	140/3146 (4.5%)
All	All	1.56	60/9280 (0.6%)	2.69	560/12584 (4.5%)

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	31
1	B	0	31
1	C	0	31
1	D	0	31
All	All	0	124

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	TYR	CG-CD1	8.18	1.49	1.39
1	B	188	TYR	CG-CD1	8.18	1.49	1.39
1	C	188	TYR	CG-CD1	8.18	1.49	1.39
1	D	188	TYR	CG-CD1	8.18	1.49	1.39
1	A	192	GLU	CD-OE1	-6.82	1.18	1.25
1	B	192	GLU	CD-OE1	-6.82	1.18	1.25
1	C	192	GLU	CD-OE1	-6.82	1.18	1.25
1	D	192	GLU	CD-OE1	-6.82	1.18	1.25
1	A	119	SER	CB-OG	6.26	1.50	1.42
1	B	119	SER	CB-OG	6.26	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	SER	CB-OG	6.26	1.50	1.42
1	D	119	SER	CB-OG	6.26	1.50	1.42
1	A	44	ILE	C-O	6.21	1.35	1.23
1	B	44	ILE	C-O	6.21	1.35	1.23
1	C	44	ILE	C-O	6.21	1.35	1.23
1	D	44	ILE	C-O	6.21	1.35	1.23
1	A	134	LEU	N-CA	5.98	1.58	1.46
1	B	134	LEU	N-CA	5.98	1.58	1.46
1	C	134	LEU	N-CA	5.98	1.58	1.46
1	D	134	LEU	N-CA	5.98	1.58	1.46
1	A	151	SER	CB-OG	5.86	1.49	1.42
1	B	151	SER	CB-OG	5.86	1.49	1.42
1	C	151	SER	CB-OG	5.86	1.49	1.42
1	D	151	SER	CB-OG	5.86	1.49	1.42
1	A	254	GLY	C-O	5.66	1.32	1.23
1	B	254	GLY	C-O	5.66	1.32	1.23
1	C	254	GLY	C-O	5.66	1.32	1.23
1	D	254	GLY	C-O	5.66	1.32	1.23
1	A	283	ARG	C-O	5.64	1.34	1.23
1	B	283	ARG	C-O	5.64	1.34	1.23
1	C	283	ARG	C-O	5.64	1.34	1.23
1	D	283	ARG	C-O	5.64	1.34	1.23
1	A	179	SER	CB-OG	5.60	1.49	1.42
1	B	179	SER	CB-OG	5.60	1.49	1.42
1	C	179	SER	CB-OG	5.60	1.49	1.42
1	D	179	SER	CB-OG	5.60	1.49	1.42
1	A	30	PHE	C-O	5.55	1.33	1.23
1	B	30	PHE	C-O	5.55	1.33	1.23
1	C	30	PHE	C-O	5.55	1.33	1.23
1	D	30	PHE	C-O	5.55	1.33	1.23
1	A	281	GLY	N-CA	5.44	1.54	1.46
1	B	281	GLY	N-CA	5.44	1.54	1.46
1	C	281	GLY	N-CA	5.44	1.54	1.46
1	D	281	GLY	N-CA	5.44	1.54	1.46
1	A	277	ASP	CA-CB	5.34	1.65	1.53
1	B	277	ASP	CA-CB	5.34	1.65	1.53
1	C	277	ASP	CA-CB	5.34	1.65	1.53
1	D	277	ASP	CA-CB	5.34	1.65	1.53
1	A	162	GLY	C-O	5.15	1.31	1.23
1	B	162	GLY	C-O	5.15	1.31	1.23
1	C	162	GLY	C-O	5.15	1.31	1.23
1	D	162	GLY	C-O	5.15	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	THR	C-O	5.04	1.32	1.23
1	B	163	THR	C-O	5.04	1.32	1.23
1	C	163	THR	C-O	5.04	1.32	1.23
1	D	163	THR	C-O	5.04	1.32	1.23
1	A	138	ASN	N-CA	5.04	1.56	1.46
1	B	138	ASN	N-CA	5.04	1.56	1.46
1	C	138	ASN	N-CA	5.04	1.56	1.46
1	D	138	ASN	N-CA	5.04	1.56	1.46

All (560) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH1	35.13	137.87	120.30
1	B	169	ARG	NE-CZ-NH1	35.13	137.87	120.30
1	C	169	ARG	NE-CZ-NH1	35.13	137.87	120.30
1	D	169	ARG	NE-CZ-NH1	35.13	137.87	120.30
1	A	260	ARG	NE-CZ-NH1	-24.16	108.22	120.30
1	B	260	ARG	NE-CZ-NH1	-24.16	108.22	120.30
1	C	260	ARG	NE-CZ-NH1	-24.16	108.22	120.30
1	D	260	ARG	NE-CZ-NH1	-24.16	108.22	120.30
1	A	171	ARG	NE-CZ-NH1	-21.05	109.78	120.30
1	B	171	ARG	NE-CZ-NH1	-21.05	109.78	120.30
1	C	171	ARG	NE-CZ-NH1	-21.05	109.78	120.30
1	D	171	ARG	NE-CZ-NH1	-21.05	109.78	120.30
1	A	228	ARG	NE-CZ-NH1	-18.78	110.91	120.30
1	B	228	ARG	NE-CZ-NH1	-18.78	110.91	120.30
1	C	228	ARG	NE-CZ-NH1	-18.78	110.91	120.30
1	D	228	ARG	NE-CZ-NH1	-18.78	110.91	120.30
1	A	111	ASP	CB-CG-OD1	17.94	134.44	118.30
1	B	111	ASP	CB-CG-OD1	17.94	134.44	118.30
1	C	111	ASP	CB-CG-OD1	17.94	134.44	118.30
1	D	111	ASP	CB-CG-OD1	17.94	134.44	118.30
1	A	249	TYR	CB-CG-CD1	16.55	130.93	121.00
1	B	249	TYR	CB-CG-CD1	16.55	130.93	121.00
1	C	249	TYR	CB-CG-CD1	16.55	130.93	121.00
1	D	249	TYR	CB-CG-CD1	16.55	130.93	121.00
1	A	249	TYR	CB-CG-CD2	-14.46	112.32	121.00
1	B	249	TYR	CB-CG-CD2	-14.46	112.32	121.00
1	C	249	TYR	CB-CG-CD2	-14.46	112.32	121.00
1	D	249	TYR	CB-CG-CD2	-14.46	112.32	121.00
1	A	276	LEU	C-N-CA	14.34	157.55	121.70
1	B	276	LEU	C-N-CA	14.34	157.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	LEU	C-N-CA	14.34	157.55	121.70
1	D	276	LEU	C-N-CA	14.34	157.55	121.70
1	A	309	ASP	CB-CG-OD2	14.14	131.02	118.30
1	B	309	ASP	CB-CG-OD2	14.14	131.02	118.30
1	C	309	ASP	CB-CG-OD2	14.14	131.02	118.30
1	D	309	ASP	CB-CG-OD2	14.14	131.02	118.30
1	A	52	ASP	CB-CG-OD1	13.43	130.39	118.30
1	B	52	ASP	CB-CG-OD1	13.43	130.39	118.30
1	C	52	ASP	CB-CG-OD1	13.43	130.39	118.30
1	D	52	ASP	CB-CG-OD1	13.43	130.39	118.30
1	A	87	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	B	87	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	C	87	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	D	87	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	A	77	ASP	CB-CG-OD2	-12.80	106.78	118.30
1	B	77	ASP	CB-CG-OD2	-12.80	106.78	118.30
1	C	77	ASP	CB-CG-OD2	-12.80	106.78	118.30
1	D	77	ASP	CB-CG-OD2	-12.80	106.78	118.30
1	A	125	MET	CG-SD-CE	12.79	120.67	100.20
1	B	125	MET	CG-SD-CE	12.79	120.67	100.20
1	C	125	MET	CG-SD-CE	12.79	120.67	100.20
1	D	125	MET	CG-SD-CE	12.79	120.67	100.20
1	A	169	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	B	169	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	C	169	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	D	169	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	A	169	ARG	CD-NE-CZ	11.87	140.22	123.60
1	B	169	ARG	CD-NE-CZ	11.87	140.22	123.60
1	C	169	ARG	CD-NE-CZ	11.87	140.22	123.60
1	D	169	ARG	CD-NE-CZ	11.87	140.22	123.60
1	A	308	ASP	CB-CG-OD1	11.75	128.88	118.30
1	B	308	ASP	CB-CG-OD1	11.75	128.88	118.30
1	C	308	ASP	CB-CG-OD1	11.75	128.88	118.30
1	D	308	ASP	CB-CG-OD1	11.75	128.88	118.30
1	A	260	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	B	260	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	C	260	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	D	260	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	A	228	ARG	CD-NE-CZ	-11.50	107.50	123.60
1	B	228	ARG	CD-NE-CZ	-11.50	107.50	123.60
1	C	228	ARG	CD-NE-CZ	-11.50	107.50	123.60
1	D	228	ARG	CD-NE-CZ	-11.50	107.50	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NH1-CZ-NH2	-11.32	106.94	119.40
1	B	169	ARG	NH1-CZ-NH2	-11.32	106.94	119.40
1	C	169	ARG	NH1-CZ-NH2	-11.32	106.94	119.40
1	D	169	ARG	NH1-CZ-NH2	-11.32	106.94	119.40
1	A	234	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	B	234	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	C	234	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	D	234	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	69	LYS	CA-CB-CG	10.46	136.42	113.40
1	B	69	LYS	CA-CB-CG	10.46	136.42	113.40
1	C	69	LYS	CA-CB-CG	10.46	136.42	113.40
1	D	69	LYS	CA-CB-CG	10.46	136.42	113.40
1	A	85	ASP	CB-CG-OD2	-10.23	109.09	118.30
1	B	85	ASP	CB-CG-OD2	-10.23	109.09	118.30
1	C	85	ASP	CB-CG-OD2	-10.23	109.09	118.30
1	D	85	ASP	CB-CG-OD2	-10.23	109.09	118.30
1	A	277	ASP	CB-CG-OD1	9.82	127.14	118.30
1	B	277	ASP	CB-CG-OD1	9.82	127.14	118.30
1	C	277	ASP	CB-CG-OD1	9.82	127.14	118.30
1	D	277	ASP	CB-CG-OD1	9.82	127.14	118.30
1	A	46	ASP	CB-CG-OD1	9.76	127.08	118.30
1	B	46	ASP	CB-CG-OD1	9.76	127.08	118.30
1	C	46	ASP	CB-CG-OD1	9.76	127.08	118.30
1	D	46	ASP	CB-CG-OD1	9.76	127.08	118.30
1	A	118	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	118	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	118	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	D	118	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	286	TYR	CB-CG-CD1	9.62	126.77	121.00
1	B	286	TYR	CB-CG-CD1	9.62	126.77	121.00
1	C	286	TYR	CB-CG-CD1	9.62	126.77	121.00
1	D	286	TYR	CB-CG-CD1	9.62	126.77	121.00
1	A	310	GLU	CA-CB-CG	9.57	134.45	113.40
1	B	310	GLU	CA-CB-CG	9.57	134.45	113.40
1	C	310	GLU	CA-CB-CG	9.57	134.45	113.40
1	D	310	GLU	CA-CB-CG	9.57	134.45	113.40
1	A	309	ASP	CA-CB-CG	9.56	134.43	113.40
1	B	309	ASP	CA-CB-CG	9.56	134.43	113.40
1	C	309	ASP	CA-CB-CG	9.56	134.43	113.40
1	D	309	ASP	CA-CB-CG	9.56	134.43	113.40
1	A	228	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	B	228	ARG	NE-CZ-NH2	9.50	125.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	D	228	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	A	309	ASP	OD1-CG-OD2	-9.38	105.47	123.30
1	B	309	ASP	OD1-CG-OD2	-9.38	105.47	123.30
1	C	309	ASP	OD1-CG-OD2	-9.38	105.47	123.30
1	D	309	ASP	OD1-CG-OD2	-9.38	105.47	123.30
1	A	87	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	B	87	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	C	87	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	D	87	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	22	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	B	22	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	C	22	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	D	22	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	276	LEU	O-C-N	-9.05	108.22	122.70
1	B	276	LEU	O-C-N	-9.05	108.22	122.70
1	C	276	LEU	O-C-N	-9.05	108.22	122.70
1	D	276	LEU	O-C-N	-9.05	108.22	122.70
1	A	326	ALA	CB-CA-C	8.97	123.56	110.10
1	B	326	ALA	CB-CA-C	8.97	123.56	110.10
1	C	326	ALA	CB-CA-C	8.97	123.56	110.10
1	D	326	ALA	CB-CA-C	8.97	123.56	110.10
1	A	281	GLY	CA-C-O	-8.64	105.05	120.60
1	B	281	GLY	CA-C-O	-8.64	105.05	120.60
1	C	281	GLY	CA-C-O	-8.64	105.05	120.60
1	D	281	GLY	CA-C-O	-8.64	105.05	120.60
1	A	111	ASP	N-CA-CB	8.58	126.05	110.60
1	B	111	ASP	N-CA-CB	8.58	126.05	110.60
1	C	111	ASP	N-CA-CB	8.58	126.05	110.60
1	D	111	ASP	N-CA-CB	8.58	126.05	110.60
1	A	89	ALA	N-CA-CB	-8.45	98.28	110.10
1	B	89	ALA	N-CA-CB	-8.45	98.28	110.10
1	C	89	ALA	N-CA-CB	-8.45	98.28	110.10
1	D	89	ALA	N-CA-CB	-8.45	98.28	110.10
1	A	299	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	B	299	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	C	299	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	D	299	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	74	LYS	N-CA-C	8.39	133.64	111.00
1	B	74	LYS	N-CA-C	8.39	133.64	111.00
1	C	74	LYS	N-CA-C	8.39	133.64	111.00
1	D	74	LYS	N-CA-C	8.39	133.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	TYR	CB-CG-CD2	8.27	125.96	121.00
1	B	248	TYR	CB-CG-CD2	8.27	125.96	121.00
1	C	248	TYR	CB-CG-CD2	8.27	125.96	121.00
1	D	248	TYR	CB-CG-CD2	8.27	125.96	121.00
1	A	84	ASP	CB-CG-OD1	8.16	125.65	118.30
1	B	84	ASP	CB-CG-OD1	8.16	125.65	118.30
1	C	84	ASP	CB-CG-OD1	8.16	125.65	118.30
1	D	84	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	260	ARG	CD-NE-CZ	-8.09	112.27	123.60
1	B	260	ARG	CD-NE-CZ	-8.09	112.27	123.60
1	C	260	ARG	CD-NE-CZ	-8.09	112.27	123.60
1	D	260	ARG	CD-NE-CZ	-8.09	112.27	123.60
1	A	171	ARG	CD-NE-CZ	-8.09	112.28	123.60
1	B	171	ARG	CD-NE-CZ	-8.09	112.28	123.60
1	C	171	ARG	CD-NE-CZ	-8.09	112.28	123.60
1	D	171	ARG	CD-NE-CZ	-8.09	112.28	123.60
1	A	308	ASP	CA-CB-CG	7.85	130.66	113.40
1	B	308	ASP	CA-CB-CG	7.85	130.66	113.40
1	C	308	ASP	CA-CB-CG	7.85	130.66	113.40
1	D	308	ASP	CA-CB-CG	7.85	130.66	113.40
1	A	57	LYS	CD-CE-NZ	7.76	129.55	111.70
1	B	57	LYS	CD-CE-NZ	7.76	129.55	111.70
1	C	57	LYS	CD-CE-NZ	7.76	129.55	111.70
1	D	57	LYS	CD-CE-NZ	7.76	129.55	111.70
1	A	197	GLU	OE1-CD-OE2	-7.71	114.04	123.30
1	B	197	GLU	OE1-CD-OE2	-7.71	114.04	123.30
1	C	197	GLU	OE1-CD-OE2	-7.71	114.04	123.30
1	D	197	GLU	OE1-CD-OE2	-7.71	114.04	123.30
1	A	242	GLU	CA-CB-CG	7.59	130.10	113.40
1	B	242	GLU	CA-CB-CG	7.59	130.10	113.40
1	C	242	GLU	CA-CB-CG	7.59	130.10	113.40
1	D	242	GLU	CA-CB-CG	7.59	130.10	113.40
1	A	174	LEU	CA-CB-CG	7.54	132.64	115.30
1	B	174	LEU	CA-CB-CG	7.54	132.64	115.30
1	C	174	LEU	CA-CB-CG	7.54	132.64	115.30
1	D	174	LEU	CA-CB-CG	7.54	132.64	115.30
1	A	108	ASP	CB-CG-OD1	7.53	125.08	118.30
1	B	108	ASP	CB-CG-OD1	7.53	125.08	118.30
1	C	108	ASP	CB-CG-OD1	7.53	125.08	118.30
1	D	108	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	47	GLU	OE1-CD-OE2	7.52	132.32	123.30
1	B	47	GLU	OE1-CD-OE2	7.52	132.32	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	GLU	OE1-CD-OE2	7.52	132.32	123.30
1	D	47	GLU	OE1-CD-OE2	7.52	132.32	123.30
1	A	111	ASP	OD1-CG-OD2	-7.35	109.33	123.30
1	B	111	ASP	OD1-CG-OD2	-7.35	109.33	123.30
1	C	111	ASP	OD1-CG-OD2	-7.35	109.33	123.30
1	D	111	ASP	OD1-CG-OD2	-7.35	109.33	123.30
1	A	46	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	B	46	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	C	46	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	D	46	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	277	ASP	OD1-CG-OD2	-7.23	109.57	123.30
1	B	277	ASP	OD1-CG-OD2	-7.23	109.57	123.30
1	C	277	ASP	OD1-CG-OD2	-7.23	109.57	123.30
1	D	277	ASP	OD1-CG-OD2	-7.23	109.57	123.30
1	A	87	ARG	O-C-N	7.16	134.16	122.70
1	B	87	ARG	O-C-N	7.16	134.16	122.70
1	C	87	ARG	O-C-N	7.16	134.16	122.70
1	D	87	ARG	O-C-N	7.16	134.16	122.70
1	A	308	ASP	CB-CA-C	7.13	124.67	110.40
1	B	308	ASP	CB-CA-C	7.13	124.67	110.40
1	C	308	ASP	CB-CA-C	7.13	124.67	110.40
1	D	308	ASP	CB-CA-C	7.13	124.67	110.40
1	A	40	MET	CG-SD-CE	-7.12	88.81	100.20
1	B	40	MET	CG-SD-CE	-7.12	88.81	100.20
1	C	40	MET	CG-SD-CE	-7.12	88.81	100.20
1	D	40	MET	CG-SD-CE	-7.12	88.81	100.20
1	A	305	GLU	CG-CD-OE2	-7.07	104.15	118.30
1	B	305	GLU	CG-CD-OE2	-7.07	104.15	118.30
1	C	305	GLU	CG-CD-OE2	-7.07	104.15	118.30
1	D	305	GLU	CG-CD-OE2	-7.07	104.15	118.30
1	A	145	TYR	CB-CG-CD1	6.97	125.18	121.00
1	B	145	TYR	CB-CG-CD1	6.97	125.18	121.00
1	C	145	TYR	CB-CG-CD1	6.97	125.18	121.00
1	D	145	TYR	CB-CG-CD1	6.97	125.18	121.00
1	A	64	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	B	64	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	C	64	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	D	64	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	A	29	GLY	O-C-N	-6.95	111.58	122.70
1	B	29	GLY	O-C-N	-6.95	111.58	122.70
1	C	29	GLY	O-C-N	-6.95	111.58	122.70
1	D	29	GLY	O-C-N	-6.95	111.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ARG	CD-NE-CZ	-6.93	113.89	123.60
1	B	327	ARG	CD-NE-CZ	-6.93	113.89	123.60
1	C	327	ARG	CD-NE-CZ	-6.93	113.89	123.60
1	D	327	ARG	CD-NE-CZ	-6.93	113.89	123.60
1	A	238	TYR	CG-CD2-CE2	6.88	126.81	121.30
1	B	238	TYR	CG-CD2-CE2	6.88	126.81	121.30
1	C	238	TYR	CG-CD2-CE2	6.88	126.81	121.30
1	D	238	TYR	CG-CD2-CE2	6.88	126.81	121.30
1	A	313	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	B	313	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	C	313	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	D	313	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	A	134	LEU	CB-CA-C	6.79	123.09	110.20
1	B	134	LEU	CB-CA-C	6.79	123.09	110.20
1	C	134	LEU	CB-CA-C	6.79	123.09	110.20
1	D	134	LEU	CB-CA-C	6.79	123.09	110.20
1	A	299	ARG	NH1-CZ-NH2	6.78	126.86	119.40
1	B	299	ARG	NH1-CZ-NH2	6.78	126.86	119.40
1	C	299	ARG	NH1-CZ-NH2	6.78	126.86	119.40
1	D	299	ARG	NH1-CZ-NH2	6.78	126.86	119.40
1	A	61	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	B	61	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	61	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	D	61	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	74	LYS	CB-CA-C	-6.66	97.08	110.40
1	B	74	LYS	CB-CA-C	-6.66	97.08	110.40
1	C	74	LYS	CB-CA-C	-6.66	97.08	110.40
1	D	74	LYS	CB-CA-C	-6.66	97.08	110.40
1	A	292	VAL	CA-CB-CG2	6.62	120.83	110.90
1	B	292	VAL	CA-CB-CG2	6.62	120.83	110.90
1	C	292	VAL	CA-CB-CG2	6.62	120.83	110.90
1	D	292	VAL	CA-CB-CG2	6.62	120.83	110.90
1	A	313	ARG	CG-CD-NE	6.59	125.64	111.80
1	B	313	ARG	CG-CD-NE	6.59	125.64	111.80
1	C	313	ARG	CG-CD-NE	6.59	125.64	111.80
1	D	313	ARG	CG-CD-NE	6.59	125.64	111.80
1	A	22	ARG	CD-NE-CZ	-6.56	114.41	123.60
1	B	22	ARG	CD-NE-CZ	-6.56	114.41	123.60
1	C	22	ARG	CD-NE-CZ	-6.56	114.41	123.60
1	D	22	ARG	CD-NE-CZ	-6.56	114.41	123.60
1	A	163	THR	CA-CB-CG2	6.56	121.59	112.40
1	B	163	THR	CA-CB-CG2	6.56	121.59	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	THR	CA-CB-CG2	6.56	121.59	112.40
1	D	163	THR	CA-CB-CG2	6.56	121.59	112.40
1	A	299	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	B	299	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	C	299	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	D	299	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	A	50	LEU	CA-CB-CG	6.51	130.28	115.30
1	B	50	LEU	CA-CB-CG	6.51	130.28	115.30
1	C	50	LEU	CA-CB-CG	6.51	130.28	115.30
1	D	50	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	50	LEU	N-CA-CB	-6.51	97.38	110.40
1	B	50	LEU	N-CA-CB	-6.51	97.38	110.40
1	C	50	LEU	N-CA-CB	-6.51	97.38	110.40
1	D	50	LEU	N-CA-CB	-6.51	97.38	110.40
1	A	78	ILE	CA-CB-CG1	6.46	123.28	111.00
1	B	78	ILE	CA-CB-CG1	6.46	123.28	111.00
1	C	78	ILE	CA-CB-CG1	6.46	123.28	111.00
1	D	78	ILE	CA-CB-CG1	6.46	123.28	111.00
1	A	161	SER	C-N-CA	6.44	135.83	122.30
1	B	161	SER	C-N-CA	6.44	135.83	122.30
1	C	161	SER	C-N-CA	6.44	135.83	122.30
1	D	161	SER	C-N-CA	6.44	135.83	122.30
1	A	157	ARG	CG-CD-NE	6.38	125.19	111.80
1	B	157	ARG	CG-CD-NE	6.38	125.19	111.80
1	C	157	ARG	CG-CD-NE	6.38	125.19	111.80
1	D	157	ARG	CG-CD-NE	6.38	125.19	111.80
1	A	323	SER	N-CA-CB	-6.36	100.96	110.50
1	B	323	SER	N-CA-CB	-6.36	100.96	110.50
1	C	323	SER	N-CA-CB	-6.36	100.96	110.50
1	D	323	SER	N-CA-CB	-6.36	100.96	110.50
1	A	191	GLY	O-C-N	-6.25	112.70	122.70
1	B	191	GLY	O-C-N	-6.25	112.70	122.70
1	C	191	GLY	O-C-N	-6.25	112.70	122.70
1	D	191	GLY	O-C-N	-6.25	112.70	122.70
1	A	296	ASN	CB-CA-C	6.22	122.85	110.40
1	B	296	ASN	CB-CA-C	6.22	122.85	110.40
1	C	296	ASN	CB-CA-C	6.22	122.85	110.40
1	D	296	ASN	CB-CA-C	6.22	122.85	110.40
1	A	289	VAL	N-CA-CB	-6.22	97.81	111.50
1	B	289	VAL	N-CA-CB	-6.22	97.81	111.50
1	C	289	VAL	N-CA-CB	-6.22	97.81	111.50
1	D	289	VAL	N-CA-CB	-6.22	97.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	LEU	CA-C-O	-6.22	107.04	120.10
1	B	279	LEU	CA-C-O	-6.22	107.04	120.10
1	C	279	LEU	CA-C-O	-6.22	107.04	120.10
1	D	279	LEU	CA-C-O	-6.22	107.04	120.10
1	A	37	PHE	CB-CG-CD2	6.22	125.15	120.80
1	B	37	PHE	CB-CG-CD2	6.22	125.15	120.80
1	C	37	PHE	CB-CG-CD2	6.22	125.15	120.80
1	D	37	PHE	CB-CG-CD2	6.22	125.15	120.80
1	A	47	GLU	CG-CD-OE2	-6.16	105.98	118.30
1	B	47	GLU	CG-CD-OE2	-6.16	105.98	118.30
1	C	47	GLU	CG-CD-OE2	-6.16	105.98	118.30
1	D	47	GLU	CG-CD-OE2	-6.16	105.98	118.30
1	A	132	LEU	CA-CB-CG	6.12	129.37	115.30
1	B	132	LEU	CA-CB-CG	6.12	129.37	115.30
1	C	132	LEU	CA-CB-CG	6.12	129.37	115.30
1	D	132	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	279	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	279	LEU	CA-CB-CG	6.10	129.33	115.30
1	C	279	LEU	CA-CB-CG	6.10	129.33	115.30
1	D	279	LEU	CA-CB-CG	6.10	129.33	115.30
1	A	76	VAL	C-N-CA	6.09	136.93	121.70
1	B	76	VAL	C-N-CA	6.09	136.93	121.70
1	C	76	VAL	C-N-CA	6.09	136.93	121.70
1	D	76	VAL	C-N-CA	6.09	136.93	121.70
1	A	313	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	B	313	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	C	313	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	D	313	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	164	ILE	CB-CG1-CD1	-6.06	96.93	113.90
1	B	164	ILE	CB-CG1-CD1	-6.06	96.93	113.90
1	C	164	ILE	CB-CG1-CD1	-6.06	96.93	113.90
1	D	164	ILE	CB-CG1-CD1	-6.06	96.93	113.90
1	A	50	LEU	CB-CA-C	5.96	121.53	110.20
1	B	50	LEU	CB-CA-C	5.96	121.53	110.20
1	C	50	LEU	CB-CA-C	5.96	121.53	110.20
1	D	50	LEU	CB-CA-C	5.96	121.53	110.20
1	A	234	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	234	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	234	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	234	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	256	ALA	CB-CA-C	5.84	118.86	110.10
1	B	256	ALA	CB-CA-C	5.84	118.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	ALA	CB-CA-C	5.84	118.86	110.10
1	D	256	ALA	CB-CA-C	5.84	118.86	110.10
1	A	276	LEU	CA-C-O	5.80	132.27	120.10
1	B	276	LEU	CA-C-O	5.80	132.27	120.10
1	C	276	LEU	CA-C-O	5.80	132.27	120.10
1	D	276	LEU	CA-C-O	5.80	132.27	120.10
1	A	144	THR	N-CA-CB	5.79	121.31	110.30
1	B	144	THR	N-CA-CB	5.79	121.31	110.30
1	C	144	THR	N-CA-CB	5.79	121.31	110.30
1	D	144	THR	N-CA-CB	5.79	121.31	110.30
1	A	166	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	166	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	166	ASP	CB-CG-OD2	5.76	123.48	118.30
1	D	166	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	181	ALA	CB-CA-C	5.74	118.72	110.10
1	B	181	ALA	CB-CA-C	5.74	118.72	110.10
1	C	181	ALA	CB-CA-C	5.74	118.72	110.10
1	D	181	ALA	CB-CA-C	5.74	118.72	110.10
1	A	205	TYR	CB-CG-CD2	5.73	124.44	121.00
1	B	205	TYR	CB-CG-CD2	5.73	124.44	121.00
1	C	205	TYR	CB-CG-CD2	5.73	124.44	121.00
1	D	205	TYR	CB-CG-CD2	5.73	124.44	121.00
1	A	294	ASN	CB-CA-C	5.72	121.84	110.40
1	B	294	ASN	CB-CA-C	5.72	121.84	110.40
1	C	294	ASN	CB-CA-C	5.72	121.84	110.40
1	D	294	ASN	CB-CA-C	5.72	121.84	110.40
1	A	184	ASN	CB-CG-ND2	5.71	130.41	116.70
1	B	184	ASN	CB-CG-ND2	5.71	130.41	116.70
1	C	184	ASN	CB-CG-ND2	5.71	130.41	116.70
1	D	184	ASN	CB-CG-ND2	5.71	130.41	116.70
1	A	171	ARG	NH1-CZ-NH2	5.65	125.61	119.40
1	B	171	ARG	NH1-CZ-NH2	5.65	125.61	119.40
1	C	171	ARG	NH1-CZ-NH2	5.65	125.61	119.40
1	D	171	ARG	NH1-CZ-NH2	5.65	125.61	119.40
1	A	284	ASP	O-C-N	5.63	131.71	122.70
1	B	284	ASP	O-C-N	5.63	131.71	122.70
1	C	284	ASP	O-C-N	5.63	131.71	122.70
1	D	284	ASP	O-C-N	5.63	131.71	122.70
1	A	286	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	B	286	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	C	286	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	D	286	TYR	CB-CG-CD2	-5.59	117.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	HIS	CA-C-O	5.57	131.80	120.10
1	B	315	HIS	CA-C-O	5.57	131.80	120.10
1	C	315	HIS	CA-C-O	5.57	131.80	120.10
1	D	315	HIS	CA-C-O	5.57	131.80	120.10
1	A	111	ASP	CA-CB-CG	5.53	125.55	113.40
1	B	111	ASP	CA-CB-CG	5.53	125.55	113.40
1	C	111	ASP	CA-CB-CG	5.53	125.55	113.40
1	D	111	ASP	CA-CB-CG	5.53	125.55	113.40
1	A	307	ASN	N-CA-CB	-5.52	100.67	110.60
1	B	307	ASN	N-CA-CB	-5.52	100.67	110.60
1	C	307	ASN	N-CA-CB	-5.52	100.67	110.60
1	D	307	ASN	N-CA-CB	-5.52	100.67	110.60
1	A	327	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	327	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	327	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	327	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	255	LEU	CB-CA-C	5.45	120.56	110.20
1	B	255	LEU	CB-CA-C	5.45	120.56	110.20
1	C	255	LEU	CB-CA-C	5.45	120.56	110.20
1	D	255	LEU	CB-CA-C	5.45	120.56	110.20
1	A	136	ALA	CA-C-N	5.44	129.18	117.20
1	B	136	ALA	CA-C-N	5.44	129.18	117.20
1	C	136	ALA	CA-C-N	5.44	129.18	117.20
1	D	136	ALA	CA-C-N	5.44	129.18	117.20
1	A	243	LYS	N-CA-CB	5.43	120.37	110.60
1	B	243	LYS	N-CA-CB	5.43	120.37	110.60
1	C	243	LYS	N-CA-CB	5.43	120.37	110.60
1	D	243	LYS	N-CA-CB	5.43	120.37	110.60
1	A	136	ALA	CA-C-O	-5.42	108.71	120.10
1	B	136	ALA	CA-C-O	-5.42	108.71	120.10
1	C	136	ALA	CA-C-O	-5.42	108.71	120.10
1	D	136	ALA	CA-C-O	-5.42	108.71	120.10
1	A	139	PRO	CA-C-O	-5.41	107.21	120.20
1	B	139	PRO	CA-C-O	-5.41	107.21	120.20
1	C	139	PRO	CA-C-O	-5.41	107.21	120.20
1	D	139	PRO	CA-C-O	-5.41	107.21	120.20
1	A	273	SER	N-CA-CB	5.36	118.54	110.50
1	B	273	SER	N-CA-CB	5.36	118.54	110.50
1	C	273	SER	N-CA-CB	5.36	118.54	110.50
1	D	273	SER	N-CA-CB	5.36	118.54	110.50
1	A	109	LEU	CB-CA-C	-5.33	100.07	110.20
1	B	109	LEU	CB-CA-C	-5.33	100.07	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	LEU	CB-CA-C	-5.33	100.07	110.20
1	D	109	LEU	CB-CA-C	-5.33	100.07	110.20
1	A	134	LEU	CB-CG-CD1	5.33	120.06	111.00
1	B	134	LEU	CB-CG-CD1	5.33	120.06	111.00
1	C	134	LEU	CB-CG-CD1	5.33	120.06	111.00
1	D	134	LEU	CB-CG-CD1	5.33	120.06	111.00
1	A	257	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	313	ARG	CB-CA-C	5.31	121.02	110.40
1	B	257	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	313	ARG	CB-CA-C	5.31	121.02	110.40
1	C	257	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	313	ARG	CB-CA-C	5.31	121.02	110.40
1	D	257	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	313	ARG	CB-CA-C	5.31	121.02	110.40
1	A	108	ASP	C-N-CA	5.30	134.96	121.70
1	A	306	LEU	CA-C-O	5.30	131.23	120.10
1	B	108	ASP	C-N-CA	5.30	134.96	121.70
1	B	306	LEU	CA-C-O	5.30	131.23	120.10
1	C	108	ASP	C-N-CA	5.30	134.96	121.70
1	C	306	LEU	CA-C-O	5.30	131.23	120.10
1	D	108	ASP	C-N-CA	5.30	134.96	121.70
1	D	306	LEU	CA-C-O	5.30	131.23	120.10
1	A	281	GLY	CA-C-N	5.30	128.86	117.20
1	B	281	GLY	CA-C-N	5.30	128.86	117.20
1	C	281	GLY	CA-C-N	5.30	128.86	117.20
1	D	281	GLY	CA-C-N	5.30	128.86	117.20
1	A	70	VAL	C-N-CA	5.29	134.92	121.70
1	B	70	VAL	C-N-CA	5.29	134.92	121.70
1	C	70	VAL	C-N-CA	5.29	134.92	121.70
1	D	70	VAL	C-N-CA	5.29	134.92	121.70
1	A	177	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	B	177	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	C	177	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	D	177	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	277	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	277	ASP	CB-CG-OD2	5.26	123.04	118.30
1	C	277	ASP	CB-CG-OD2	5.26	123.04	118.30
1	D	277	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	49	VAL	CG1-CB-CG2	5.24	119.28	110.90
1	B	49	VAL	CG1-CB-CG2	5.24	119.28	110.90
1	C	49	VAL	CG1-CB-CG2	5.24	119.28	110.90
1	D	49	VAL	CG1-CB-CG2	5.24	119.28	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	GLU	CA-CB-CG	5.22	124.89	113.40
1	B	266	GLU	CA-CB-CG	5.22	124.89	113.40
1	C	266	GLU	CA-CB-CG	5.22	124.89	113.40
1	D	266	GLU	CA-CB-CG	5.22	124.89	113.40
1	A	84	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	B	84	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	C	84	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	D	84	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	A	327	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	327	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	327	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	327	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	85	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	85	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	85	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	85	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	283	ARG	CA-C-N	5.16	128.55	117.20
1	B	283	ARG	CA-C-N	5.16	128.55	117.20
1	C	283	ARG	CA-C-N	5.16	128.55	117.20
1	D	283	ARG	CA-C-N	5.16	128.55	117.20
1	A	282	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	B	282	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	C	282	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	D	282	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	A	77	ASP	OD1-CG-OD2	5.15	133.08	123.30
1	A	132	LEU	N-CA-CB	-5.15	100.11	110.40
1	B	77	ASP	OD1-CG-OD2	5.15	133.08	123.30
1	B	132	LEU	N-CA-CB	-5.15	100.11	110.40
1	C	77	ASP	OD1-CG-OD2	5.15	133.08	123.30
1	C	132	LEU	N-CA-CB	-5.15	100.11	110.40
1	D	77	ASP	OD1-CG-OD2	5.15	133.08	123.30
1	D	132	LEU	N-CA-CB	-5.15	100.11	110.40
1	A	227	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	B	227	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	C	227	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	D	227	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	A	309	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	309	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	309	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	309	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	166	ASP	OD1-CG-OD2	-5.12	113.57	123.30
1	B	166	ASP	OD1-CG-OD2	-5.12	113.57	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	ASP	OD1-CG-OD2	-5.12	113.57	123.30
1	D	166	ASP	OD1-CG-OD2	-5.12	113.57	123.30
1	A	114	ILE	CB-CG1-CD1	5.12	128.23	113.90
1	B	114	ILE	CB-CG1-CD1	5.12	128.23	113.90
1	C	114	ILE	CB-CG1-CD1	5.12	128.23	113.90
1	D	114	ILE	CB-CG1-CD1	5.12	128.23	113.90
1	A	305	GLU	CG-CD-OE1	5.10	128.49	118.30
1	B	305	GLU	CG-CD-OE1	5.10	128.49	118.30
1	C	305	GLU	CG-CD-OE1	5.10	128.49	118.30
1	D	305	GLU	CG-CD-OE1	5.10	128.49	118.30
1	A	37	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	B	37	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	C	37	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	D	37	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	A	247	THR	CA-CB-CG2	5.04	119.45	112.40
1	B	247	THR	CA-CB-CG2	5.04	119.45	112.40
1	C	247	THR	CA-CB-CG2	5.04	119.45	112.40
1	D	247	THR	CA-CB-CG2	5.04	119.45	112.40
1	A	112	LYS	CA-C-N	-5.03	106.13	117.20
1	B	112	LYS	CA-C-N	-5.03	106.13	117.20
1	C	112	LYS	CA-C-N	-5.03	106.13	117.20
1	D	112	LYS	CA-C-N	-5.03	106.13	117.20
1	A	62	ALA	CB-CA-C	5.03	117.64	110.10
1	B	62	ALA	CB-CA-C	5.03	117.64	110.10
1	C	62	ALA	CB-CA-C	5.03	117.64	110.10
1	D	62	ALA	CB-CA-C	5.03	117.64	110.10

There are no chirality outliers.

All (124) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Mainchain
1	A	134	LEU	Mainchain
1	A	147	THR	Mainchain
1	A	152	GLY	Mainchain
1	A	154	PRO	Mainchain
1	A	167	THR	Mainchain
1	A	170	PHE	Sidechain
1	A	171	ARG	Sidechain
1	A	184	ASN	Mainchain
1	A	188	TYR	Mainchain
1	A	191	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	206	ILE	Mainchain
1	A	207	GLY	Mainchain
1	A	229	ILE	Mainchain
1	A	23	VAL	Mainchain
1	A	275	TYR	Sidechain
1	A	281	GLY	Mainchain
1	A	285	VAL	Mainchain
1	A	286	TYR	Sidechain
1	A	295	ARG	Mainchain
1	A	30	PHE	Sidechain
1	A	300	GLU	Mainchain
1	A	301	VAL	Mainchain
1	A	310	GLU	Mainchain
1	A	312	ASN	Mainchain
1	A	323	SER	Mainchain
1	A	325	LEU	Mainchain
1	A	49	VAL	Mainchain
1	A	62	ALA	Mainchain
1	A	77	ASP	Mainchain
1	A	94	ILE	Mainchain
1	B	111	ASP	Mainchain
1	B	134	LEU	Mainchain
1	B	147	THR	Mainchain
1	B	152	GLY	Mainchain
1	B	154	PRO	Mainchain
1	B	167	THR	Mainchain
1	B	170	PHE	Sidechain
1	B	171	ARG	Sidechain
1	B	184	ASN	Mainchain
1	B	188	TYR	Mainchain
1	B	191	GLY	Mainchain
1	B	206	ILE	Mainchain
1	B	207	GLY	Mainchain
1	B	229	ILE	Mainchain
1	B	23	VAL	Mainchain
1	B	275	TYR	Sidechain
1	B	281	GLY	Mainchain
1	B	285	VAL	Mainchain
1	B	286	TYR	Sidechain
1	B	295	ARG	Mainchain
1	B	30	PHE	Sidechain
1	B	300	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	B	301	VAL	Mainchain
1	B	310	GLU	Mainchain
1	B	312	ASN	Mainchain
1	B	323	SER	Mainchain
1	B	325	LEU	Mainchain
1	B	49	VAL	Mainchain
1	B	62	ALA	Mainchain
1	B	77	ASP	Mainchain
1	B	94	ILE	Mainchain
1	C	111	ASP	Mainchain
1	C	134	LEU	Mainchain
1	C	147	THR	Mainchain
1	C	152	GLY	Mainchain
1	C	154	PRO	Mainchain
1	C	167	THR	Mainchain
1	C	170	PHE	Sidechain
1	C	171	ARG	Sidechain
1	C	184	ASN	Mainchain
1	C	188	TYR	Mainchain
1	C	191	GLY	Mainchain
1	C	206	ILE	Mainchain
1	C	207	GLY	Mainchain
1	C	229	ILE	Mainchain
1	C	23	VAL	Mainchain
1	C	275	TYR	Sidechain
1	C	281	GLY	Mainchain
1	C	285	VAL	Mainchain
1	C	286	TYR	Sidechain
1	C	295	ARG	Mainchain
1	C	30	PHE	Sidechain
1	C	300	GLU	Mainchain
1	C	301	VAL	Mainchain
1	C	310	GLU	Mainchain
1	C	312	ASN	Mainchain
1	C	323	SER	Mainchain
1	C	325	LEU	Mainchain
1	C	49	VAL	Mainchain
1	C	62	ALA	Mainchain
1	C	77	ASP	Mainchain
1	C	94	ILE	Mainchain
1	D	111	ASP	Mainchain
1	D	134	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	D	147	THR	Mainchain
1	D	152	GLY	Mainchain
1	D	154	PRO	Mainchain
1	D	167	THR	Mainchain
1	D	170	PHE	Sidechain
1	D	171	ARG	Sidechain
1	D	184	ASN	Mainchain
1	D	188	TYR	Mainchain
1	D	191	GLY	Mainchain
1	D	206	ILE	Mainchain
1	D	207	GLY	Mainchain
1	D	229	ILE	Mainchain
1	D	23	VAL	Mainchain
1	D	275	TYR	Sidechain
1	D	281	GLY	Mainchain
1	D	285	VAL	Mainchain
1	D	286	TYR	Sidechain
1	D	295	ARG	Mainchain
1	D	30	PHE	Sidechain
1	D	300	GLU	Mainchain
1	D	301	VAL	Mainchain
1	D	310	GLU	Mainchain
1	D	312	ASN	Mainchain
1	D	323	SER	Mainchain
1	D	325	LEU	Mainchain
1	D	49	VAL	Mainchain
1	D	62	ALA	Mainchain
1	D	77	ASP	Mainchain
1	D	94	ILE	Mainchain

## 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	2277	0	2251	199	46
1	B	2277	0	2251	193	0
1	C	2277	0	2251	194	11
1	D	2277	0	2251	200	57

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	2	0
3	A	1	0	0	1	0
All	All	9119	0	9004	733	57

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 40.

All (733) 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:B:87:ARG:HG3	1:B:88:ASP:H	1.12	1.15
1:C:87:ARG:HG3	1:C:88:ASP:H	1.12	1.15
1:C:142:ILE:HD13	1:C:324:VAL:HG11	1.32	1.12
1:B:142:ILE:HD13	1:B:324:VAL:HG11	1.32	1.11
1:D:87:ARG:HG3	1:D:88:ASP:H	1.12	1.11
1:A:87:ARG:HG3	1:A:88:ASP:H	1.12	1.10
1:D:142:ILE:HD13	1:D:324:VAL:HG11	1.32	1.09
1:A:142:ILE:HD13	1:A:324:VAL:HG11	1.32	1.09
1:C:265:ASN:HD22	1:C:295:ARG:HB2	1.18	1.08
1:B:265:ASN:HD22	1:B:295:ARG:HB2	1.18	1.08
1:C:18:ASN:N	1:C:18:ASN:HD22	1.50	1.03
1:A:265:ASN:HD22	1:A:295:ARG:HB2	1.18	1.03
1:D:265:ASN:HD22	1:D:295:ARG:HB2	1.18	1.03
1:B:18:ASN:HD22	1:B:18:ASN:N	1.50	1.03
1:D:311:LYS:HA	1:D:315:HIS:HB2	1.40	1.03
1:A:311:LYS:HA	1:A:315:HIS:HB2	1.40	1.02
1:D:18:ASN:N	1:D:18:ASN:HD22	1.50	1.02
1:A:18:ASN:N	1:A:18:ASN:HD22	1.50	1.01
1:B:311:LYS:HA	1:B:315:HIS:HB2	1.40	1.01
1:C:311:LYS:HA	1:C:315:HIS:HB2	1.40	1.01
1:D:310:GLU:O	1:D:312:ASN:N	1.93	1.00
1:A:310:GLU:O	1:A:312:ASN:N	1.93	1.00
1:C:310:GLU:O	1:C:312:ASN:N	1.93	1.00
1:B:310:GLU:O	1:B:312:ASN:N	1.93	1.00
1:A:18:ASN:H	1:A:18:ASN:ND2	1.53	0.98
1:D:18:ASN:ND2	1:D:18:ASN:H	1.53	0.98
1:B:18:ASN:ND2	1:B:18:ASN:H	1.53	0.97
1:C:18:ASN:ND2	1:C:18:ASN:H	1.53	0.97
1:D:87:ARG:CG	1:D:88:ASP:H	1.77	0.92
1:A:87:ARG:CG	1:A:88:ASP:H	1.77	0.92
1:A:87:ARG:HG3	1:A:88:ASP:N	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:HG3	1:D:88:ASP:N	1.86	0.91
1:C:265:ASN:ND2	1:C:295:ARG:HB2	1.85	0.91
1:A:265:ASN:ND2	1:A:295:ARG:HB2	1.85	0.91
1:D:265:ASN:ND2	1:D:295:ARG:HB2	1.85	0.91
1:C:87:ARG:CG	1:C:88:ASP:H	1.77	0.90
1:B:265:ASN:ND2	1:B:295:ARG:HB2	1.85	0.90
1:B:87:ARG:HG3	1:B:88:ASP:N	1.86	0.90
1:B:87:ARG:CG	1:B:88:ASP:H	1.77	0.90
1:C:87:ARG:HG3	1:C:88:ASP:N	1.86	0.90
1:D:87:ARG:HB2	1:D:87:ARG:NH1	1.89	0.88
1:A:87:ARG:NH1	1:A:87:ARG:HB2	1.89	0.88
1:A:142:ILE:CD1	1:A:324:VAL:HG11	2.04	0.87
1:C:142:ILE:CD1	1:C:324:VAL:HG11	2.04	0.87
1:D:142:ILE:CD1	1:D:324:VAL:HG11	2.04	0.87
1:B:142:ILE:CD1	1:B:324:VAL:HG11	2.04	0.87
1:A:295:ARG:HH11	1:A:295:ARG:HG3	1.40	0.86
1:D:295:ARG:HH11	1:D:295:ARG:HG3	1.40	0.86
1:B:87:ARG:NH1	1:B:87:ARG:HB2	1.89	0.86
1:C:87:ARG:HB2	1:C:87:ARG:NH1	1.89	0.86
1:B:295:ARG:HG3	1:B:295:ARG:HH11	1.40	0.86
1:C:295:ARG:HG3	1:C:295:ARG:HH11	1.40	0.86
1:B:70:VAL:HG22	1:D:182:PRO:HB2	1.57	0.86
1:A:182:PRO:HB2	1:C:70:VAL:HG22	1.57	0.86
1:A:200:VAL:HG11	1:A:304:ILE:HD12	1.56	0.85
1:D:200:VAL:HG11	1:D:304:ILE:HD12	1.56	0.85
1:C:200:VAL:HG11	1:C:304:ILE:HD12	1.56	0.85
1:A:244:LYS:O	1:A:244:LYS:HG2	1.77	0.84
1:D:244:LYS:HG2	1:D:244:LYS:O	1.77	0.84
1:B:200:VAL:HG11	1:B:304:ILE:HD12	1.56	0.84
1:A:70:VAL:HG22	1:C:182:PRO:HB2	1.57	0.84
1:B:182:PRO:HB2	1:D:70:VAL:HG22	1.57	0.84
1:C:311:LYS:HA	1:C:315:HIS:CB	2.07	0.84
1:B:311:LYS:HA	1:B:315:HIS:CB	2.07	0.84
1:D:109:LEU:O	1:D:113:ASN:HB2	1.78	0.84
1:A:109:LEU:O	1:A:113:ASN:HB2	1.78	0.83
1:B:244:LYS:HG2	1:B:244:LYS:O	1.77	0.83
1:D:55:GLU:O	1:D:59:ILE:HD12	1.78	0.83
1:C:244:LYS:O	1:C:244:LYS:HG2	1.77	0.83
1:A:55:GLU:O	1:A:59:ILE:HD12	1.78	0.83
1:D:311:LYS:HA	1:D:315:HIS:CB	2.07	0.83
1:A:311:LYS:HA	1:A:315:HIS:CB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:O	1:B:59:ILE:HD12	1.78	0.83
1:C:55:GLU:O	1:C:59:ILE:HD12	1.78	0.82
1:B:109:LEU:O	1:B:113:ASN:HB2	1.78	0.82
1:C:109:LEU:O	1:C:113:ASN:HB2	1.78	0.82
1:B:328:ALA:O	1:B:329:PHE:HB2	1.80	0.81
1:B:200:VAL:HG11	1:B:304:ILE:CD1	2.11	0.81
1:C:200:VAL:HG11	1:C:304:ILE:CD1	2.11	0.81
1:C:328:ALA:O	1:C:329:PHE:HB2	1.80	0.81
1:A:15:MET:HE2	1:A:18:ASN:HA	1.61	0.80
1:C:240:ILE:CG1	1:C:247:THR:HG22	2.12	0.80
1:B:240:ILE:CG1	1:B:247:THR:HG22	2.12	0.80
1:D:15:MET:HE2	1:D:18:ASN:HA	1.62	0.80
1:A:270:LEU:HD12	1:A:293:ILE:HD12	1.64	0.80
1:A:200:VAL:HG11	1:A:304:ILE:CD1	2.11	0.80
1:D:270:LEU:HD12	1:D:293:ILE:HD12	1.64	0.80
1:D:200:VAL:HG11	1:D:304:ILE:CD1	2.11	0.80
1:D:328:ALA:O	1:D:329:PHE:HB2	1.80	0.79
1:A:328:ALA:O	1:A:329:PHE:HB2	1.80	0.79
1:D:130:GLN:O	1:D:157:ARG:NH1	2.15	0.79
1:A:130:GLN:O	1:A:157:ARG:NH1	2.15	0.79
1:A:163:THR:O	1:A:167:THR:HG23	1.83	0.79
1:A:240:ILE:CG1	1:A:247:THR:HG22	2.12	0.79
1:D:163:THR:O	1:D:167:THR:HG23	1.83	0.79
1:D:240:ILE:CG1	1:D:247:THR:HG22	2.12	0.79
1:C:270:LEU:HD12	1:C:293:ILE:HD12	1.64	0.79
1:B:270:LEU:HD12	1:B:293:ILE:HD12	1.64	0.79
1:C:15:MET:HE2	1:C:18:ASN:HA	1.64	0.78
1:A:244:LYS:HE3	1:C:61:ASP:OD1	1.83	0.78
1:B:61:ASP:OD1	1:D:244:LYS:HE3	1.83	0.78
1:A:178:PHE:CE1	1:A:206:ILE:CD1	2.66	0.78
1:B:130:GLN:O	1:B:157:ARG:NH1	2.15	0.78
1:D:178:PHE:CE1	1:D:206:ILE:CD1	2.66	0.78
1:C:130:GLN:O	1:C:157:ARG:NH1	2.15	0.78
1:B:15:MET:HE2	1:B:18:ASN:HA	1.64	0.78
1:C:178:PHE:CE1	1:C:206:ILE:CD1	2.66	0.78
1:B:178:PHE:CE1	1:B:206:ILE:CD1	2.66	0.78
1:B:244:LYS:HE3	1:D:61:ASP:OD1	1.83	0.78
1:A:61:ASP:OD1	1:C:244:LYS:HE3	1.83	0.78
1:B:163:THR:O	1:B:167:THR:HG23	1.83	0.77
1:C:163:THR:O	1:C:167:THR:HG23	1.83	0.77
1:C:18:ASN:HD22	1:C:18:ASN:H	0.77	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASN:HD22	1:B:18:ASN:H	0.77	0.75
1:A:310:GLU:C	1:A:312:ASN:H	1.90	0.75
1:D:310:GLU:C	1:D:312:ASN:H	1.90	0.75
1:C:310:GLU:C	1:C:312:ASN:H	1.90	0.74
1:A:178:PHE:CE1	1:A:206:ILE:HD11	2.23	0.74
1:D:178:PHE:CE1	1:D:206:ILE:HD11	2.23	0.74
1:B:310:GLU:C	1:B:312:ASN:H	1.90	0.74
1:B:178:PHE:CE1	1:B:206:ILE:HD11	2.23	0.73
1:C:178:PHE:CE1	1:C:206:ILE:HD11	2.23	0.73
1:D:306:LEU:O	1:D:307:ASN:O	2.06	0.72
1:A:306:LEU:O	1:A:307:ASN:O	2.06	0.72
1:C:15:MET:CE	1:C:18:ASN:HA	2.18	0.72
1:B:55:GLU:HG3	1:B:59:ILE:HD11	1.71	0.72
1:C:55:GLU:HG3	1:C:59:ILE:HD11	1.71	0.72
1:B:15:MET:CE	1:B:18:ASN:HA	2.18	0.72
1:C:306:LEU:O	1:C:307:ASN:O	2.06	0.72
1:B:306:LEU:O	1:B:307:ASN:O	2.06	0.72
1:D:18:ASN:N	1:D:18:ASN:ND2	2.24	0.72
1:A:18:ASN:N	1:A:18:ASN:ND2	2.24	0.72
1:D:15:MET:CE	1:D:18:ASN:HA	2.18	0.71
1:B:118:ARG:O	1:B:122:GLU:HG2	1.90	0.71
1:C:118:ARG:O	1:C:122:GLU:HG2	1.90	0.71
1:A:15:MET:CE	1:A:18:ASN:HA	2.18	0.71
1:A:55:GLU:HG3	1:A:59:ILE:HD11	1.71	0.71
1:D:24:VAL:HG22	1:D:49:VAL:HB	1.73	0.71
1:D:55:GLU:HG3	1:D:59:ILE:HD11	1.71	0.71
1:A:24:VAL:HG22	1:A:49:VAL:HB	1.73	0.71
1:B:24:VAL:HG22	1:B:49:VAL:HB	1.73	0.71
1:C:257:ARG:NH2	1:C:266:GLU:OE2	2.18	0.71
1:C:24:VAL:HG22	1:C:49:VAL:HB	1.73	0.71
1:B:257:ARG:NH2	1:B:266:GLU:OE2	2.18	0.71
1:D:118:ARG:O	1:D:122:GLU:HG2	1.90	0.70
1:D:87:ARG:HB2	1:D:87:ARG:CZ	2.20	0.70
1:A:87:ARG:CZ	1:A:87:ARG:HB2	2.20	0.70
1:D:86:CYS:HA	1:D:89:ALA:CB	2.22	0.70
1:A:118:ARG:O	1:A:122:GLU:HG2	1.90	0.70
1:A:86:CYS:HA	1:A:89:ALA:CB	2.22	0.70
1:B:68:GLY:O	1:B:71:PHE:HB2	1.92	0.70
1:C:68:GLY:O	1:C:71:PHE:HB2	1.92	0.70
1:A:18:ASN:H	1:A:18:ASN:HD22	0.77	0.69
1:C:86:CYS:HA	1:C:89:ALA:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:GLU:C	1:D:312:ASN:N	2.42	0.69
1:B:86:CYS:HA	1:B:89:ALA:CB	2.22	0.69
1:D:18:ASN:HD22	1:D:18:ASN:H	0.77	0.69
1:B:279:LEU:HD23	1:B:301:VAL:CG1	2.22	0.69
1:C:279:LEU:HD23	1:C:301:VAL:CG1	2.22	0.69
1:A:310:GLU:C	1:A:312:ASN:N	2.42	0.69
1:A:279:LEU:HD23	1:A:301:VAL:CG1	2.22	0.69
1:D:283:ARG:H	1:D:322:LYS:NZ	1.90	0.69
1:D:279:LEU:HD23	1:D:301:VAL:CG1	2.22	0.69
1:C:87:ARG:CZ	1:C:87:ARG:HB2	2.20	0.69
1:A:283:ARG:H	1:A:322:LYS:NZ	1.90	0.69
1:B:87:ARG:HB2	1:B:87:ARG:CZ	2.20	0.69
1:C:83:TYR:C	1:C:85:ASP:H	1.97	0.69
1:D:167:THR:HG22	1:D:189:ILE:H	1.56	0.69
1:B:167:THR:HG22	1:B:189:ILE:H	1.56	0.69
1:B:83:TYR:C	1:B:85:ASP:H	1.97	0.69
1:A:167:THR:HG22	1:A:189:ILE:H	1.56	0.68
1:C:283:ARG:H	1:C:322:LYS:NZ	1.90	0.68
1:A:68:GLY:O	1:A:71:PHE:HB2	1.92	0.68
1:B:283:ARG:H	1:B:322:LYS:NZ	1.90	0.68
1:C:167:THR:HG22	1:C:189:ILE:H	1.56	0.68
1:D:68:GLY:O	1:D:71:PHE:HB2	1.92	0.68
1:B:125:MET:HE3	1:B:129:PHE:HB3	1.75	0.68
1:C:125:MET:HE3	1:C:129:PHE:HB3	1.74	0.68
1:C:189:ILE:CG2	1:C:197:GLU:HG3	2.24	0.67
1:D:189:ILE:CD1	1:D:233:VAL:HG11	2.24	0.67
1:B:189:ILE:CG2	1:B:197:GLU:HG3	2.24	0.67
1:A:125:MET:HE3	1:A:129:PHE:HB3	1.77	0.67
1:A:189:ILE:CD1	1:A:233:VAL:HG11	2.24	0.67
1:D:125:MET:HE3	1:D:129:PHE:HB3	1.77	0.67
1:B:189:ILE:CD1	1:B:233:VAL:HG11	2.24	0.67
1:A:83:TYR:C	1:A:85:ASP:H	1.97	0.67
1:A:189:ILE:CG2	1:A:197:GLU:HG3	2.24	0.67
1:D:83:TYR:C	1:D:85:ASP:H	1.97	0.67
1:D:189:ILE:CG2	1:D:197:GLU:HG3	2.24	0.67
1:C:189:ILE:CD1	1:C:233:VAL:HG11	2.24	0.66
1:A:257:ARG:NH2	1:A:266:GLU:OE2	2.18	0.66
1:D:257:ARG:NH2	1:D:266:GLU:OE2	2.18	0.66
1:A:87:ARG:CG	1:A:88:ASP:N	2.52	0.66
1:C:310:GLU:C	1:C:312:ASN:N	2.42	0.66
1:D:87:ARG:CG	1:D:88:ASP:N	2.52	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:C	1:B:312:ASN:N	2.42	0.66
1:B:257:ARG:HG3	1:B:257:ARG:NH1	2.10	0.66
1:C:257:ARG:NH1	1:C:257:ARG:HG3	2.10	0.66
1:D:257:ARG:NH1	1:D:257:ARG:HG3	2.10	0.66
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.10	0.65
1:D:257:ARG:HH11	1:D:257:ARG:HG3	1.62	0.65
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.62	0.65
1:B:110:VAL:O	1:B:114:ILE:HG13	1.97	0.65
1:C:110:VAL:O	1:C:114:ILE:HG13	1.97	0.64
1:C:42:GLN:OE1	1:C:44:ILE:HD11	1.97	0.64
1:D:110:VAL:O	1:D:114:ILE:HG13	1.97	0.64
1:B:42:GLN:OE1	1:B:44:ILE:HD11	1.97	0.64
1:A:110:VAL:O	1:A:114:ILE:HG13	1.97	0.64
1:A:192:GLU:HB2	1:A:321:LEU:HD11	1.80	0.64
1:D:192:GLU:HB2	1:D:321:LEU:HD11	1.80	0.64
1:B:257:ARG:HG3	1:B:257:ARG:HH11	1.62	0.64
1:C:257:ARG:HH11	1:C:257:ARG:HG3	1.62	0.64
1:D:15:MET:HE2	1:D:18:ASN:CA	2.28	0.64
1:A:15:MET:HE2	1:A:18:ASN:CA	2.28	0.64
1:A:49:VAL:HG22	1:A:78:ILE:HD12	1.79	0.64
1:D:49:VAL:HG22	1:D:78:ILE:HD12	1.79	0.63
1:B:49:VAL:HG22	1:B:78:ILE:HD12	1.79	0.63
1:B:142:ILE:HD13	1:B:324:VAL:CG1	2.21	0.63
1:C:49:VAL:HG22	1:C:78:ILE:HD12	1.79	0.63
1:A:42:GLN:OE1	1:A:44:ILE:HD11	1.97	0.63
1:B:265:ASN:ND2	1:B:295:ARG:CB	2.60	0.63
1:D:42:GLN:OE1	1:D:44:ILE:HD11	1.97	0.63
1:C:142:ILE:HD13	1:C:324:VAL:CG1	2.21	0.63
1:C:265:ASN:ND2	1:C:295:ARG:CB	2.60	0.63
1:A:182:PRO:CB	1:C:70:VAL:HG22	2.29	0.63
1:B:35:TYR:O	1:B:38:ALA:HB3	1.98	0.62
1:C:35:TYR:O	1:C:38:ALA:HB3	1.98	0.62
1:D:35:TYR:O	1:D:38:ALA:HB3	1.98	0.62
1:C:18:ASN:ND2	1:C:18:ASN:N	2.24	0.62
1:A:35:TYR:O	1:A:38:ALA:HB3	1.98	0.62
1:B:18:ASN:ND2	1:B:18:ASN:N	2.24	0.62
1:B:192:GLU:HB2	1:B:321:LEU:HD11	1.80	0.62
1:D:324:VAL:O	1:D:328:ALA:HB3	2.00	0.62
1:C:192:GLU:HB2	1:C:321:LEU:HD11	1.80	0.62
1:C:324:VAL:O	1:C:328:ALA:HB3	2.00	0.62
1:B:324:VAL:O	1:B:328:ALA:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ILE:HD13	1:D:324:VAL:CG1	2.21	0.62
1:A:324:VAL:O	1:A:328:ALA:HB3	2.00	0.62
1:B:129:PHE:CZ	1:B:131:GLY:HA3	2.35	0.62
1:C:129:PHE:CZ	1:C:131:GLY:HA3	2.35	0.62
1:B:15:MET:HE2	1:B:18:ASN:CA	2.29	0.62
1:A:142:ILE:HD13	1:A:324:VAL:CG1	2.21	0.61
1:C:15:MET:HE2	1:C:18:ASN:CA	2.29	0.61
1:A:59:ILE:HG22	1:C:243:LYS:HD3	1.82	0.61
1:B:243:LYS:HD3	1:D:59:ILE:HG22	1.82	0.61
1:A:265:ASN:ND2	1:A:295:ARG:CB	2.60	0.61
1:A:129:PHE:CZ	1:A:131:GLY:HA3	2.35	0.61
1:D:129:PHE:CZ	1:D:131:GLY:HA3	2.35	0.61
1:B:28:ALA:HB2	1:B:50:LEU:CD1	2.31	0.61
1:C:28:ALA:HB2	1:C:50:LEU:CD1	2.31	0.61
1:D:265:ASN:ND2	1:D:295:ARG:CB	2.60	0.61
1:A:190:ILE:HD13	1:A:200:VAL:HG21	1.82	0.61
1:A:70:VAL:HG22	1:C:182:PRO:CB	2.29	0.61
1:B:182:PRO:CB	1:D:70:VAL:HG22	2.29	0.61
1:D:190:ILE:HD13	1:D:200:VAL:HG21	1.82	0.61
1:D:73:PRO:O	1:D:74:LYS:HB2	2.01	0.61
1:A:73:PRO:O	1:A:74:LYS:HB2	2.01	0.61
1:C:73:PRO:O	1:C:74:LYS:HB2	2.01	0.61
1:A:178:PHE:CD1	1:A:206:ILE:HD13	2.36	0.61
1:D:178:PHE:CD1	1:D:206:ILE:HD13	2.36	0.61
1:B:73:PRO:O	1:B:74:LYS:HB2	2.01	0.61
1:C:132:LEU:HD12	1:C:262:ILE:HG21	1.82	0.60
1:B:132:LEU:HD12	1:B:262:ILE:HG21	1.82	0.60
1:A:28:ALA:HB2	1:A:50:LEU:CD1	2.31	0.60
1:B:87:ARG:HB2	1:B:87:ARG:HH11	1.66	0.60
1:C:178:PHE:CD1	1:C:206:ILE:HD13	2.36	0.60
1:B:189:ILE:HD11	1:B:233:VAL:HG11	1.84	0.60
1:D:132:LEU:HD12	1:D:262:ILE:HG21	1.82	0.60
1:D:28:ALA:HB2	1:D:50:LEU:CD1	2.31	0.60
1:B:178:PHE:CD1	1:B:206:ILE:HD13	2.36	0.60
1:C:189:ILE:HD11	1:C:233:VAL:HG11	1.84	0.60
1:A:132:LEU:HD12	1:A:262:ILE:HG21	1.82	0.60
1:C:87:ARG:HH11	1:C:87:ARG:HB2	1.66	0.60
1:A:189:ILE:HD11	1:A:233:VAL:HG11	1.84	0.60
1:B:59:ILE:HG22	1:D:243:LYS:HD3	1.82	0.59
1:D:189:ILE:HD11	1:D:233:VAL:HG11	1.84	0.59
1:A:243:LYS:HD3	1:C:59:ILE:HG22	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:CG	1:B:88:ASP:N	2.52	0.59
1:D:324:VAL:HG12	1:D:324:VAL:O	2.02	0.59
1:A:324:VAL:HG12	1:A:324:VAL:O	2.02	0.59
1:A:192:GLU:O	1:A:197:GLU:HB3	2.03	0.59
1:D:192:GLU:O	1:D:197:GLU:HB3	2.03	0.59
1:B:324:VAL:HG12	1:B:324:VAL:O	2.02	0.59
1:C:87:ARG:CG	1:C:88:ASP:N	2.52	0.59
1:C:324:VAL:HG12	1:C:324:VAL:O	2.02	0.59
1:C:190:ILE:HD13	1:C:200:VAL:HG21	1.82	0.59
1:B:272:VAL:O	1:B:288:GLY:HA2	2.03	0.59
1:C:272:VAL:O	1:C:288:GLY:HA2	2.03	0.59
1:A:169:ARG:NH1	2:A:1:SO4:O2	2.35	0.59
1:B:190:ILE:HD13	1:B:200:VAL:HG21	1.82	0.59
1:B:192:GLU:O	1:B:197:GLU:HB3	2.03	0.59
1:C:192:GLU:O	1:C:197:GLU:HB3	2.03	0.59
1:D:324:VAL:CG1	1:D:324:VAL:O	2.51	0.58
1:A:324:VAL:CG1	1:A:324:VAL:O	2.51	0.58
1:B:324:VAL:CG1	1:B:324:VAL:O	2.51	0.58
1:A:179:SER:O	1:D:299:ARG:NH1	2.36	0.58
1:C:324:VAL:O	1:C:324:VAL:CG1	2.51	0.58
1:B:70:VAL:HG22	1:D:182:PRO:CB	2.29	0.58
1:B:55:GLU:HG3	1:B:59:ILE:CD1	2.33	0.58
1:C:55:GLU:HG3	1:C:59:ILE:CD1	2.33	0.58
1:A:272:VAL:O	1:A:288:GLY:HA2	2.03	0.58
1:D:272:VAL:O	1:D:288:GLY:HA2	2.03	0.58
1:D:15:MET:CG	1:D:16:LYS:H	2.17	0.58
1:A:15:MET:CG	1:A:16:LYS:H	2.17	0.58
1:A:83:TYR:C	1:A:85:ASP:N	2.57	0.58
1:C:15:MET:CG	1:C:16:LYS:N	2.67	0.57
1:B:15:MET:CG	1:B:16:LYS:N	2.67	0.57
1:A:15:MET:HG3	1:A:16:LYS:N	2.19	0.57
1:D:55:GLU:HG3	1:D:59:ILE:CD1	2.33	0.57
1:D:83:TYR:C	1:D:85:ASP:N	2.57	0.57
1:D:15:MET:CG	1:D:16:LYS:N	2.67	0.57
1:D:15:MET:HG3	1:D:16:LYS:N	2.19	0.57
1:A:15:MET:CG	1:A:16:LYS:N	2.67	0.57
1:A:55:GLU:HG3	1:A:59:ILE:CD1	2.33	0.57
1:C:83:TYR:C	1:C:85:ASP:N	2.57	0.57
1:B:83:TYR:C	1:B:85:ASP:N	2.57	0.57
1:A:132:LEU:HD12	1:A:262:ILE:CG2	2.34	0.57
1:D:132:LEU:HD12	1:D:262:ILE:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ILE:HG23	1:C:197:GLU:HG3	1.86	0.57
1:D:306:LEU:C	1:D:307:ASN:O	2.40	0.57
1:A:306:LEU:C	1:A:307:ASN:O	2.40	0.57
1:B:189:ILE:HG23	1:B:197:GLU:HG3	1.86	0.57
1:C:15:MET:HG3	1:C:16:LYS:N	2.19	0.57
1:C:15:MET:CG	1:C:16:LYS:H	2.17	0.57
1:B:15:MET:CG	1:B:16:LYS:H	2.17	0.57
1:C:240:ILE:HG13	1:C:247:THR:HG22	1.86	0.57
1:B:240:ILE:HG13	1:B:247:THR:HG22	1.86	0.57
1:B:132:LEU:HD12	1:B:262:ILE:CG2	2.34	0.57
1:C:32:GLY:O	1:C:36:VAL:HG23	2.05	0.57
1:A:87:ARG:HB2	1:A:87:ARG:HH11	1.66	0.57
1:B:15:MET:HG3	1:B:16:LYS:N	2.19	0.57
1:C:132:LEU:HD12	1:C:262:ILE:CG2	2.34	0.57
1:B:32:GLY:O	1:B:36:VAL:HG23	2.05	0.57
1:A:189:ILE:HG23	1:A:197:GLU:HG3	1.86	0.56
1:D:87:ARG:HH11	1:D:87:ARG:HB2	1.66	0.56
1:D:189:ILE:HG23	1:D:197:GLU:HG3	1.86	0.56
1:C:170:PHE:HB2	1:C:189:ILE:HD12	1.88	0.56
1:B:170:PHE:HB2	1:B:189:ILE:HD12	1.88	0.56
1:A:170:PHE:HB2	1:A:189:ILE:HD12	1.88	0.56
1:D:170:PHE:HB2	1:D:189:ILE:HD12	1.88	0.56
1:A:32:GLY:O	1:A:36:VAL:HG23	2.05	0.56
1:B:275:TYR:O	1:B:277:ASP:OD1	2.24	0.56
1:C:275:TYR:O	1:C:277:ASP:OD1	2.24	0.56
1:A:240:ILE:HG13	1:A:247:THR:HG22	1.86	0.56
1:D:240:ILE:HG13	1:D:247:THR:HG22	1.86	0.56
1:D:32:GLY:O	1:D:36:VAL:HG23	2.05	0.56
1:C:331:ARG:C	1:C:331:ARG:HD3	2.26	0.55
1:C:306:LEU:C	1:C:307:ASN:O	2.40	0.55
1:A:275:TYR:O	1:A:277:ASP:OD1	2.24	0.55
1:D:275:TYR:O	1:D:277:ASP:OD1	2.24	0.55
1:B:22:ARG:NH2	1:B:47:GLU:OE1	2.37	0.55
1:B:331:ARG:C	1:B:331:ARG:HD3	2.26	0.55
1:A:64:ASP:OD2	1:C:244:LYS:NZ	2.40	0.55
1:B:179:SER:O	1:C:299:ARG:NH1	2.36	0.55
1:C:279:LEU:HG	1:C:303:GLU:HG3	1.88	0.55
1:B:244:LYS:NZ	1:D:64:ASP:OD2	2.40	0.55
1:B:299:ARG:NH1	1:C:179:SER:O	2.36	0.55
1:B:306:LEU:C	1:B:307:ASN:O	2.40	0.55
1:C:22:ARG:NH2	1:C:47:GLU:OE1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LEU:HG	1:B:303:GLU:HG3	1.88	0.55
1:A:244:LYS:NZ	1:C:64:ASP:OD2	2.40	0.55
1:B:64:ASP:OD2	1:D:244:LYS:NZ	2.40	0.55
1:A:279:LEU:HG	1:A:303:GLU:HG3	1.88	0.55
1:D:331:ARG:HD3	1:D:331:ARG:C	2.26	0.55
1:D:279:LEU:HG	1:D:303:GLU:HG3	1.88	0.55
1:A:28:ALA:HB2	1:A:50:LEU:HD11	1.88	0.55
1:A:331:ARG:C	1:A:331:ARG:HD3	2.26	0.55
1:C:74:LYS:HE2	1:D:266:GLU:HG2	1.89	0.55
1:D:28:ALA:HB2	1:D:50:LEU:HD11	1.88	0.55
1:A:266:GLU:HG2	1:B:74:LYS:HE2	1.89	0.54
1:C:28:ALA:HB2	1:C:50:LEU:HD11	1.88	0.54
1:B:113:ASN:ND2	1:B:116:ILE:HD12	2.22	0.54
1:A:279:LEU:HD23	1:A:301:VAL:HG12	1.89	0.54
1:C:295:ARG:HG3	1:C:295:ARG:NH1	2.15	0.54
1:C:113:ASN:ND2	1:C:116:ILE:HD12	2.22	0.54
1:B:28:ALA:HB2	1:B:50:LEU:HD11	1.88	0.54
1:B:295:ARG:NH1	1:B:295:ARG:HG3	2.15	0.54
1:D:279:LEU:HD23	1:D:301:VAL:HG12	1.89	0.54
1:B:112:LYS:NZ	1:B:112:LYS:CB	2.70	0.54
1:C:206:ILE:HD11	1:C:211:ILE:HD11	1.88	0.54
1:B:206:ILE:HD11	1:B:211:ILE:HD11	1.88	0.54
1:A:113:ASN:ND2	1:A:116:ILE:HD12	2.22	0.54
1:C:112:LYS:NZ	1:C:112:LYS:CB	2.70	0.54
1:D:206:ILE:HD11	1:D:211:ILE:HD11	1.88	0.54
1:D:15:MET:CE	1:D:18:ASN:CA	2.86	0.54
1:A:15:MET:CE	1:A:18:ASN:CA	2.86	0.54
1:A:206:ILE:HD11	1:A:211:ILE:HD11	1.88	0.54
1:D:113:ASN:ND2	1:D:116:ILE:HD12	2.22	0.54
1:A:112:LYS:CB	1:A:112:LYS:NZ	2.70	0.54
1:D:229:ILE:O	1:D:233:VAL:HG23	2.08	0.54
1:D:112:LYS:CB	1:D:112:LYS:NZ	2.70	0.54
1:A:229:ILE:O	1:A:233:VAL:HG23	2.08	0.54
1:C:167:THR:CG2	1:C:189:ILE:H	2.22	0.53
1:A:206:ILE:HD11	1:A:211:ILE:CD1	2.38	0.53
1:C:206:ILE:HD11	1:C:211:ILE:CD1	2.38	0.53
1:B:167:THR:CG2	1:B:189:ILE:H	2.22	0.53
1:D:178:PHE:CD1	1:D:206:ILE:CD1	2.92	0.53
1:D:206:ILE:HD11	1:D:211:ILE:CD1	2.38	0.53
1:C:229:ILE:O	1:C:233:VAL:HG23	2.08	0.53
1:A:178:PHE:CD1	1:A:206:ILE:CD1	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HD11	1:B:211:ILE:CD1	2.38	0.53
1:B:229:ILE:O	1:B:233:VAL:HG23	2.08	0.53
1:C:86:CYS:HA	1:C:89:ALA:HB2	1.90	0.53
1:B:86:CYS:HA	1:B:89:ALA:HB2	1.90	0.53
1:B:253:MET:CE	1:D:72:ALA:HB2	2.39	0.53
1:A:113:ASN:HB3	1:A:143:LEU:HD21	1.91	0.53
1:A:72:ALA:HB2	1:C:253:MET:CE	2.39	0.53
1:D:113:ASN:HB3	1:D:143:LEU:HD21	1.91	0.53
1:A:189:ILE:HD13	1:A:233:VAL:HG11	1.91	0.53
1:B:189:ILE:HD13	1:B:233:VAL:HG11	1.91	0.53
1:D:93:VAL:HG22	1:D:134:LEU:HD23	1.91	0.53
1:A:93:VAL:HG22	1:A:134:LEU:HD23	1.91	0.53
1:D:189:ILE:HD13	1:D:233:VAL:HG11	1.91	0.53
1:C:189:ILE:HD13	1:C:233:VAL:HG11	1.91	0.53
1:A:26:ILE:HD12	1:A:92:VAL:CG1	2.39	0.53
1:C:93:VAL:HG22	1:C:134:LEU:HD23	1.91	0.53
1:C:178:PHE:CD1	1:C:206:ILE:CD1	2.92	0.52
1:B:178:PHE:CD1	1:B:206:ILE:CD1	2.92	0.52
1:C:266:GLU:HG2	1:D:74:LYS:HE2	1.89	0.52
1:A:74:LYS:HE2	1:B:266:GLU:HG2	1.89	0.52
1:B:93:VAL:HG22	1:B:134:LEU:HD23	1.91	0.52
1:D:26:ILE:HD12	1:D:92:VAL:CG1	2.39	0.52
1:C:15:MET:HG2	1:D:296:ASN:OD1	2.10	0.52
1:A:296:ASN:OD1	1:B:15:MET:HG2	2.10	0.52
1:C:15:MET:CE	1:C:18:ASN:CA	2.86	0.52
1:A:295:ARG:NH1	1:A:295:ARG:HG3	2.15	0.52
1:C:279:LEU:HD23	1:C:301:VAL:HG12	1.89	0.52
1:D:295:ARG:NH1	1:D:295:ARG:HG3	2.15	0.52
1:B:15:MET:CE	1:B:18:ASN:CA	2.86	0.52
1:A:253:MET:CE	1:C:72:ALA:HB2	2.39	0.52
1:A:299:ARG:NH1	1:D:179:SER:O	2.36	0.52
1:B:279:LEU:HD23	1:B:301:VAL:HG12	1.89	0.52
1:C:283:ARG:H	1:C:322:LYS:HZ2	1.56	0.52
1:B:249:TYR:O	1:B:250:GLY:C	2.47	0.52
1:C:249:TYR:O	1:C:250:GLY:C	2.47	0.52
1:B:72:ALA:HB2	1:D:253:MET:CE	2.39	0.52
1:B:26:ILE:HD12	1:B:92:VAL:CG1	2.39	0.52
1:C:26:ILE:HD12	1:C:92:VAL:CG1	2.39	0.52
1:A:26:ILE:HG21	1:A:120:ILE:HD13	1.92	0.52
1:D:26:ILE:HG21	1:D:120:ILE:HD13	1.92	0.52
1:B:26:ILE:HG21	1:B:120:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ILE:HG21	1:C:120:ILE:HD13	1.92	0.52
1:A:200:VAL:HG11	1:A:304:ILE:HD11	1.92	0.52
1:B:113:ASN:HB3	1:B:143:LEU:HD21	1.91	0.51
1:C:113:ASN:HB3	1:C:143:LEU:HD21	1.91	0.51
1:C:307:ASN:C	1:C:309:ASP:H	2.12	0.51
1:D:200:VAL:HG11	1:D:304:ILE:HD11	1.92	0.51
1:B:28:ALA:CB	1:B:50:LEU:HD11	2.41	0.51
1:C:28:ALA:CB	1:C:50:LEU:HD11	2.41	0.51
1:D:249:TYR:O	1:D:250:GLY:C	2.47	0.51
1:C:296:ASN:OD1	1:D:15:MET:HG2	2.10	0.51
1:A:15:MET:HG2	1:B:296:ASN:OD1	2.10	0.51
1:B:307:ASN:C	1:B:309:ASP:H	2.12	0.51
1:D:307:ASN:C	1:D:309:ASP:H	2.12	0.51
1:A:307:ASN:C	1:A:309:ASP:H	2.12	0.51
1:B:283:ARG:H	1:B:322:LYS:HZ2	1.57	0.51
1:C:267:ASN:ND2	1:C:299:ARG:CZ	2.74	0.51
1:B:267:ASN:ND2	1:B:299:ARG:CZ	2.74	0.51
1:A:86:CYS:HA	1:A:89:ALA:HB2	1.90	0.51
1:A:26:ILE:HD12	1:A:92:VAL:HG13	1.93	0.51
1:D:26:ILE:HD12	1:D:92:VAL:HG13	1.93	0.51
1:D:15:MET:CE	1:D:18:ASN:N	2.74	0.51
1:A:15:MET:CE	1:A:18:ASN:N	2.74	0.51
1:D:167:THR:CG2	1:D:189:ILE:H	2.22	0.51
1:C:15:MET:CE	1:C:18:ASN:N	2.74	0.50
1:D:86:CYS:HA	1:D:89:ALA:HB2	1.90	0.50
1:A:22:ARG:NH2	1:A:47:GLU:OE1	2.37	0.50
1:B:15:MET:CE	1:B:18:ASN:N	2.74	0.50
1:A:167:THR:CG2	1:A:189:ILE:H	2.22	0.50
1:D:22:ARG:NH2	1:D:47:GLU:OE1	2.37	0.50
1:C:267:ASN:ND2	1:C:294:ASN:OD1	2.45	0.50
1:B:267:ASN:ND2	1:B:294:ASN:OD1	2.45	0.50
1:D:267:ASN:ND2	1:D:299:ARG:CZ	2.74	0.50
1:A:267:ASN:ND2	1:A:299:ARG:CZ	2.74	0.50
1:A:270:LEU:CD1	1:A:293:ILE:HD12	2.40	0.50
1:A:267:ASN:ND2	1:A:294:ASN:OD1	2.45	0.50
1:D:267:ASN:ND2	1:D:294:ASN:OD1	2.45	0.50
1:C:125:MET:O	1:C:128:GLY:N	2.45	0.50
1:B:125:MET:O	1:B:128:GLY:N	2.45	0.50
1:A:249:TYR:O	1:A:250:GLY:C	2.47	0.50
1:B:200:VAL:HG11	1:B:304:ILE:HD11	1.92	0.50
1:D:270:LEU:CD1	1:D:293:ILE:HD12	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:VAL:HG11	1:C:304:ILE:HD11	1.92	0.49
1:D:28:ALA:CB	1:D:50:LEU:HD11	2.41	0.49
1:A:28:ALA:CB	1:A:50:LEU:HD11	2.41	0.49
1:A:280:TYR:HB2	1:A:314:PHE:CE2	2.47	0.49
1:A:125:MET:O	1:A:128:GLY:N	2.45	0.49
1:D:125:MET:O	1:D:128:GLY:N	2.45	0.49
1:D:280:TYR:HB2	1:D:314:PHE:CE2	2.47	0.49
1:B:26:ILE:HD12	1:B:92:VAL:HG13	1.93	0.49
1:C:26:ILE:HD12	1:C:92:VAL:HG13	1.93	0.49
1:C:280:TYR:HB2	1:C:314:PHE:CE2	2.47	0.49
1:B:280:TYR:HB2	1:B:314:PHE:CE2	2.47	0.49
1:A:170:PHE:HB2	1:A:189:ILE:CD1	2.43	0.48
1:D:170:PHE:HB2	1:D:189:ILE:CD1	2.43	0.48
1:A:279:LEU:CD2	1:A:301:VAL:HB	2.43	0.48
1:D:279:LEU:CD2	1:D:301:VAL:HB	2.43	0.48
1:C:112:LYS:O	1:C:116:ILE:HG13	2.14	0.48
1:B:170:PHE:HB2	1:B:189:ILE:CD1	2.43	0.48
1:C:170:PHE:HB2	1:C:189:ILE:CD1	2.43	0.48
1:B:26:ILE:CG2	1:B:120:ILE:HD13	2.44	0.48
1:C:26:ILE:CG2	1:C:120:ILE:HD13	2.44	0.48
1:B:112:LYS:O	1:B:116:ILE:HG13	2.14	0.48
1:A:26:ILE:CG2	1:A:120:ILE:HD13	2.44	0.48
1:D:26:ILE:CG2	1:D:120:ILE:HD13	2.44	0.48
1:C:279:LEU:CD2	1:C:301:VAL:HB	2.43	0.48
1:B:279:LEU:CD2	1:B:301:VAL:HB	2.43	0.48
1:C:324:VAL:O	1:C:328:ALA:CB	2.62	0.48
1:B:324:VAL:O	1:B:328:ALA:CB	2.62	0.48
1:D:283:ARG:H	1:D:322:LYS:HZ2	1.59	0.48
1:D:112:LYS:O	1:D:116:ILE:HG13	2.14	0.47
1:B:328:ALA:O	1:B:329:PHE:CB	2.59	0.47
1:A:112:LYS:O	1:A:116:ILE:HG13	2.14	0.47
1:A:206:ILE:CD1	1:A:211:ILE:HD11	2.44	0.47
1:D:206:ILE:CD1	1:D:211:ILE:HD11	2.44	0.47
1:D:232:ASN:HD22	1:D:232:ASN:HA	1.41	0.47
1:B:206:ILE:CD1	1:B:211:ILE:HD11	2.44	0.47
1:C:206:ILE:CD1	1:C:211:ILE:HD11	2.44	0.47
1:C:328:ALA:O	1:C:329:PHE:CB	2.59	0.47
1:B:59:ILE:HG13	1:B:79:TRP:CD1	2.50	0.47
1:C:59:ILE:HG13	1:C:79:TRP:CD1	2.50	0.47
1:D:96:ALA:O	1:D:137:THR:HG21	2.15	0.47
1:A:96:ALA:O	1:A:137:THR:HG21	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:CD1	1:B:293:ILE:HD12	2.40	0.47
1:A:283:ARG:H	1:A:322:LYS:HZ2	1.60	0.47
1:B:160:GLY:HA3	1:B:273:SER:HB2	1.97	0.47
1:C:160:GLY:HA3	1:C:273:SER:HB2	1.97	0.47
1:D:24:VAL:HA	1:D:49:VAL:O	2.15	0.47
1:A:24:VAL:HA	1:A:49:VAL:O	2.15	0.47
1:D:160:GLY:HA3	1:D:273:SER:HB2	1.97	0.47
1:D:59:ILE:HG13	1:D:79:TRP:CD1	2.50	0.47
1:A:293:ILE:O	1:A:294:ASN:HB3	2.15	0.47
1:A:160:GLY:HA3	1:A:273:SER:HB2	1.97	0.47
1:A:59:ILE:HG13	1:A:79:TRP:CD1	2.50	0.46
1:B:59:ILE:CG2	1:D:243:LYS:HD3	2.45	0.46
1:A:243:LYS:HD3	1:C:59:ILE:CG2	2.45	0.46
1:D:293:ILE:O	1:D:294:ASN:HB3	2.15	0.46
1:C:270:LEU:CD1	1:C:293:ILE:HD12	2.40	0.46
1:C:42:GLN:OE1	1:C:44:ILE:CD1	2.63	0.46
1:A:240:ILE:CD1	1:A:247:THR:HG22	2.46	0.46
1:B:24:VAL:HA	1:B:49:VAL:O	2.15	0.46
1:D:240:ILE:CD1	1:D:247:THR:HG22	2.46	0.46
1:C:24:VAL:HA	1:C:49:VAL:O	2.15	0.46
1:A:42:GLN:OE1	1:A:44:ILE:CD1	2.63	0.46
1:D:42:GLN:OE1	1:D:44:ILE:CD1	2.63	0.46
1:D:22:ARG:O	1:D:90:ASP:HB2	2.15	0.46
1:D:228:ARG:HA	1:D:228:ARG:HD2	1.56	0.46
1:D:149:LYS:HA	1:D:149:LYS:HD3	1.73	0.46
1:A:324:VAL:O	1:A:328:ALA:CB	2.62	0.46
1:B:129:PHE:CZ	1:B:131:GLY:CA	2.99	0.46
1:A:22:ARG:O	1:A:90:ASP:HB2	2.15	0.46
1:D:138:ASN:HA	1:D:140:VAL:N	2.31	0.46
1:A:228:ARG:HA	1:A:228:ARG:HD2	1.56	0.46
1:D:324:VAL:O	1:D:328:ALA:CB	2.62	0.46
1:C:129:PHE:CZ	1:C:131:GLY:CA	2.99	0.46
1:B:22:ARG:O	1:B:90:ASP:HB2	2.15	0.46
1:A:138:ASN:HA	1:A:140:VAL:N	2.31	0.46
1:C:22:ARG:O	1:C:90:ASP:HB2	2.15	0.46
1:C:327:ARG:HH11	1:C:327:ARG:HD3	1.59	0.46
1:B:260:ARG:HH11	1:B:260:ARG:HD3	1.04	0.46
1:A:129:PHE:CZ	1:A:131:GLY:CA	2.99	0.46
1:D:129:PHE:CZ	1:D:131:GLY:CA	2.99	0.46
1:C:167:THR:HG22	1:C:189:ILE:HB	1.98	0.46
1:A:149:LYS:HA	1:A:149:LYS:HD3	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ASN:HA	1:B:140:VAL:N	2.31	0.46
1:C:96:ALA:O	1:C:137:THR:HG21	2.15	0.46
1:C:138:ASN:HA	1:C:140:VAL:N	2.31	0.46
1:B:167:THR:HG22	1:B:189:ILE:HB	1.98	0.46
1:B:96:ALA:O	1:B:137:THR:HG21	2.15	0.46
1:A:327:ARG:HD3	1:A:327:ARG:HH11	1.59	0.45
1:A:15:MET:HE3	1:A:18:ASN:ND2	2.31	0.45
1:A:59:ILE:CG2	1:C:243:LYS:HD3	2.45	0.45
1:B:234:ARG:O	1:B:234:ARG:HG2	2.17	0.45
1:C:234:ARG:HG2	1:C:234:ARG:O	2.17	0.45
1:B:243:LYS:HD3	1:D:59:ILE:CG2	2.45	0.45
1:C:240:ILE:CD1	1:C:247:THR:HG22	2.46	0.45
1:B:293:ILE:O	1:B:294:ASN:HB3	2.15	0.45
1:C:260:ARG:HH11	1:C:260:ARG:HD3	1.04	0.45
1:B:240:ILE:CD1	1:B:247:THR:HG22	2.46	0.45
1:C:293:ILE:O	1:C:294:ASN:HB3	2.15	0.45
1:D:321:LEU:C	1:D:323:SER:H	2.19	0.45
1:D:302:ILE:HD13	1:D:302:ILE:HG21	1.60	0.45
1:C:164:ILE:HD13	1:C:164:ILE:HG21	1.53	0.45
1:C:118:ARG:CZ	1:C:122:GLU:OE2	2.64	0.45
1:B:48:ILE:HD13	1:B:48:ILE:HG21	1.75	0.45
1:D:327:ARG:HD3	1:D:327:ARG:HH11	1.59	0.45
1:A:321:LEU:C	1:A:323:SER:H	2.19	0.45
1:B:118:ARG:CZ	1:B:122:GLU:OE2	2.64	0.45
1:D:118:ARG:CZ	1:D:122:GLU:OE2	2.64	0.45
1:C:48:ILE:HD13	1:C:48:ILE:HG21	1.75	0.45
1:A:118:ARG:CZ	1:A:122:GLU:OE2	2.64	0.45
1:A:302:ILE:HD13	1:A:302:ILE:HG21	1.60	0.45
1:A:181:ALA:HA	1:A:182:PRO:HD3	1.82	0.44
1:D:167:THR:HG22	1:D:189:ILE:HB	1.98	0.44
1:A:167:THR:HG22	1:A:189:ILE:HB	1.98	0.44
1:D:181:ALA:HA	1:D:182:PRO:HD3	1.82	0.44
1:B:258:VAL:HG13	1:B:293:ILE:HD13	1.99	0.44
1:B:42:GLN:OE1	1:B:44:ILE:CD1	2.63	0.44
1:B:149:LYS:HD3	1:B:149:LYS:HA	1.73	0.44
1:B:164:ILE:HD13	1:B:164:ILE:HG21	1.53	0.44
1:A:161:SER:OG	1:A:251:ILE:HD11	2.18	0.44
1:C:258:VAL:HG13	1:C:293:ILE:HD13	1.99	0.44
1:D:161:SER:OG	1:D:251:ILE:HD11	2.18	0.44
1:D:234:ARG:HG2	1:D:234:ARG:O	2.17	0.44
1:D:15:MET:HE3	1:D:18:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ILE:HD13	1:D:304:ILE:HG21	1.74	0.44
1:D:55:GLU:C	1:D:59:ILE:HD12	2.38	0.44
1:B:321:LEU:C	1:B:323:SER:H	2.19	0.44
1:C:321:LEU:C	1:C:323:SER:H	2.19	0.44
2:A:2:SO4:O2	1:D:186:HIS:NE2	2.43	0.44
1:A:55:GLU:C	1:A:59:ILE:HD12	2.38	0.44
1:A:232:ASN:HD22	1:A:232:ASN:HA	1.41	0.44
1:A:234:ARG:HG2	1:A:234:ARG:O	2.17	0.44
1:C:149:LYS:HA	1:C:149:LYS:HD3	1.73	0.44
1:B:190:ILE:HD13	1:B:200:VAL:CG2	2.48	0.44
1:C:240:ILE:HD11	1:C:247:THR:HG22	2.00	0.44
1:B:240:ILE:HD11	1:B:247:THR:HG22	2.00	0.44
1:B:279:LEU:HD23	1:B:301:VAL:HG11	1.99	0.43
1:C:279:LEU:HD23	1:C:301:VAL:HG11	1.99	0.43
1:D:190:ILE:HD13	1:D:200:VAL:CG2	2.48	0.43
1:D:244:LYS:HE2	1:D:248:TYR:CZ	2.53	0.43
1:A:190:ILE:HD13	1:A:200:VAL:CG2	2.48	0.43
1:A:304:ILE:HG21	1:A:304:ILE:HD13	1.74	0.43
1:A:244:LYS:HE2	1:A:248:TYR:CZ	2.53	0.43
1:D:258:VAL:HG13	1:D:293:ILE:HD13	1.99	0.43
1:B:138:ASN:HA	1:B:140:VAL:H	1.84	0.43
1:C:138:ASN:HA	1:C:140:VAL:H	1.84	0.43
1:B:136:ALA:HB2	1:B:255:LEU:HD21	2.00	0.43
1:A:258:VAL:HG13	1:A:293:ILE:HD13	1.99	0.43
1:D:240:ILE:HD11	1:D:247:THR:HG22	2.00	0.43
1:B:229:ILE:HG22	1:B:229:ILE:O	2.18	0.43
1:C:279:LEU:C	1:C:281:GLY:H	2.22	0.43
1:A:240:ILE:HD11	1:A:247:THR:HG22	2.00	0.43
1:B:279:LEU:C	1:B:281:GLY:H	2.22	0.43
1:A:322:LYS:HA	1:A:325:LEU:HD12	2.00	0.43
1:B:161:SER:OG	1:B:251:ILE:HD11	2.18	0.43
1:C:136:ALA:HB2	1:C:255:LEU:HD21	2.00	0.43
1:C:229:ILE:O	1:C:229:ILE:HG22	2.18	0.43
1:D:322:LYS:HA	1:D:325:LEU:HD12	2.00	0.43
1:C:322:LYS:HA	1:C:325:LEU:HD12	2.00	0.43
1:A:138:ASN:HA	1:A:140:VAL:H	1.84	0.43
1:C:161:SER:OG	1:C:251:ILE:HD11	2.18	0.43
1:A:260:ARG:HH11	1:A:260:ARG:HD3	1.04	0.43
1:B:322:LYS:HA	1:B:325:LEU:HD12	2.00	0.43
1:D:138:ASN:HA	1:D:140:VAL:H	1.84	0.43
1:D:270:LEU:HD23	1:D:270:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ILE:HD13	1:C:304:ILE:HG21	1.74	0.42
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.78	0.42
1:A:269:ILE:HD12	1:D:184:ASN:HB3	2.01	0.42
1:C:244:LYS:HE2	1:C:248:TYR:CZ	2.53	0.42
1:A:184:ASN:HB3	1:D:269:ILE:HD12	2.01	0.42
1:D:260:ARG:HH11	1:D:260:ARG:HD3	1.04	0.42
1:B:244:LYS:HE2	1:B:248:TYR:CZ	2.53	0.42
1:B:55:GLU:C	1:B:59:ILE:HD12	2.38	0.42
1:C:55:GLU:C	1:C:59:ILE:HD12	2.38	0.42
1:A:136:ALA:HB2	1:A:255:LEU:HD21	2.00	0.42
1:D:136:ALA:HB2	1:D:255:LEU:HD21	2.00	0.42
1:C:270:LEU:HA	1:C:270:LEU:HD23	1.78	0.42
1:B:270:LEU:HA	1:B:270:LEU:HD23	1.78	0.42
1:C:321:LEU:C	1:C:323:SER:N	2.73	0.42
1:A:161:SER:CB	3:A:332:HOH:O	2.66	0.42
1:A:75:PRO:O	1:A:75:PRO:CD	2.67	0.42
1:B:321:LEU:C	1:B:323:SER:N	2.73	0.42
1:D:75:PRO:CD	1:D:75:PRO:O	2.67	0.42
1:D:311:LYS:CA	1:D:315:HIS:CB	2.90	0.42
1:C:311:LYS:CA	1:C:315:HIS:CB	2.90	0.42
1:B:304:ILE:HD13	1:B:304:ILE:HG21	1.74	0.42
1:D:167:THR:HG22	1:D:189:ILE:N	2.30	0.42
1:B:184:ASN:HB3	1:C:269:ILE:HD12	2.01	0.42
1:B:269:ILE:HD12	1:C:184:ASN:HB3	2.01	0.42
1:A:304:ILE:HA	1:D:209:MET:SD	2.60	0.42
1:A:209:MET:SD	1:D:304:ILE:HA	2.60	0.42
1:B:167:THR:O	1:B:171:ARG:HG3	2.20	0.42
1:C:167:THR:O	1:C:171:ARG:HG3	2.20	0.42
1:A:311:LYS:CA	1:A:315:HIS:CB	2.90	0.42
1:A:229:ILE:O	1:A:229:ILE:HG22	2.18	0.42
1:A:279:LEU:C	1:A:281:GLY:H	2.22	0.42
1:D:279:LEU:C	1:D:281:GLY:H	2.22	0.42
1:A:280:TYR:CE2	1:A:289:VAL:CG2	3.04	0.41
1:C:165:LEU:O	1:C:169:ARG:HG3	2.20	0.41
1:B:311:LYS:CA	1:B:315:HIS:CB	2.90	0.41
1:A:167:THR:HG22	1:A:189:ILE:N	2.30	0.41
1:D:229:ILE:HG22	1:D:229:ILE:O	2.18	0.41
1:A:279:LEU:HD23	1:A:301:VAL:HG11	1.99	0.41
1:D:280:TYR:CE2	1:D:289:VAL:CG2	3.04	0.41
1:B:165:LEU:O	1:B:169:ARG:HG3	2.20	0.41
1:B:209:MET:SD	1:C:304:ILE:HA	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LYS:HZ3	1:B:112:LYS:HB3	1.85	0.41
1:C:112:LYS:HB3	1:C:112:LYS:HZ3	1.85	0.41
1:D:279:LEU:HD23	1:D:301:VAL:HG11	1.99	0.41
1:A:165:LEU:O	1:A:169:ARG:HG3	2.20	0.41
1:B:136:ALA:HA	1:B:161:SER:HB2	2.03	0.41
1:C:136:ALA:HA	1:C:161:SER:HB2	2.03	0.41
1:C:75:PRO:O	1:C:75:PRO:CD	2.67	0.41
1:B:304:ILE:HA	1:C:209:MET:SD	2.60	0.41
1:D:132:LEU:CD1	1:D:262:ILE:CG2	2.98	0.41
1:A:132:LEU:CD1	1:A:262:ILE:CG2	2.98	0.41
1:D:165:LEU:O	1:D:169:ARG:HG3	2.20	0.41
1:B:75:PRO:O	1:B:75:PRO:CD	2.67	0.41
1:B:232:ASN:HA	1:B:232:ASN:HD22	1.41	0.41
1:A:167:THR:O	1:A:171:ARG:HG3	2.20	0.41
1:B:71:PHE:CE1	1:D:168:ALA:HB2	2.56	0.41
1:A:168:ALA:HB2	1:C:71:PHE:CE1	2.56	0.41
1:D:112:LYS:HZ3	1:D:112:LYS:HB3	1.85	0.41
1:D:167:THR:O	1:D:171:ARG:HG3	2.20	0.41
1:B:206:ILE:CD1	1:B:211:ILE:CD1	2.98	0.41
1:A:71:PHE:CE1	1:C:168:ALA:HB2	2.56	0.41
1:B:132:LEU:CD1	1:B:262:ILE:CG2	2.98	0.41
1:B:168:ALA:HB2	1:D:71:PHE:CE1	2.56	0.41
1:C:190:ILE:HD13	1:C:200:VAL:CG2	2.48	0.41
1:D:206:ILE:CD1	1:D:211:ILE:CD1	2.98	0.41
1:C:206:ILE:CD1	1:C:211:ILE:CD1	2.98	0.41
1:C:132:LEU:CD1	1:C:262:ILE:CG2	2.98	0.41
1:D:112:LYS:HB3	1:D:112:LYS:NZ	2.36	0.41
1:A:206:ILE:CD1	1:A:211:ILE:CD1	2.98	0.41
1:A:136:ALA:HA	1:A:161:SER:HB2	2.03	0.41
1:D:136:ALA:HA	1:D:161:SER:HB2	2.03	0.41
1:C:232:ASN:HD22	1:C:232:ASN:HA	1.41	0.41
1:A:112:LYS:HB3	1:A:112:LYS:NZ	2.36	0.40
1:A:243:LYS:HE3	1:A:243:LYS:HB3	1.88	0.40
1:D:199:PRO:HG2	1:D:199:PRO:O	2.21	0.40
1:A:199:PRO:O	1:A:199:PRO:HG2	2.21	0.40
1:C:199:PRO:HG2	1:C:199:PRO:O	2.21	0.40
1:D:209:MET:C	1:D:210:PRO:O	2.60	0.40
1:C:280:TYR:CE2	1:C:289:VAL:CG2	3.04	0.40
1:B:199:PRO:HG2	1:B:199:PRO:O	2.21	0.40
1:A:209:MET:C	1:A:210:PRO:O	2.60	0.40
1:D:243:LYS:HB3	1:D:243:LYS:HE3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:TYR:CE2	1:B:289:VAL:CG2	3.04	0.40
1:C:27:GLY:O	1:C:32:GLY:HA3	2.21	0.40
1:B:27:GLY:O	1:B:32:GLY:HA3	2.21	0.40
1:A:208:VAL:HB	1:D:203:GLN:O	2.22	0.40
1:D:313:ARG:HH11	1:D:313:ARG:HG2	1.87	0.40

All (57) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:N	1:D:331:ARG:CB[6_665]	0.71	1.49
1:A:326:ALA:C	1:D:331:ARG:C[6_665]	0.78	1.42
1:A:325:LEU:C	1:D:331:ARG:CB[6_665]	0.88	1.32
1:C:316:HIS:CE1	1:D:316:HIS:CE1[6_655]	1.07	1.13
1:C:316:HIS:NE2	1:D:316:HIS:CE1[6_655]	1.09	1.11
1:A:326:ALA:N	1:D:331:ARG:CA[6_665]	1.12	1.08
1:A:326:ALA:CA	1:D:331:ARG:C[6_665]	1.23	0.97
1:A:323:SER:C	1:D:330:THR:CB[6_665]	1.24	0.96
1:C:316:HIS:NE2	1:D:316:HIS:NE2[6_655]	1.24	0.96
1:A:325:LEU:O	1:D:331:ARG:CG[6_665]	1.29	0.91
1:A:327:ARG:CB	1:D:330:THR:O[6_665]	1.32	0.88
1:C:235:ASP:OD2	1:D:235:ASP:OD2[6_655]	1.34	0.86
1:A:327:ARG:N	1:D:331:ARG:C[6_665]	1.42	0.78
1:A:323:SER:O	1:D:330:THR:CA[6_665]	1.42	0.78
1:A:323:SER:O	1:D:330:THR:CB[6_665]	1.42	0.78
1:C:316:HIS:CE1	1:D:316:HIS:NE2[6_655]	1.48	0.72
1:A:326:ALA:CA	1:D:331:ARG:CA[6_665]	1.54	0.66
1:A:325:LEU:O	1:D:331:ARG:CB[6_665]	1.55	0.65
1:A:326:ALA:C	1:D:331:ARG:CA[6_665]	1.57	0.63
1:A:327:ARG:CA	1:D:330:THR:O[6_665]	1.59	0.61
1:A:327:ARG:N	1:D:331:ARG:CA[6_665]	1.59	0.61
1:A:326:ALA:CA	1:D:331:ARG:CB[6_665]	1.60	0.60
1:A:323:SER:O	1:D:330:THR:C[6_665]	1.60	0.60
1:A:324:VAL:N	1:D:330:THR:CB[6_665]	1.67	0.53
1:A:323:SER:O	1:D:330:THR:OG1[6_665]	1.68	0.52
1:A:326:ALA:CB	1:D:331:ARG:O[6_665]	1.70	0.50
1:A:323:SER:O	1:D:331:ARG:N[6_665]	1.70	0.50
1:A:323:SER:CB	1:D:330:THR:OG1[6_665]	1.72	0.48
1:A:326:ALA:CA	1:D:331:ARG:CG[6_665]	1.85	0.35
1:C:316:HIS:CD2	1:D:316:HIS:NE2[6_655]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:C	1:D:330:THR:OG1[6_665]	1.89	0.31
1:A:326:ALA:N	1:D:331:ARG:N[6_665]	1.89	0.31
1:A:326:ALA:CA	1:D:331:ARG:CD[6_665]	1.90	0.30
1:A:325:LEU:C	1:D:331:ARG:CG[6_665]	1.91	0.29
1:A:323:SER:OG	1:D:330:THR:CG2[6_665]	1.93	0.27
1:A:323:SER:CA	1:D:330:THR:OG1[6_665]	1.93	0.27
1:A:327:ARG:N	1:D:331:ARG:N[6_665]	1.95	0.25
1:A:326:ALA:O	1:D:331:ARG:C[6_665]	1.95	0.25
1:C:316:HIS:NE2	1:D:316:HIS:ND1[6_655]	1.97	0.23
1:A:326:ALA:CA	1:D:331:ARG:O[6_665]	1.97	0.23
1:A:326:ALA:CB	1:D:331:ARG:C[6_665]	2.00	0.20
1:A:327:ARG:CB	1:D:330:THR:C[6_665]	2.01	0.19
1:A:327:ARG:N	1:D:330:THR:O[6_665]	2.02	0.18
1:A:326:ALA:C	1:D:331:ARG:O[6_665]	2.02	0.18
1:C:327:ARG:NH1	1:D:312:ASN:CG[6_655]	2.05	0.15
1:A:327:ARG:N	1:D:330:THR:C[6_665]	2.07	0.13
1:C:316:HIS:ND1	1:D:316:HIS:NE2[6_655]	2.11	0.09
1:A:325:LEU:C	1:D:331:ARG:CA[6_665]	2.11	0.09
1:A:327:ARG:C	1:D:330:THR:O[6_665]	2.12	0.08
1:A:327:ARG:N	1:D:331:ARG:O[6_665]	2.13	0.07
1:C:316:HIS:NE2	1:D:316:HIS:CD2[6_655]	2.14	0.06
1:A:327:ARG:CB	1:D:329:PHE:O[6_665]	2.14	0.06
1:A:323:SER:CA	1:D:330:THR:CB[6_665]	2.14	0.06
1:A:326:ALA:N	1:D:331:ARG:CG[6_665]	2.16	0.04
1:C:228:ARG:NE	1:D:242:GLU:OE2[6_655]	2.17	0.03
1:A:326:ALA:CB	1:D:331:ARG:CD[6_665]	2.18	0.02
1:A:323:SER:C	1:D:330:THR:CA[6_665]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	286/317 (90%)	233 (82%)	37 (13%)	16 (6%)	<b>2</b> <b>6</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	286/317 (90%)	233 (82%)	37 (13%)	16 (6%)	2	6
1	C	286/317 (90%)	233 (82%)	37 (13%)	16 (6%)	2	6
1	D	286/317 (90%)	233 (82%)	37 (13%)	16 (6%)	2	6
All	All	1144/1268 (90%)	932 (82%)	148 (13%)	64 (6%)	2	6

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	98	ALA
1	A	307	ASN
1	A	311	LYS
1	A	329	PHE
1	B	18	ASN
1	B	98	ALA
1	B	307	ASN
1	B	311	LYS
1	B	329	PHE
1	C	18	ASN
1	C	98	ALA
1	C	307	ASN
1	C	311	LYS
1	C	329	PHE
1	D	18	ASN
1	D	98	ALA
1	D	307	ASN
1	D	311	LYS
1	D	329	PHE
1	A	75	PRO
1	A	330	THR
1	B	75	PRO
1	B	330	THR
1	C	75	PRO
1	C	330	THR
1	D	75	PRO
1	D	330	THR
1	A	284	ASP
1	B	284	ASP
1	C	284	ASP
1	D	284	ASP
1	A	250	GLY

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Mol	Chain	Res	Type
1	B	250	GLY
1	C	250	GLY
1	D	250	GLY
1	A	248	TYR
1	B	248	TYR
1	C	248	TYR
1	D	248	TYR
1	A	210	PRO
1	A	267	ASN
1	B	210	PRO
1	B	267	ASN
1	C	210	PRO
1	C	267	ASN
1	D	210	PRO
1	D	267	ASN
1	A	74	LYS
1	B	74	LYS
1	C	74	LYS
1	D	74	LYS
1	A	73	PRO
1	B	73	PRO
1	C	73	PRO
1	D	73	PRO
1	A	180	VAL
1	B	180	VAL
1	C	180	VAL
1	D	180	VAL
1	A	139	PRO
1	B	139	PRO
1	C	139	PRO
1	D	139	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/255 (92%)	207 (88%)	29 (12%)	6	18
1	B	236/255 (92%)	207 (88%)	29 (12%)	6	18
1	C	236/255 (92%)	207 (88%)	29 (12%)	6	18
1	D	236/255 (92%)	207 (88%)	29 (12%)	6	18
All	All	944/1020 (92%)	828 (88%)	116 (12%)	6	18

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	18	ASN
1	A	74	LYS
1	A	77	ASP
1	A	87	ARG
1	A	90	ASP
1	A	99	ASN
1	A	112	LYS
1	A	113	ASN
1	A	119	SER
1	A	134	LEU
1	A	179	SER
1	A	183	GLN
1	A	192	GLU
1	A	197	GLU
1	A	198	LEU
1	A	203	GLN
1	A	227	GLU
1	A	228	ARG
1	A	243	LYS
1	A	257	ARG
1	A	265	ASN
1	A	266	GLU
1	A	277	ASP
1	A	283	ARG
1	A	289	VAL
1	A	294	ASN
1	A	295	ARG
1	A	331	ARG
1	B	15	MET

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Mol	Chain	Res	Type
1	B	18	ASN
1	B	74	LYS
1	B	77	ASP
1	B	87	ARG
1	B	90	ASP
1	B	99	ASN
1	B	112	LYS
1	B	113	ASN
1	B	119	SER
1	B	134	LEU
1	B	179	SER
1	B	183	GLN
1	B	192	GLU
1	B	197	GLU
1	B	198	LEU
1	B	203	GLN
1	B	227	GLU
1	B	228	ARG
1	B	243	LYS
1	B	257	ARG
1	B	265	ASN
1	B	266	GLU
1	B	277	ASP
1	B	283	ARG
1	B	289	VAL
1	B	294	ASN
1	B	295	ARG
1	B	331	ARG
1	C	15	MET
1	C	18	ASN
1	C	74	LYS
1	C	77	ASP
1	C	87	ARG
1	C	90	ASP
1	C	99	ASN
1	C	112	LYS
1	C	113	ASN
1	C	119	SER
1	C	134	LEU
1	C	179	SER
1	C	183	GLN
1	C	192	GLU

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Mol	Chain	Res	Type
1	C	197	GLU
1	C	198	LEU
1	C	203	GLN
1	C	227	GLU
1	C	228	ARG
1	C	243	LYS
1	C	257	ARG
1	C	265	ASN
1	C	266	GLU
1	C	277	ASP
1	C	283	ARG
1	C	289	VAL
1	C	294	ASN
1	C	295	ARG
1	C	331	ARG
1	D	15	MET
1	D	18	ASN
1	D	74	LYS
1	D	77	ASP
1	D	87	ARG
1	D	90	ASP
1	D	99	ASN
1	D	112	LYS
1	D	113	ASN
1	D	119	SER
1	D	134	LEU
1	D	179	SER
1	D	183	GLN
1	D	192	GLU
1	D	197	GLU
1	D	198	LEU
1	D	203	GLN
1	D	227	GLU
1	D	228	ARG
1	D	243	LYS
1	D	257	ARG
1	D	265	ASN
1	D	266	GLU
1	D	277	ASP
1	D	283	ARG
1	D	289	VAL
1	D	294	ASN

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Mol	Chain	Res	Type
1	D	295	ARG
1	D	331	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	99	ASN
1	A	113	ASN
1	A	138	ASN
1	A	232	ASN
1	A	239	GLN
1	A	265	ASN
1	A	267	ASN
1	A	294	ASN
1	A	307	ASN
1	B	18	ASN
1	B	99	ASN
1	B	113	ASN
1	B	138	ASN
1	B	193	HIS
1	B	232	ASN
1	B	239	GLN
1	B	265	ASN
1	B	267	ASN
1	B	294	ASN
1	B	307	ASN
1	C	18	ASN
1	C	99	ASN
1	C	113	ASN
1	C	138	ASN
1	C	193	HIS
1	C	232	ASN
1	C	239	GLN
1	C	265	ASN
1	C	267	ASN
1	C	294	ASN
1	C	307	ASN
1	D	18	ASN
1	D	99	ASN
1	D	113	ASN
1	D	138	ASN

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Mol	Chain	Res	Type
1	D	193	HIS
1	D	232	ASN
1	D	239	GLN
1	D	265	ASN
1	D	267	ASN
1	D	294	ASN
1	D	307	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	SO4	A	1	-	4,4,4	1.35	1 (25%)	6,6,6	0.79	0
2	SO4	A	2	-	4,4,4	1.97	2 (50%)	6,6,6	0.71	0

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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	SO4	O3-S	2.19	1.55	1.47
2	A	1	SO4	O1-S	2.52	1.55	1.47
2	A	2	SO4	O2-S	3.07	1.57	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SO4	1	0
2	A	2	SO4	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.