



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 07:24 PM EDT

PDB ID : 1X0R  
Title : Thioredoxin Peroxidase from *Aeropyrum pernix* K1  
Authors : Nakamura, T.; Yamamoto, T.; Inoue, T.; Matsumura, H.; Kobayashi, A.;  
Hagihara, Y.; Uegaki, K.; Ataka, M.; Kai, Y.; Ishikawa, K.  
Deposited on : 2005-03-28  
Resolution : 2.00 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

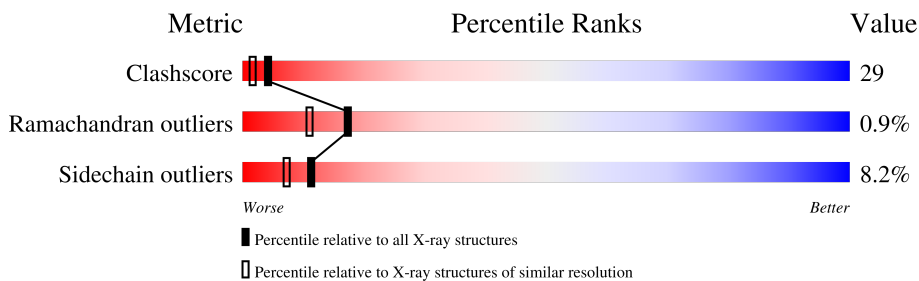
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)


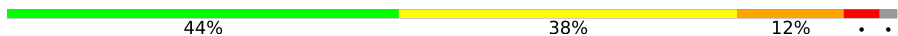
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	249	
1	B	249	
1	C	249	
1	D	249	
1	E	249	
1	F	249	
1	G	249	
1	H	249	

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Mol	Chain	Length	Quality of chain
1	I	249	
1	J	249	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	2001	-	X	X	-
2	EDO	A	2012	-	X	X	-
2	EDO	A	2016	-	X	-	-
2	EDO	A	2017	-	X	-	-
2	EDO	A	2029	-	X	X	-
2	EDO	A	2063	-	X	X	-
2	EDO	A	2065	-	X	X	-
2	EDO	A	2116	-	X	-	-
2	EDO	A	2122	-	-	X	-
2	EDO	A	2124	-	X	X	-
2	EDO	B	2002	-	X	X	-
2	EDO	B	2013	-	X	-	-
2	EDO	B	2018	-	X	-	-
2	EDO	B	2021	-	-	X	-
2	EDO	B	2025	-	X	-	-
2	EDO	B	2028	-	X	X	-
2	EDO	B	2030	-	-	X	-
2	EDO	B	2070	-	X	-	-
2	EDO	B	2125	-	X	X	-
2	EDO	C	2004	-	X	X	-
2	EDO	C	2024	-	X	X	-
2	EDO	C	2036	-	X	-	-
2	EDO	C	2064	-	X	-	-
2	EDO	C	2067	-	-	X	-
2	EDO	C	2075	-	X	X	-
2	EDO	C	2080	-	X	-	-
2	EDO	C	2081	-	X	-	-
2	EDO	C	2083	-	X	-	-
2	EDO	C	2085	-	X	X	-
2	EDO	C	2126	-	X	X	-
2	EDO	C	2128	-	X	X	-
2	EDO	D	2003	-	X	X	-
2	EDO	D	2031	-	X	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	D	2033	-	X	-	-
2	EDO	D	2035	-	-	X	-
2	EDO	D	2071	-	X	-	-
2	EDO	D	2072	-	X	-	-
2	EDO	D	2073	-	X	-	-
2	EDO	D	2074	-	X	-	-
2	EDO	D	2118	-	X	X	-
2	EDO	D	2119	-	X	-	-
2	EDO	E	2005	-	X	X	-
2	EDO	E	2039	-	X	-	-
2	EDO	E	2042	-	X	-	-
2	EDO	E	2076	-	X	X	-
2	EDO	E	2077	-	X	-	-
2	EDO	E	2079	-	X	-	-
2	EDO	E	2088	-	X	-	-
2	EDO	E	2089	-	X	X	-
2	EDO	E	2090	-	X	X	-
2	EDO	E	2091	-	X	X	-
2	EDO	E	2092	-	X	-	-
2	EDO	E	2120	-	X	X	-
2	EDO	E	2127	-	X	X	-
2	EDO	F	2006	-	X	-	-
2	EDO	F	2034	-	-	X	-
2	EDO	F	2037	-	X	-	-
2	EDO	F	2038	-	-	X	-
2	EDO	F	2043	-	-	X	-
2	EDO	F	2086	-	X	X	-
2	EDO	F	2094	-	X	-	-
2	EDO	F	2096	-	X	-	-
2	EDO	F	2097	-	X	X	-
2	EDO	F	2098	-	X	-	-
2	EDO	G	2009	-	X	X	-
2	EDO	G	2050	-	-	X	-
2	EDO	G	2056	-	X	X	-
2	EDO	G	2057	-	-	X	-
2	EDO	G	2093	-	X	X	-
2	EDO	G	2101	-	X	-	-
2	EDO	H	2010	-	X	X	-
2	EDO	H	2044	-	-	X	-
2	EDO	H	2058	-	X	X	-
2	EDO	H	2059	-	X	-	-
2	EDO	H	2060	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	H	2111	-	X	-	-
2	EDO	H	2113	-	-	X	-
2	EDO	I	2007	-	X	X	-
2	EDO	I	2045	-	X	-	-
2	EDO	I	2046	-	-	X	-
2	EDO	I	2051	-	-	X	-
2	EDO	I	2052	-	X	-	-
2	EDO	I	2099	-	X	-	-
2	EDO	I	2103	-	X	X	-
2	EDO	I	2107	-	-	X	-
2	EDO	I	2115	-	-	X	-
2	EDO	I	2121	-	-	X	-
2	EDO	J	2008	-	X	X	-
2	EDO	J	2048	-	X	-	-
2	EDO	J	2049	-	-	X	-
2	EDO	J	2053	-	X	-	-
2	EDO	J	2068	-	X	X	-
2	EDO	J	2069	-	X	-	-
2	EDO	J	2104	-	X	X	-
2	EDO	J	2105	-	-	X	-
2	EDO	J	2109	-	-	X	-
2	EDO	J	2123	-	X	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21431 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 Probable peroxiredoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	244	1973	1268	347	352	2	4	0	0	0
1	B	244	1973	1268	347	352	2	4	0	0	0
1	C	244	1973	1268	347	352	2	4	0	0	0
1	D	244	1973	1268	347	352	2	4	0	0	0
1	E	244	1973	1268	347	352	2	4	0	0	0
1	F	244	1973	1268	347	352	2	4	0	0	0
1	G	244	1973	1268	347	352	2	4	0	0	0
1	H	244	1973	1268	347	352	2	4	0	0	0
1	I	244	1973	1268	347	352	2	4	0	0	0
1	J	244	1973	1268	347	352	2	4	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MSE	MET	modified residue	UNP Q9Y9L0
A	140	MSE	MET	modified residue	UNP Q9Y9L0
A	145	MSE	MET	modified residue	UNP Q9Y9L0
A	200	MSE	MET	modified residue	UNP Q9Y9L0
A	207	SER	CYS	engineered mutation	UNP Q9Y9L0
B	15	MSE	MET	modified residue	UNP Q9Y9L0
B	140	MSE	MET	modified residue	UNP Q9Y9L0
B	145	MSE	MET	modified residue	UNP Q9Y9L0
B	200	MSE	MET	modified residue	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	207	SER	CYS	engineered mutation	UNP Q9Y9L0
C	15	MSE	MET	modified residue	UNP Q9Y9L0
C	140	MSE	MET	modified residue	UNP Q9Y9L0
C	145	MSE	MET	modified residue	UNP Q9Y9L0
C	200	MSE	MET	modified residue	UNP Q9Y9L0
C	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	15	MSE	MET	modified residue	UNP Q9Y9L0
D	140	MSE	MET	modified residue	UNP Q9Y9L0
D	145	MSE	MET	modified residue	UNP Q9Y9L0
D	200	MSE	MET	modified residue	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
E	15	MSE	MET	modified residue	UNP Q9Y9L0
E	140	MSE	MET	modified residue	UNP Q9Y9L0
E	145	MSE	MET	modified residue	UNP Q9Y9L0
E	200	MSE	MET	modified residue	UNP Q9Y9L0
E	207	SER	CYS	engineered mutation	UNP Q9Y9L0
F	15	MSE	MET	modified residue	UNP Q9Y9L0
F	140	MSE	MET	modified residue	UNP Q9Y9L0
F	145	MSE	MET	modified residue	UNP Q9Y9L0
F	200	MSE	MET	modified residue	UNP Q9Y9L0
F	207	SER	CYS	engineered mutation	UNP Q9Y9L0
G	15	MSE	MET	modified residue	UNP Q9Y9L0
G	140	MSE	MET	modified residue	UNP Q9Y9L0
G	145	MSE	MET	modified residue	UNP Q9Y9L0
G	200	MSE	MET	modified residue	UNP Q9Y9L0
G	207	SER	CYS	engineered mutation	UNP Q9Y9L0
H	15	MSE	MET	modified residue	UNP Q9Y9L0
H	140	MSE	MET	modified residue	UNP Q9Y9L0
H	145	MSE	MET	modified residue	UNP Q9Y9L0
H	200	MSE	MET	modified residue	UNP Q9Y9L0
H	207	SER	CYS	engineered mutation	UNP Q9Y9L0
I	15	MSE	MET	modified residue	UNP Q9Y9L0
I	140	MSE	MET	modified residue	UNP Q9Y9L0
I	145	MSE	MET	modified residue	UNP Q9Y9L0
I	200	MSE	MET	modified residue	UNP Q9Y9L0
I	207	SER	CYS	engineered mutation	UNP Q9Y9L0
J	15	MSE	MET	modified residue	UNP Q9Y9L0
J	140	MSE	MET	modified residue	UNP Q9Y9L0
J	145	MSE	MET	modified residue	UNP Q9Y9L0
J	200	MSE	MET	modified residue	UNP Q9Y9L0
J	207	SER	CYS	engineered mutation	UNP Q9Y9L0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

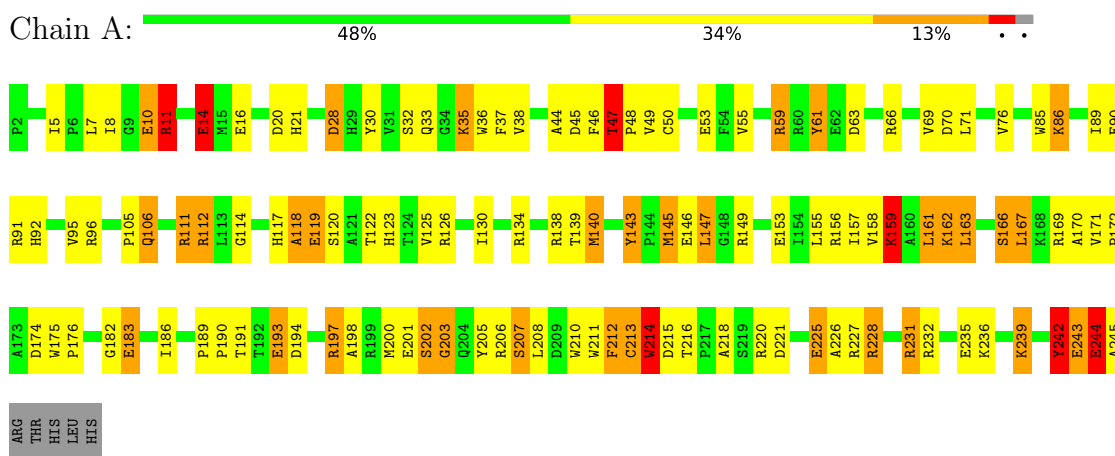
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	140	Total O 140 140	0	0
3	B	120	Total O 120 120	0	0
3	C	136	Total O 136 136	0	0
3	D	132	Total O 132 132	0	0
3	E	133	Total O 133 133	0	0
3	F	115	Total O 115 115	0	0
3	G	98	Total O 98 98	0	0
3	H	94	Total O 94 94	0	0
3	I	106	Total O 106 106	0	0
3	J	115	Total O 115 115	0	0

### 3 Residue-property plots [i](#)

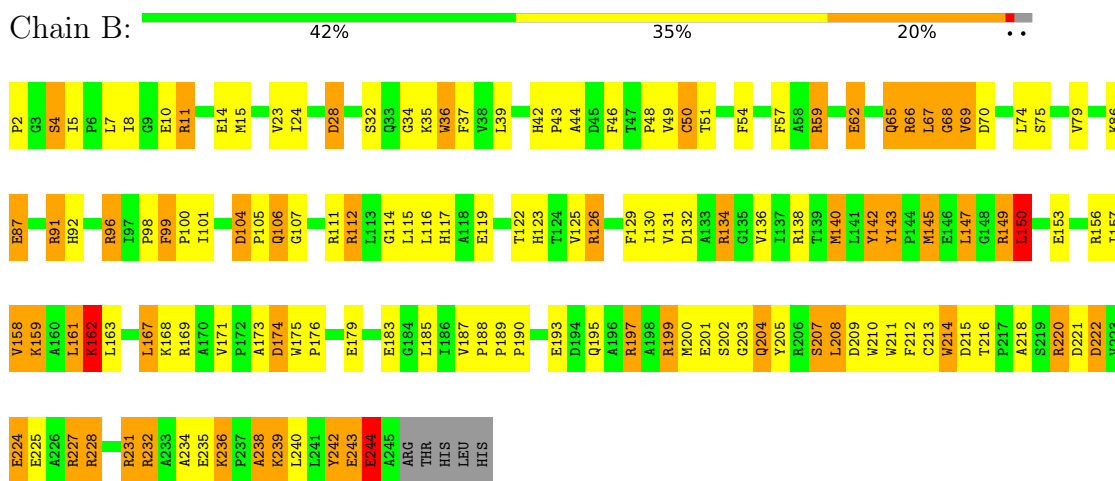
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Probable peroxiredoxin

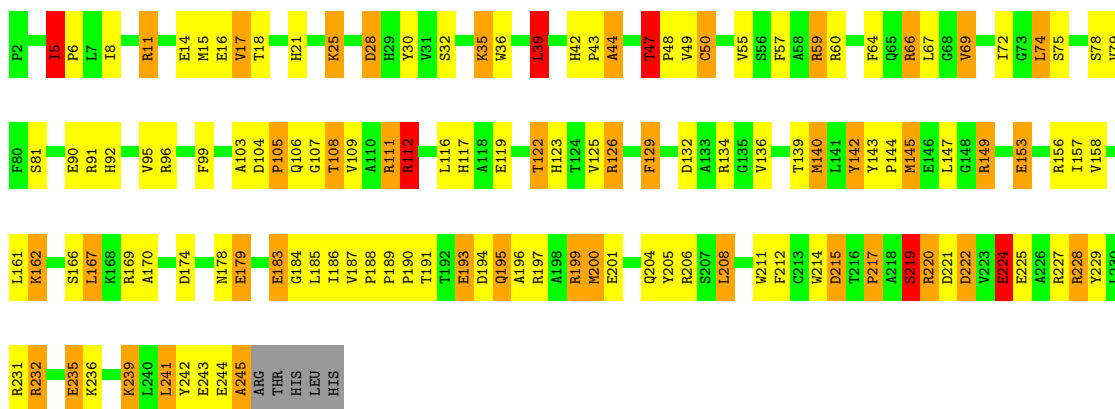


- Molecule 1: Probable peroxiredoxin



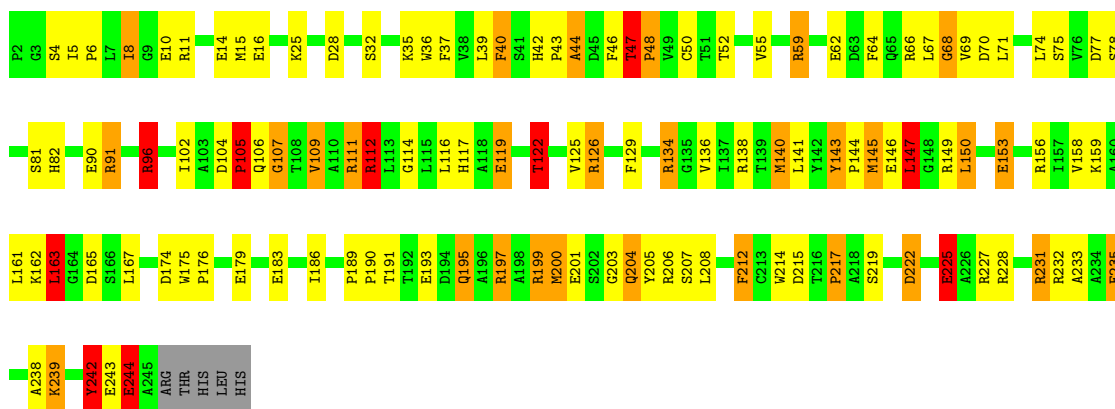
- Molecule 1: Probable peroxiredoxin





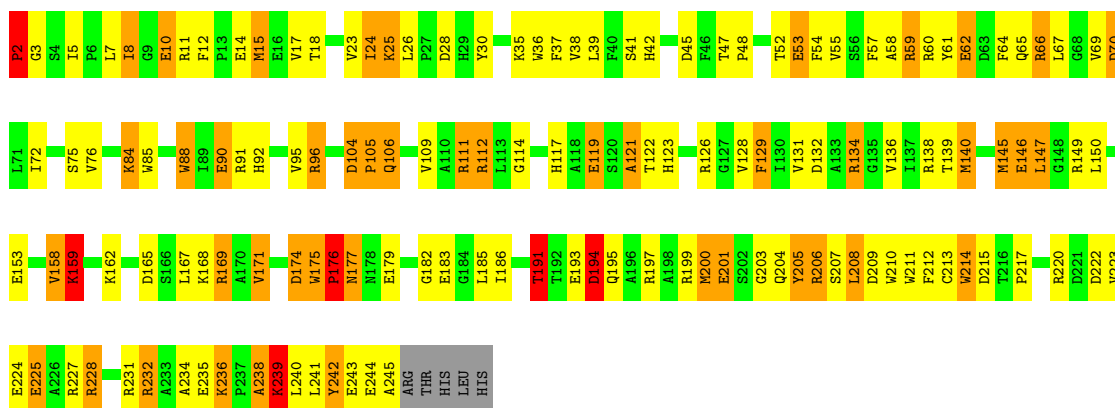
- Molecule 1: Probable peroxiredoxin

Chain D: 50% 33% 12% ..



- Molecule 1: Probable peroxiredoxin

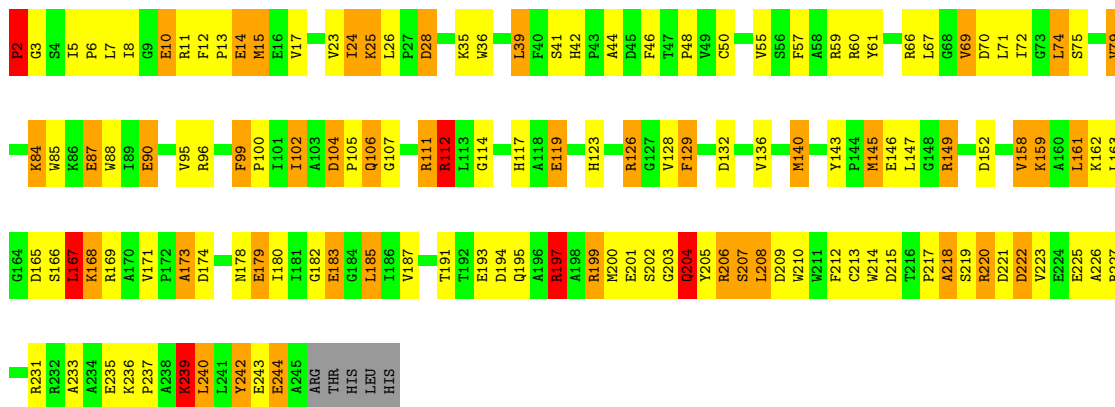
Chain E: 41% 37% 18% ..



- Molecule 1: Probable peroxiredoxin

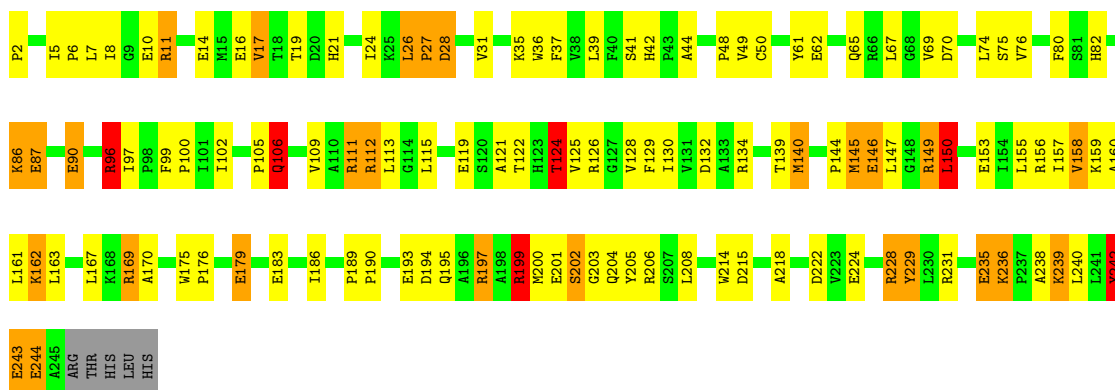
Chain F: 44% 35% 17% ..





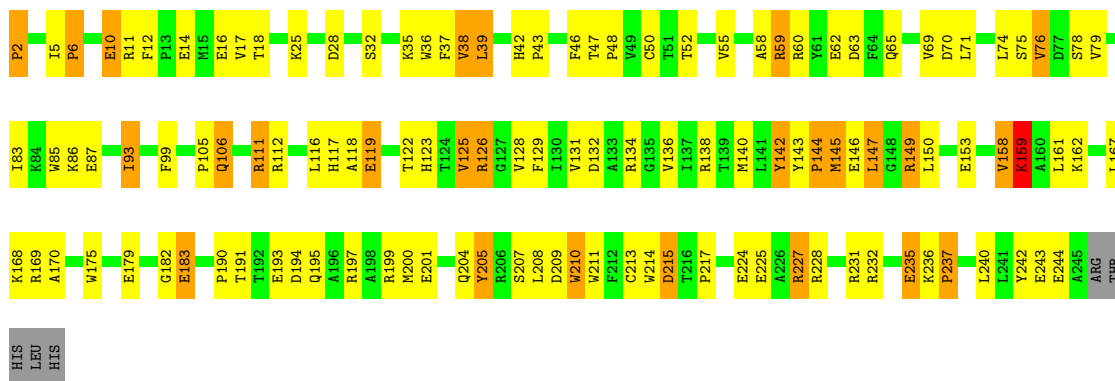
- Molecule 1: Probable peroxiredoxin

Chain G: 49% 35% 11% ..



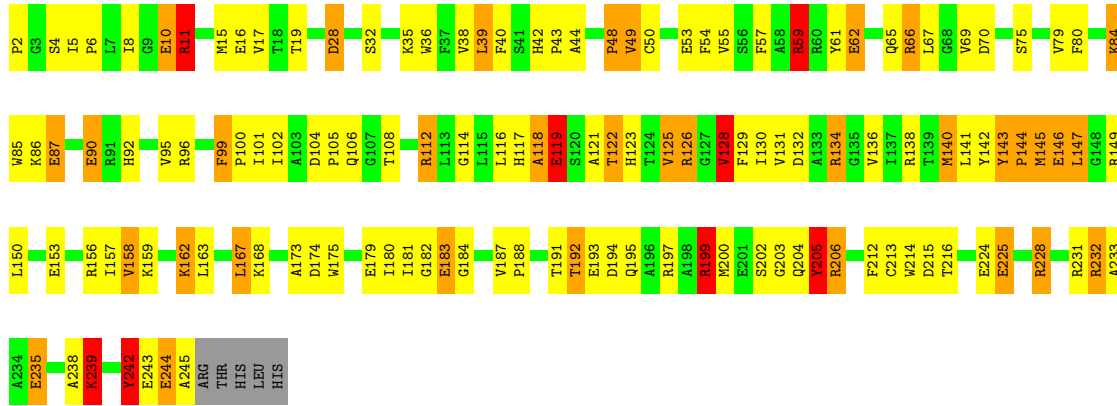
- Molecule 1: Probable peroxiredoxin

Chain H: 50% 37% 10% .

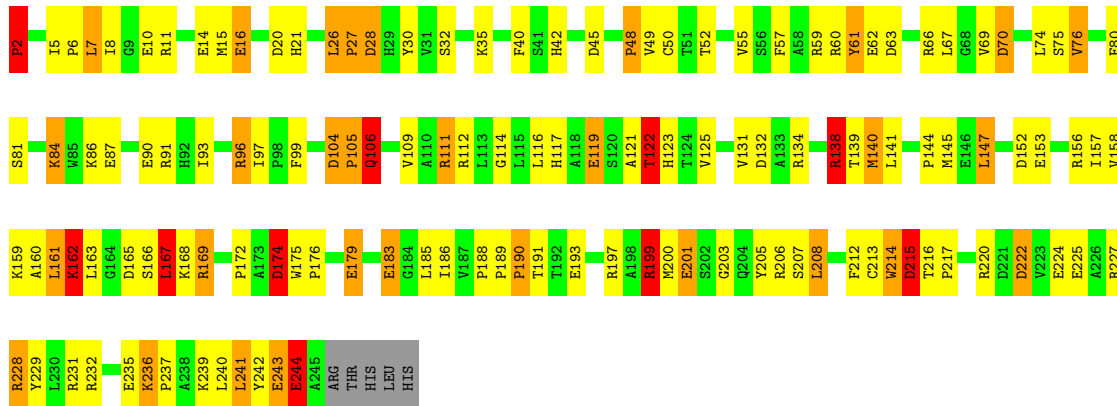


- Molecule 1: Probable peroxiredoxin

Chain I: 44% 37% 14% ..



• Molecule 1: Probable peroxiredoxin



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.63Å 101.79Å 102.89Å 105.37° 105.28° 93.32°	Depositor
Resolution (Å)	29.89 – 2.00	Depositor
% Data completeness (in resolution range)	89.9 (29.89-2.00)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.164 , 0.171	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	21431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

## 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: EDO

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	2.20	78/2024 (3.9%)	1.70	37/2745 (1.3%)
1	B	2.16	79/2024 (3.9%)	1.91	55/2745 (2.0%)
1	C	2.16	79/2024 (3.9%)	1.76	55/2745 (2.0%)
1	D	2.17	68/2024 (3.4%)	1.68	39/2745 (1.4%)
1	E	2.25	96/2024 (4.7%)	1.91	51/2745 (1.9%)
1	F	2.14	74/2024 (3.7%)	1.78	50/2745 (1.8%)
1	G	2.12	65/2024 (3.2%)	1.74	36/2745 (1.3%)
1	H	2.15	74/2024 (3.7%)	1.62	28/2745 (1.0%)
1	I	2.12	74/2024 (3.7%)	1.75	43/2745 (1.6%)
1	J	2.21	63/2024 (3.1%)	2.32	78/2745 (2.8%)
All	All	2.17	750/20240 (3.7%)	1.83	472/27450 (1.7%)

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	2
1	B	0	1
1	D	0	2
1	E	0	1
1	G	0	3
1	H	0	1
1	I	0	2
1	J	0	4
All	All	0	16

All (750) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	GLU	CG-CD	15.52	1.75	1.51
1	H	62	GLU	CD-OE2	15.03	1.42	1.25
1	B	162	LYS	CE-NZ	14.24	1.84	1.49
1	J	214	TRP	CG-CD1	14.23	1.56	1.36
1	D	68	GLY	N-CA	13.91	1.67	1.46
1	G	26	LEU	C-N	12.91	1.58	1.34
1	E	224	GLU	CG-CD	12.75	1.71	1.51
1	J	224	GLU	CD-OE1	12.59	1.39	1.25
1	D	243	GLU	CG-CD	12.54	1.70	1.51
1	F	225	GLU	CG-CD	12.52	1.70	1.51
1	I	145	MSE	CB-CG	12.37	1.89	1.52
1	E	119	GLU	CD-OE2	12.37	1.39	1.25
1	A	242	TYR	CE2-CZ	12.12	1.54	1.38
1	B	243	GLU	CG-CD	11.98	1.70	1.51
1	A	145	MSE	CB-CG	11.98	1.88	1.52
1	A	183	GLU	CD-OE2	11.76	1.38	1.25
1	F	90	GLU	CG-CD	11.74	1.69	1.51
1	J	16	GLU	CG-CD	11.70	1.69	1.51
1	B	104	ASP	CB-CG	-11.66	1.27	1.51
1	J	243	GLU	CG-CD	11.59	1.69	1.51
1	E	121	ALA	CA-CB	11.35	1.76	1.52
1	E	243	GLU	CG-CD	11.35	1.69	1.51
1	F	90	GLU	CD-OE2	11.33	1.38	1.25
1	I	87	GLU	CB-CG	-11.27	1.30	1.52
1	D	225	GLU	CG-CD	11.12	1.68	1.51
1	J	27	PRO	CA-C	10.72	1.74	1.52
1	G	242	TYR	CD2-CE2	10.67	1.55	1.39
1	B	153	GLU	CG-CD	10.64	1.68	1.51
1	J	215	ASP	CB-CG	-10.56	1.29	1.51
1	G	62	GLU	CD-OE1	10.54	1.37	1.25
1	D	179	GLU	CG-CD	10.44	1.67	1.51
1	A	228	ARG	CZ-NH1	10.35	1.46	1.33
1	J	244	GLU	CG-CD	10.34	1.67	1.51
1	E	242	TYR	CD1-CE1	10.30	1.54	1.39
1	I	235	GLU	CG-CD	10.25	1.67	1.51
1	D	183	GLU	CD-OE2	10.21	1.36	1.25
1	E	214	TRP	CG-CD1	10.21	1.51	1.36
1	D	207	SER	CB-OG	-10.13	1.29	1.42
1	D	136	VAL	CB-CG2	10.10	1.74	1.52
1	C	214	TRP	CG-CD1	10.08	1.50	1.36
1	C	224	GLU	CG-CD	10.06	1.67	1.51
1	H	145	MSE	CB-CG	10.05	1.82	1.52
1	B	79	VAL	CB-CG2	10.00	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	158	VAL	CB-CG1	9.73	1.73	1.52
1	J	49	VAL	CB-CG2	9.71	1.73	1.52
1	E	145	MSE	CB-CG	9.69	1.81	1.52
1	F	225	GLU	CB-CG	9.67	1.70	1.52
1	C	205	TYR	CD2-CE2	9.63	1.53	1.39
1	E	243	GLU	CD-OE2	9.59	1.36	1.25
1	I	225	GLU	CG-CD	9.57	1.66	1.51
1	E	224	GLU	CD-OE1	9.54	1.36	1.25
1	C	242	TYR	CG-CD1	9.53	1.51	1.39
1	C	224	GLU	CD-OE1	9.51	1.36	1.25
1	H	193	GLU	CB-CG	-9.44	1.34	1.52
1	A	153	GLU	CB-CG	9.44	1.70	1.52
1	A	119	GLU	CD-OE2	9.39	1.35	1.25
1	F	193	GLU	CB-CG	-9.39	1.34	1.52
1	G	235	GLU	CG-CD	9.38	1.66	1.51
1	I	183	GLU	CD-OE2	9.37	1.35	1.25
1	C	219	SER	CB-OG	-9.37	1.30	1.42
1	E	62	GLU	CG-CD	9.25	1.65	1.51
1	A	225	GLU	CB-CG	9.24	1.69	1.52
1	I	183	GLU	CG-CD	9.20	1.65	1.51
1	I	125	VAL	CB-CG2	-9.16	1.33	1.52
1	A	162	LYS	CD-CE	9.12	1.74	1.51
1	F	225	GLU	CD-OE2	9.10	1.35	1.25
1	G	62	GLU	CD-OE2	9.04	1.35	1.25
1	I	242	TYR	CE1-CZ	9.04	1.50	1.38
1	G	153	GLU	CG-CD	8.98	1.65	1.51
1	C	242	TYR	CE1-CZ	8.98	1.50	1.38
1	J	62	GLU	CD-OE1	8.96	1.35	1.25
1	H	214	TRP	CE3-CZ3	-8.83	1.23	1.38
1	J	224	GLU	CG-CD	8.78	1.65	1.51
1	I	243	GLU	CG-CD	8.71	1.65	1.51
1	B	69	VAL	CB-CG2	8.70	1.71	1.52
1	E	242	TYR	CG-CD1	8.67	1.50	1.39
1	F	44	ALA	CA-CB	8.65	1.70	1.52
1	H	214	TRP	CE2-CZ2	-8.65	1.25	1.39
1	J	104	ASP	CA-CB	8.61	1.72	1.53
1	C	145	MSE	CB-CG	8.57	1.78	1.52
1	F	179	GLU	CD-OE1	8.54	1.35	1.25
1	B	242	TYR	CD1-CE1	8.53	1.52	1.39
1	C	79	VAL	CB-CG2	8.53	1.70	1.52
1	H	175	TRP	CB-CG	8.53	1.65	1.50
1	A	214	TRP	CG-CD1	8.49	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	162	LYS	CE-NZ	8.44	1.70	1.49
1	A	182	GLY	C-O	8.43	1.37	1.23
1	E	76	VAL	CB-CG1	8.43	1.70	1.52
1	D	145	MSE	CB-CG	8.42	1.77	1.52
1	A	183	GLU	CG-CD	8.41	1.64	1.51
1	E	171	VAL	CB-CG2	8.40	1.70	1.52
1	F	87	GLU	CG-CD	8.38	1.64	1.51
1	E	225	GLU	CD-OE1	8.38	1.34	1.25
1	D	193	GLU	CB-CG	-8.37	1.36	1.52
1	D	225	GLU	CD-OE1	8.36	1.34	1.25
1	D	243	GLU	CD-OE2	8.36	1.34	1.25
1	E	146	GLU	CG-CD	8.36	1.64	1.51
1	D	201	GLU	CD-OE1	8.35	1.34	1.25
1	H	168	LYS	CD-CE	8.33	1.72	1.51
1	D	16	GLU	CD-OE1	8.31	1.34	1.25
1	A	193	GLU	CB-CG	-8.30	1.36	1.52
1	E	90	GLU	CG-CD	8.30	1.64	1.51
1	H	179	GLU	CD-OE2	8.30	1.34	1.25
1	A	76	VAL	CB-CG1	8.27	1.70	1.52
1	I	224	GLU	CG-CD	8.24	1.64	1.51
1	D	225	GLU	CD-OE2	8.21	1.34	1.25
1	D	37	PHE	CE1-CZ	8.20	1.52	1.37
1	E	70	ASP	CG-OD1	8.18	1.44	1.25
1	E	236	LYS	CD-CE	8.18	1.71	1.51
1	D	243	GLU	CD-OE1	8.17	1.34	1.25
1	G	242	TYR	CE2-CZ	8.17	1.49	1.38
1	B	4	SER	CB-OG	8.16	1.52	1.42
1	G	242	TYR	CE1-CZ	8.16	1.49	1.38
1	C	211	TRP	CB-CG	8.15	1.65	1.50
1	G	235	GLU	CD-OE2	8.13	1.34	1.25
1	F	168	LYS	CE-NZ	8.12	1.69	1.49
1	C	90	GLU	CB-CG	-8.11	1.36	1.52
1	A	85	TRP	CZ3-CH2	8.05	1.52	1.40
1	B	225	GLU	CD-OE1	8.04	1.34	1.25
1	E	55	VAL	CB-CG1	8.04	1.69	1.52
1	H	214	TRP	CB-CG	-8.03	1.35	1.50
1	B	162	LYS	CD-CE	8.02	1.71	1.51
1	E	35	LYS	CD-CE	8.01	1.71	1.51
1	D	96	ARG	CZ-NH1	8.01	1.43	1.33
1	C	244	GLU	CG-CD	8.00	1.64	1.51
1	I	153	GLU	CB-CG	7.98	1.67	1.52
1	G	236	LYS	CE-NZ	7.95	1.69	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	121	ALA	CA-CB	7.94	1.69	1.52
1	A	90	GLU	CB-CG	-7.93	1.37	1.52
1	J	16	GLU	CD-OE1	7.88	1.34	1.25
1	C	235	GLU	CD-OE1	7.87	1.34	1.25
1	C	47	THR	CB-CG2	-7.82	1.26	1.52
1	J	176	PRO	CG-CD	-7.80	1.25	1.50
1	H	62	GLU	CB-CG	-7.77	1.37	1.52
1	B	214	TRP	CE3-CZ3	-7.74	1.25	1.38
1	F	183	GLU	CD-OE2	7.74	1.34	1.25
1	J	138	ARG	CD-NE	-7.74	1.33	1.46
1	J	215	ASP	CA-CB	7.73	1.71	1.53
1	J	140	MSE	SE-CE	-7.72	1.50	1.95
1	D	222	ASP	CG-OD2	7.69	1.43	1.25
1	G	179	GLU	CD-OE2	7.69	1.34	1.25
1	I	87	GLU	CG-CD	7.67	1.63	1.51
1	G	229	TYR	CD2-CE2	7.65	1.50	1.39
1	G	193	GLU	CD-OE2	7.64	1.34	1.25
1	I	235	GLU	CD-OE1	7.62	1.34	1.25
1	G	61	TYR	CD2-CE2	7.61	1.50	1.39
1	G	44	ALA	CA-CB	7.61	1.68	1.52
1	F	243	GLU	CG-CD	7.60	1.63	1.51
1	H	179	GLU	CD-OE1	7.60	1.34	1.25
1	B	199	ARG	CB-CG	-7.59	1.32	1.52
1	J	220	ARG	CG-CD	7.58	1.70	1.51
1	C	16	GLU	CD-OE1	7.57	1.33	1.25
1	F	119	GLU	CD-OE2	7.56	1.33	1.25
1	G	76	VAL	CB-CG1	7.53	1.68	1.52
1	F	57	PHE	CE2-CZ	7.51	1.51	1.37
1	G	197	ARG	CG-CD	7.51	1.70	1.51
1	F	207	SER	CB-OG	-7.49	1.32	1.42
1	A	214	TRP	CE3-CZ3	-7.46	1.25	1.38
1	A	69	VAL	CB-CG2	7.46	1.68	1.52
1	C	243	GLU	CG-CD	7.44	1.63	1.51
1	B	158	VAL	CB-CG2	-7.43	1.37	1.52
1	J	30	TYR	CE2-CZ	7.43	1.48	1.38
1	B	131	VAL	CB-CG2	7.43	1.68	1.52
1	B	87	GLU	CB-CG	-7.41	1.38	1.52
1	F	166	SER	CB-OG	-7.41	1.32	1.42
1	I	61	TYR	CD2-CE2	7.41	1.50	1.39
1	H	136	VAL	CB-CG2	7.41	1.68	1.52
1	F	242	TYR	CG-CD1	7.40	1.48	1.39
1	I	197	ARG	CZ-NH2	7.40	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	25	LYS	CE-NZ	7.39	1.67	1.49
1	B	134	ARG	CG-CD	7.39	1.70	1.51
1	I	244	GLU	CB-CG	7.37	1.66	1.52
1	B	68	GLY	N-CA	7.35	1.57	1.46
1	H	197	ARG	CG-CD	7.32	1.70	1.51
1	C	69	VAL	CA-CB	7.30	1.70	1.54
1	A	30	TYR	CE1-CZ	-7.29	1.29	1.38
1	J	119	GLU	CD-OE2	7.29	1.33	1.25
1	F	202	SER	CB-OG	7.28	1.51	1.42
1	B	179	GLU	CD-OE1	7.26	1.33	1.25
1	B	207	SER	CB-OG	-7.26	1.32	1.42
1	G	179	GLU	CB-CG	7.25	1.66	1.52
1	J	231	ARG	CG-CD	7.24	1.70	1.51
1	A	242	TYR	CD1-CE1	7.22	1.50	1.39
1	A	242	TYR	CG-CD1	7.21	1.48	1.39
1	D	138	ARG	CB-CG	7.20	1.72	1.52
1	E	104	ASP	CB-CG	-7.19	1.36	1.51
1	H	62	GLU	CD-OE1	7.19	1.33	1.25
1	F	112	ARG	CG-CD	7.18	1.70	1.51
1	C	242	TYR	CD2-CE2	7.18	1.50	1.39
1	J	26	LEU	C-N	7.18	1.47	1.34
1	I	146	GLU	CB-CG	7.17	1.65	1.52
1	C	99	PHE	CD2-CE2	7.14	1.53	1.39
1	J	214	TRP	CE2-CZ2	-7.12	1.27	1.39
1	G	242	TYR	CZ-OH	7.12	1.50	1.37
1	D	14	GLU	CD-OE2	7.10	1.33	1.25
1	G	128	VAL	CB-CG2	-7.10	1.38	1.52
1	C	140	MSE	SE-CE	-7.10	1.53	1.95
1	F	85	TRP	CZ3-CH2	7.09	1.51	1.40
1	E	30	TYR	CE2-CZ	7.07	1.47	1.38
1	A	146	GLU	CD-OE2	7.07	1.33	1.25
1	A	166	SER	CB-OG	-7.07	1.33	1.42
1	E	225	GLU	CD-OE2	7.07	1.33	1.25
1	I	16	GLU	CD-OE2	7.06	1.33	1.25
1	A	242	TYR	CD2-CE2	7.06	1.50	1.39
1	H	235	GLU	CD-OE1	7.06	1.33	1.25
1	B	214	TRP	CB-CG	-7.05	1.37	1.50
1	D	112	ARG	CG-CD	7.04	1.69	1.51
1	A	225	GLU	CD-OE2	7.04	1.33	1.25
1	G	86	LYS	CD-CE	-7.03	1.33	1.51
1	H	224	GLU	CD-OE1	7.02	1.33	1.25
1	G	243	GLU	CD-OE1	7.01	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	144	PRO	CG-CD	6.99	1.73	1.50
1	H	242	TYR	CE1-CZ	6.97	1.47	1.38
1	F	204	GLN	CB-CG	-6.96	1.33	1.52
1	F	183	GLU	CG-CD	6.96	1.62	1.51
1	D	90	GLU	CG-CD	6.95	1.62	1.51
1	E	239	LYS	N-CA	6.95	1.60	1.46
1	G	228	ARG	CG-CD	6.95	1.69	1.51
1	B	140	MSE	CG-SE	6.94	2.19	1.95
1	I	159	LYS	CG-CD	-6.94	1.28	1.52
1	H	76	VAL	CB-CG1	6.91	1.67	1.52
1	B	119	GLU	CB-CG	-6.91	1.39	1.52
1	I	140	MSE	CG-SE	6.89	2.18	1.95
1	D	212	PHE	CB-CG	6.88	1.63	1.51
1	A	95	VAL	CB-CG1	6.88	1.67	1.52
1	D	233	ALA	CA-CB	6.87	1.66	1.52
1	H	214	TRP	CG-CD2	-6.84	1.32	1.43
1	G	31	VAL	CB-CG1	6.82	1.67	1.52
1	J	61	TYR	CG-CD1	-6.82	1.30	1.39
1	E	37	PHE	CD1-CE1	6.82	1.52	1.39
1	E	61	TYR	CD1-CE1	6.82	1.49	1.39
1	E	66	ARG	CG-CD	6.81	1.69	1.51
1	H	224	GLU	CG-CD	6.80	1.62	1.51
1	B	220	ARG	CG-CD	6.80	1.69	1.51
1	E	38	VAL	CB-CG1	6.79	1.67	1.52
1	J	201	GLU	CG-CD	6.79	1.62	1.51
1	B	143	TYR	CD1-CE1	6.78	1.49	1.39
1	F	25	LYS	CE-NZ	6.78	1.66	1.49
1	G	244	GLU	CG-CD	6.77	1.62	1.51
1	I	202	SER	CB-OG	6.77	1.51	1.42
1	E	214	TRP	CE3-CZ3	-6.77	1.26	1.38
1	I	173	ALA	CA-CB	6.76	1.66	1.52
1	B	145	MSE	CB-CG	6.76	1.72	1.52
1	A	225	GLU	CD-OE1	6.75	1.33	1.25
1	F	129	PHE	CE2-CZ	6.74	1.50	1.37
1	C	57	PHE	CE2-CZ	6.73	1.50	1.37
1	H	211	TRP	CB-CG	6.70	1.62	1.50
1	I	239	LYS	CD-CE	6.70	1.68	1.51
1	J	40	PHE	CE1-CZ	6.68	1.50	1.37
1	B	37	PHE	CE2-CZ	6.68	1.50	1.37
1	E	12	PHE	CB-CG	-6.67	1.40	1.51
1	F	225	GLU	CD-OE1	6.67	1.32	1.25
1	G	179	GLU	CG-CD	6.67	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	61	TYR	CD2-CE2	6.66	1.49	1.39
1	G	140	MSE	SE-CE	-6.66	1.56	1.95
1	H	214	TRP	CG-CD1	6.65	1.46	1.36
1	I	95	VAL	CB-CG2	6.64	1.66	1.52
1	D	96	ARG	CZ-NH2	6.63	1.41	1.33
1	I	162	LYS	CD-CE	6.63	1.67	1.51
1	I	32	SER	CB-OG	-6.60	1.33	1.42
1	G	201	GLU	CD-OE1	6.59	1.32	1.25
1	F	223	VAL	CA-CB	6.59	1.68	1.54
1	A	243	GLU	CD-OE2	6.59	1.32	1.25
1	C	134	ARG	NE-CZ	6.59	1.41	1.33
1	I	231	ARG	CG-CD	6.59	1.68	1.51
1	C	243	GLU	CD-OE1	6.57	1.32	1.25
1	D	239	LYS	CE-NZ	6.57	1.65	1.49
1	J	62	GLU	CD-OE2	6.56	1.32	1.25
1	I	53	GLU	CD-OE2	-6.56	1.18	1.25
1	E	14	GLU	CD-OE1	6.56	1.32	1.25
1	D	235	GLU	CB-CG	-6.54	1.39	1.52
1	J	239	LYS	CE-NZ	6.53	1.65	1.49
1	C	157	ILE	CA-CB	6.53	1.69	1.54
1	G	90	GLU	CG-CD	6.52	1.61	1.51
1	H	228	ARG	CG-CD	6.52	1.68	1.51
1	I	119	GLU	CG-CD	6.52	1.61	1.51
1	J	14	GLU	CD-OE2	6.51	1.32	1.25
1	F	57	PHE	CB-CG	-6.51	1.40	1.51
1	F	14	GLU	CB-CG	-6.49	1.39	1.52
1	I	70	ASP	CG-OD1	6.49	1.40	1.25
1	H	16	GLU	CG-CD	6.48	1.61	1.51
1	J	80	PHE	CE1-CZ	6.48	1.49	1.37
1	E	243	GLU	CD-OE1	6.46	1.32	1.25
1	A	211	TRP	CE3-CZ3	6.46	1.49	1.38
1	G	37	PHE	CE1-CZ	6.46	1.49	1.37
1	H	242	TYR	CD2-CE2	6.45	1.49	1.39
1	H	183	GLU	CD-OE1	6.45	1.32	1.25
1	C	187	VAL	CB-CG2	6.45	1.66	1.52
1	C	229	TYR	CD1-CE1	6.42	1.49	1.39
1	C	99	PHE	CE1-CZ	6.41	1.49	1.37
1	F	111	ARG	CZ-NH1	6.40	1.41	1.33
1	H	205	TYR	CD1-CE1	-6.40	1.29	1.39
1	E	111	ARG	CZ-NH2	6.40	1.41	1.33
1	F	239	LYS	CD-CE	6.40	1.67	1.51
1	A	212	PHE	CD1-CE1	6.39	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	214	TRP	CE3-CZ3	6.39	1.49	1.38
1	A	36	TRP	CG-CD1	6.38	1.45	1.36
1	E	153	GLU	CB-CG	6.36	1.64	1.52
1	C	112	ARG	CG-CD	6.36	1.67	1.51
1	C	201	GLU	CD-OE1	6.36	1.32	1.25
1	A	243	GLU	CD-OE1	6.36	1.32	1.25
1	E	211	TRP	CE3-CZ3	6.35	1.49	1.38
1	F	79	VAL	CB-CG2	6.35	1.66	1.52
1	A	70	ASP	CG-OD1	6.34	1.40	1.25
1	D	174	ASP	CB-CG	6.34	1.65	1.51
1	F	112	ARG	CZ-NH2	6.34	1.41	1.33
1	I	179	GLU	CD-OE2	6.33	1.32	1.25
1	B	36	TRP	CE3-CZ3	6.32	1.49	1.38
1	E	179	GLU	CG-CD	6.32	1.61	1.51
1	E	140	MSE	SE-CE	-6.31	1.58	1.95
1	D	227	ARG	CG-CD	6.31	1.67	1.51
1	E	60	ARG	CG-CD	6.31	1.67	1.51
1	F	179	GLU	CD-OE2	6.30	1.32	1.25
1	C	96	ARG	CZ-NH2	6.30	1.41	1.33
1	D	81	SER	CB-OG	6.30	1.50	1.42
1	E	232	ARG	CB-CG	6.30	1.69	1.52
1	J	242	TYR	CD1-CE1	6.29	1.48	1.39
1	C	64	PHE	CE2-CZ	6.29	1.49	1.37
1	H	243	GLU	CG-CD	6.29	1.61	1.51
1	E	90	GLU	CD-OE2	6.28	1.32	1.25
1	H	58	ALA	CA-CB	6.28	1.65	1.52
1	B	158	VAL	CB-CG1	-6.28	1.39	1.52
1	F	242	TYR	CE1-CZ	6.28	1.46	1.38
1	B	14	GLU	CB-CG	-6.28	1.40	1.52
1	G	119	GLU	CD-OE2	6.26	1.32	1.25
1	C	228	ARG	CD-NE	6.25	1.57	1.46
1	C	170	ALA	CA-CB	6.25	1.65	1.52
1	J	111	ARG	CZ-NH2	6.24	1.41	1.33
1	E	88	TRP	CG-CD1	6.24	1.45	1.36
1	D	78	SER	CB-OG	6.24	1.50	1.42
1	C	81	SER	CB-OG	6.23	1.50	1.42
1	F	235	GLU	CD-OE2	6.21	1.32	1.25
1	A	86	LYS	CD-CE	6.21	1.66	1.51
1	H	244	GLU	CD-OE1	6.21	1.32	1.25
1	E	197	ARG	CZ-NH1	6.19	1.41	1.33
1	I	131	VAL	CB-CG1	6.19	1.65	1.52
1	E	231	ARG	CZ-NH2	6.19	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	193	GLU	CD-OE1	6.19	1.32	1.25
1	H	111	ARG	CZ-NH2	6.18	1.41	1.33
1	A	47	THR	CB-CG2	-6.18	1.31	1.52
1	I	44	ALA	CA-CB	6.18	1.65	1.52
1	A	158	VAL	CB-CG2	6.17	1.65	1.52
1	D	10	GLU	CB-CG	-6.17	1.40	1.52
1	A	220	ARG	CZ-NH2	6.17	1.41	1.33
1	B	156	ARG	CZ-NH1	6.17	1.41	1.33
1	A	95	VAL	C-O	6.15	1.35	1.23
1	E	61	TYR	CE2-CZ	-6.14	1.30	1.38
1	J	160	ALA	CA-CB	6.14	1.65	1.52
1	A	210	TRP	CB-CG	6.14	1.61	1.50
1	G	242	TYR	CD1-CE1	6.13	1.48	1.39
1	F	55	VAL	CB-CG2	6.13	1.65	1.52
1	E	41	SER	CA-CB	6.13	1.62	1.52
1	G	96	ARG	CB-CG	-6.12	1.36	1.52
1	I	136	VAL	CB-CG2	6.12	1.65	1.52
1	B	224	GLU	CD-OE2	6.11	1.32	1.25
1	E	85	TRP	CZ3-CH2	6.10	1.49	1.40
1	B	179	GLU	CG-CD	6.10	1.61	1.51
1	E	168	LYS	CE-NZ	6.09	1.64	1.49
1	A	35	LYS	CD-CE	6.08	1.66	1.51
1	C	228	ARG	NE-CZ	6.08	1.41	1.33
1	I	54	PHE	CD2-CE2	6.08	1.51	1.39
1	J	57	PHE	CE2-CZ	6.08	1.48	1.37
1	A	85	TRP	CG-CD1	6.07	1.45	1.36
1	I	90	GLU	CD-OE1	6.07	1.32	1.25
1	C	32	SER	CA-CB	6.06	1.62	1.52
1	F	242	TYR	CE2-CZ	6.05	1.46	1.38
1	I	125	VAL	CB-CG1	-6.05	1.40	1.52
1	A	69	VAL	CB-CG1	6.04	1.65	1.52
1	C	242	TYR	CE2-CZ	6.04	1.46	1.38
1	F	193	GLU	CD-OE2	6.04	1.32	1.25
1	B	193	GLU	CD-OE2	6.04	1.32	1.25
1	E	183	GLU	CG-CD	6.03	1.60	1.51
1	J	153	GLU	CB-CG	6.03	1.63	1.52
1	A	214	TRP	CG-CD2	-6.03	1.33	1.43
1	E	169	ARG	CZ-NH2	6.03	1.40	1.33
1	E	193	GLU	CG-CD	6.02	1.60	1.51
1	A	10	GLU	CD-OE1	6.01	1.32	1.25
1	F	12	PHE	CD2-CE2	-6.01	1.27	1.39
1	G	244	GLU	CB-CG	6.00	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	193	GLU	CG-CD	5.99	1.60	1.51
1	A	143	TYR	CB-CG	-5.99	1.42	1.51
1	D	153	GLU	CG-CD	5.99	1.60	1.51
1	E	220	ARG	CZ-NH1	5.99	1.40	1.33
1	A	212	PHE	CD2-CE2	5.99	1.51	1.39
1	F	136	VAL	CB-CG2	5.99	1.65	1.52
1	I	55	VAL	CB-CG1	5.98	1.65	1.52
1	C	78	SER	CB-OG	5.97	1.50	1.42
1	B	202	SER	CB-OG	5.97	1.50	1.42
1	E	179	GLU	CD-OE1	5.96	1.32	1.25
1	F	99	PHE	CD2-CE2	5.96	1.51	1.39
1	E	69	VAL	CB-CG2	5.96	1.65	1.52
1	B	232	ARG	CB-CG	5.96	1.68	1.52
1	F	129	PHE	CD1-CE1	5.96	1.51	1.39
1	G	145	MSE	CB-CG	5.95	1.70	1.52
1	B	224	GLU	CG-CD	5.94	1.60	1.51
1	H	134	ARG	CG-CD	5.94	1.66	1.51
1	H	142	TYR	CE1-CZ	5.94	1.46	1.38
1	F	210	TRP	CE3-CZ3	-5.94	1.28	1.38
1	H	162	LYS	CD-CE	5.94	1.66	1.51
1	F	55	VAL	CB-CG1	5.94	1.65	1.52
1	H	179	GLU	CG-CD	5.94	1.60	1.51
1	C	195	GLN	CB-CG	-5.93	1.36	1.52
1	C	184	GLY	C-O	5.93	1.33	1.23
1	D	119	GLU	CB-CG	-5.93	1.40	1.52
1	B	87	GLU	CG-CD	5.92	1.60	1.51
1	F	15	MSE	CG-SE	5.92	2.15	1.95
1	F	244	GLU	CD-OE1	5.91	1.32	1.25
1	E	136	VAL	CB-CG2	5.91	1.65	1.52
1	D	111	ARG	CZ-NH2	5.90	1.40	1.33
1	J	69	VAL	CB-CG2	5.89	1.65	1.52
1	H	210	TRP	CG-CD1	5.89	1.45	1.36
1	A	66	ARG	CZ-NH2	5.88	1.40	1.33
1	A	138	ARG	CG-CD	5.88	1.66	1.51
1	A	125	VAL	CB-CG2	-5.88	1.40	1.52
1	F	17	VAL	CA-CB	5.88	1.67	1.54
1	B	214	TRP	CG-CD1	5.88	1.45	1.36
1	D	90	GLU	CD-OE2	5.87	1.32	1.25
1	H	46	PHE	CE2-CZ	5.87	1.48	1.37
1	H	38	VAL	CB-CG1	5.87	1.65	1.52
1	C	214	TRP	CG-CD2	-5.87	1.33	1.43
1	D	146	GLU	CG-CD	5.86	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	143	TYR	CG-CD2	5.85	1.46	1.39
1	H	32	SER	CA-CB	5.85	1.61	1.52
1	J	144	PRO	CG-CD	5.85	1.70	1.50
1	C	16	GLU	CG-CD	5.84	1.60	1.51
1	F	129	PHE	CE1-CZ	-5.84	1.26	1.37
1	E	214	TRP	CB-CG	-5.83	1.39	1.50
1	G	170	ALA	CA-CB	5.82	1.64	1.52
1	H	126	ARG	CZ-NH1	5.82	1.40	1.33
1	G	195	GLN	CG-CD	5.82	1.64	1.51
1	J	66	ARG	CZ-NH2	5.82	1.40	1.33
1	D	204	GLN	CB-CG	-5.81	1.36	1.52
1	B	224	GLU	CD-OE1	5.81	1.32	1.25
1	J	179	GLU	CD-OE1	5.81	1.32	1.25
1	F	2	PRO	CA-C	-5.80	1.41	1.52
1	G	37	PHE	CG-CD2	5.80	1.47	1.38
1	B	119	GLU	CD-OE1	5.80	1.32	1.25
1	C	193	GLU	CB-CG	-5.80	1.41	1.52
1	A	37	PHE	CE2-CZ	5.80	1.48	1.37
1	C	214	TRP	CE2-CZ2	-5.80	1.29	1.39
1	D	25	LYS	CE-NZ	5.79	1.63	1.49
1	J	243	GLU	CB-CG	5.79	1.63	1.52
1	I	239	LYS	CE-NZ	5.79	1.63	1.49
1	A	191	THR	CB-CG2	5.79	1.71	1.52
1	E	231	ARG	CG-CD	5.79	1.66	1.51
1	F	233	ALA	CA-CB	5.79	1.64	1.52
1	I	206	ARG	CZ-NH1	5.79	1.40	1.33
1	H	193	GLU	CD-OE2	5.78	1.32	1.25
1	D	44	ALA	CA-CB	5.78	1.64	1.52
1	H	236	LYS	CE-NZ	5.78	1.63	1.49
1	C	235	GLU	CG-CD	5.77	1.60	1.51
1	H	224	GLU	CD-OE2	5.77	1.31	1.25
1	C	162	LYS	CD-CE	5.77	1.65	1.51
1	B	204	GLN	CB-CG	-5.76	1.36	1.52
1	H	209	ASP	CB-CG	5.75	1.63	1.51
1	G	26	LEU	C-O	5.75	1.34	1.23
1	H	143	TYR	CB-CG	-5.75	1.43	1.51
1	B	57	PHE	CE2-CZ	5.75	1.48	1.37
1	B	242	TYR	CD2-CE2	5.75	1.48	1.39
1	J	14	GLU	CG-CD	5.74	1.60	1.51
1	G	158	VAL	CB-CG1	5.74	1.64	1.52
1	C	143	TYR	CE2-CZ	5.73	1.46	1.38
1	C	224	GLU	CD-OE2	5.73	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	119	GLU	N-CA	5.72	1.57	1.46
1	C	239	LYS	CE-NZ	5.72	1.63	1.49
1	J	199	ARG	CB-CG	-5.72	1.37	1.52
1	D	40	PHE	CE1-CZ	5.71	1.48	1.37
1	C	153	GLU	CG-CD	5.71	1.60	1.51
1	H	85	TRP	CZ3-CH2	5.71	1.49	1.40
1	E	129	PHE	CD1-CE1	5.71	1.50	1.39
1	B	96	ARG	CZ-NH1	5.71	1.40	1.33
1	A	220	ARG	CG-CD	5.71	1.66	1.51
1	C	229	TYR	CE2-CZ	5.69	1.46	1.38
1	D	244	GLU	CG-CD	5.69	1.60	1.51
1	G	111	ARG	CZ-NH2	5.69	1.40	1.33
1	E	66	ARG	CZ-NH1	5.68	1.40	1.33
1	A	14	GLU	CD-OE2	5.67	1.31	1.25
1	H	162	LYS	CE-NZ	5.67	1.63	1.49
1	J	104	ASP	CB-CG	-5.67	1.39	1.51
1	A	205	TYR	CG-CD2	5.66	1.46	1.39
1	D	231	ARG	CG-CD	5.65	1.66	1.51
1	I	187	VAL	CB-CG2	5.65	1.64	1.52
1	J	224	GLU	CD-OE2	5.65	1.31	1.25
1	B	34	GLY	C-O	5.65	1.32	1.23
1	A	85	TRP	CD2-CE2	5.64	1.48	1.41
1	A	214	TRP	CZ3-CH2	-5.64	1.31	1.40
1	J	55	VAL	CB-CG1	5.63	1.64	1.52
1	E	23	VAL	CB-CG1	5.63	1.64	1.52
1	G	61	TYR	CG-CD1	-5.63	1.31	1.39
1	E	234	ALA	CA-CB	5.63	1.64	1.52
1	C	44	ALA	CA-CB	5.62	1.64	1.52
1	D	64	PHE	CE1-CZ	5.61	1.48	1.37
1	B	23	VAL	CB-CG1	5.61	1.64	1.52
1	F	226	ALA	CA-CB	5.61	1.64	1.52
1	B	218	ALA	CA-CB	5.60	1.64	1.52
1	F	243	GLU	CD-OE2	5.60	1.31	1.25
1	C	235	GLU	CB-CG	-5.60	1.41	1.52
1	E	225	GLU	CG-CD	5.60	1.60	1.51
1	I	168	LYS	CD-CE	5.60	1.65	1.51
1	B	234	ALA	CA-CB	5.60	1.64	1.52
1	J	162	LYS	CD-CE	5.59	1.65	1.51
1	G	194	ASP	CB-CG	5.59	1.63	1.51
1	H	237	PRO	CB-CG	5.58	1.77	1.50
1	B	129	PHE	CD1-CE1	5.58	1.50	1.39
1	D	242	TYR	CD2-CE2	5.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	242	TYR	CD2-CE2	5.57	1.47	1.39
1	I	140	MSE	SE-CE	-5.56	1.62	1.95
1	D	107	GLY	C-O	5.56	1.32	1.23
1	A	38	VAL	CB-CG1	5.55	1.64	1.52
1	A	236	LYS	CE-NZ	5.55	1.62	1.49
1	A	61	TYR	CD2-CE2	5.55	1.47	1.39
1	C	179	GLU	CG-CD	5.54	1.60	1.51
1	B	62	GLU	CD-OE1	5.54	1.31	1.25
1	I	16	GLU	CG-CD	5.54	1.60	1.51
1	F	187	VAL	CB-CG1	5.54	1.64	1.52
1	C	244	GLU	CD-OE2	5.53	1.31	1.25
1	D	111	ARG	CZ-NH1	5.53	1.40	1.33
1	H	153	GLU	CB-CG	5.53	1.62	1.52
1	C	211	TRP	CE3-CZ3	5.53	1.47	1.38
1	D	47	THR	CB-CG2	-5.53	1.34	1.52
1	C	59	ARG	CZ-NH1	5.53	1.40	1.33
1	D	40	PHE	CE2-CZ	5.53	1.47	1.37
1	H	37	PHE	CE2-CZ	5.52	1.47	1.37
1	G	90	GLU	CD-OE2	5.52	1.31	1.25
1	F	173	ALA	CA-CB	5.52	1.64	1.52
1	D	46	PHE	CE2-CZ	5.52	1.47	1.37
1	E	53	GLU	CD-OE1	5.51	1.31	1.25
1	F	61	TYR	CG-CD2	5.51	1.46	1.39
1	H	146	GLU	CG-CD	5.51	1.60	1.51
1	D	109	VAL	CB-CG2	-5.51	1.41	1.52
1	G	160	ALA	CA-CB	5.51	1.64	1.52
1	A	197	ARG	CG-CD	5.50	1.65	1.51
1	G	146	GLU	CD-OE1	5.50	1.31	1.25
1	J	244	GLU	CD-OE2	5.50	1.31	1.25
1	I	35	LYS	CE-NZ	5.50	1.62	1.49
1	G	197	ARG	CZ-NH1	5.49	1.40	1.33
1	A	226	ALA	CA-CB	5.49	1.64	1.52
1	J	99	PHE	CE2-CZ	5.49	1.47	1.37
1	E	214	TRP	CE2-CZ2	-5.49	1.30	1.39
1	F	222	ASP	C-O	-5.49	1.12	1.23
1	A	159	LYS	CG-CD	-5.49	1.33	1.52
1	B	193	GLU	CG-CD	5.49	1.60	1.51
1	B	159	LYS	CG-CD	-5.48	1.33	1.52
1	F	70	ASP	CG-OD1	5.48	1.38	1.25
1	H	131	VAL	CB-CG1	5.48	1.64	1.52
1	H	235	GLU	CB-CG	-5.48	1.41	1.52
1	G	134	ARG	CZ-NH1	5.47	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	172	PRO	CG-CD	5.47	1.68	1.50
1	C	109	VAL	CB-CG1	-5.46	1.41	1.52
1	A	59	ARG	CG-CD	-5.46	1.38	1.51
1	J	199	ARG	CZ-NH2	5.46	1.40	1.33
1	A	244	GLU	CD-OE2	5.46	1.31	1.25
1	E	54	PHE	CB-CG	-5.45	1.42	1.51
1	E	227	ARG	CB-CG	-5.45	1.37	1.52
1	I	243	GLU	CB-CG	5.45	1.62	1.52
1	E	227	ARG	CG-CD	5.44	1.65	1.51
1	B	66	ARG	CZ-NH2	5.44	1.40	1.33
1	B	174	ASP	CB-CG	5.44	1.63	1.51
1	G	214	TRP	CG-CD1	5.44	1.44	1.36
1	B	66	ARG	NE-CZ	5.44	1.40	1.33
1	B	239	LYS	CE-NZ	5.44	1.62	1.49
1	B	183	GLU	CD-OE2	5.43	1.31	1.25
1	G	121	ALA	CA-CB	5.43	1.63	1.52
1	J	168	LYS	CE-NZ	5.43	1.62	1.49
1	B	175	TRP	CG-CD1	5.42	1.44	1.36
1	I	233	ALA	CA-CB	5.42	1.63	1.52
1	E	84	LYS	CE-NZ	5.41	1.62	1.49
1	F	179	GLU	CB-CG	5.40	1.62	1.52
1	E	37	PHE	CD2-CE2	5.40	1.50	1.39
1	J	193	GLU	CD-OE2	5.40	1.31	1.25
1	J	30	TYR	CE1-CZ	-5.39	1.31	1.38
1	I	121	ALA	CA-CB	5.39	1.63	1.52
1	A	55	VAL	CB-CG1	5.38	1.64	1.52
1	J	55	VAL	CB-CG2	5.38	1.64	1.52
1	D	238	ALA	CA-CB	5.38	1.63	1.52
1	H	128	VAL	CB-CG1	5.38	1.64	1.52
1	G	124	THR	CB-CG2	-5.38	1.34	1.52
1	G	16	GLU	CD-OE1	5.38	1.31	1.25
1	B	44	ALA	CA-CB	5.37	1.63	1.52
1	B	50	CYS	N-CA	5.37	1.57	1.46
1	C	236	LYS	CD-CE	5.37	1.64	1.51
1	E	131	VAL	CB-CG2	5.36	1.64	1.52
1	I	197	ARG	CZ-NH1	5.36	1.40	1.33
1	F	165	ASP	CB-CG	5.36	1.63	1.51
1	B	115	LEU	CG-CD2	5.36	1.71	1.51
1	F	145	MSE	CB-CG	5.35	1.68	1.52
1	I	242	TYR	CG-CD2	5.35	1.46	1.39
1	C	196	ALA	CA-CB	5.34	1.63	1.52
1	B	243	GLU	CB-CG	5.34	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	GLU	CD-OE1	5.34	1.31	1.25
1	E	10	GLU	CD-OE1	5.33	1.31	1.25
1	I	122	THR	C-O	5.33	1.33	1.23
1	J	188	PRO	N-CA	5.33	1.56	1.47
1	C	30	TYR	CD1-CE1	5.33	1.47	1.39
1	H	62	GLU	CG-CD	5.32	1.59	1.51
1	E	205	TYR	CD1-CE1	-5.32	1.31	1.39
1	A	111	ARG	CD-NE	5.32	1.55	1.46
1	E	58	ALA	CA-CB	5.32	1.63	1.52
1	C	225	GLU	CD-OE2	5.32	1.31	1.25
1	E	201	GLU	CD-OE1	5.32	1.31	1.25
1	F	140	MSE	CG-SE	5.32	2.13	1.95
1	G	202	SER	CB-OG	5.32	1.49	1.42
1	H	205	TYR	CB-CG	-5.30	1.43	1.51
1	G	149	ARG	CZ-NH2	5.30	1.40	1.33
1	I	79	VAL	CB-CG2	5.30	1.64	1.52
1	A	214	TRP	CB-CG	-5.30	1.40	1.50
1	I	57	PHE	CE2-CZ	5.30	1.47	1.37
1	H	228	ARG	CB-CG	-5.29	1.38	1.52
1	A	119	GLU	CG-CD	5.29	1.59	1.51
1	C	108	THR	CB-CG2	-5.29	1.34	1.52
1	E	134	ARG	CB-CG	5.29	1.66	1.52
1	B	145	MSE	CG-SE	-5.28	1.77	1.95
1	B	162	LYS	CG-CD	5.28	1.70	1.52
1	E	62	GLU	CD-OE1	5.28	1.31	1.25
1	H	119	GLU	CG-CD	5.28	1.59	1.51
1	H	153	GLU	CG-CD	5.28	1.59	1.51
1	C	95	VAL	CB-CG2	5.28	1.64	1.52
1	C	96	ARG	NE-CZ	5.28	1.40	1.33
1	E	177	ASN	N-CA	5.28	1.56	1.46
1	F	23	VAL	CA-CB	5.27	1.65	1.54
1	I	85	TRP	CZ3-CH2	5.27	1.48	1.40
1	F	201	GLU	CD-OE2	5.27	1.31	1.25
1	G	36	TRP	CE3-CZ3	5.27	1.47	1.38
1	I	242	TYR	CG-CD1	5.26	1.46	1.39
1	J	76	VAL	CB-CG1	5.26	1.64	1.52
1	H	119	GLU	CD-OE1	5.26	1.31	1.25
1	D	206	ARG	CZ-NH1	5.26	1.39	1.33
1	A	139	THR	CB-CG2	5.25	1.69	1.52
1	F	46	PHE	CE2-CZ	5.25	1.47	1.37
1	C	25	LYS	CD-CE	5.25	1.64	1.51
1	B	244	GLU	CB-CG	5.24	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	146	GLU	CD-OE1	5.24	1.31	1.25
1	A	170	ALA	CA-CB	5.24	1.63	1.52
1	E	85	TRP	CE3-CZ3	5.24	1.47	1.38
1	D	143	TYR	CE2-CZ	5.24	1.45	1.38
1	D	153	GLU	CB-CG	5.23	1.62	1.52
1	G	218	ALA	CA-CB	5.23	1.63	1.52
1	I	65	GLN	CG-CD	5.23	1.63	1.51
1	E	174	ASP	CB-CG	5.23	1.62	1.51
1	D	179	GLU	CD-OE1	5.23	1.31	1.25
1	D	201	GLU	CG-CD	5.22	1.59	1.51
1	D	55	VAL	C-O	5.22	1.33	1.23
1	E	194	ASP	CB-CG	-5.21	1.40	1.51
1	D	70	ASP	CG-OD1	5.21	1.37	1.25
1	I	99	PHE	CE1-CZ	5.21	1.47	1.37
1	E	138	ARG	CZ-NH2	5.21	1.39	1.33
1	B	244	GLU	CD-OE1	5.20	1.31	1.25
1	C	245	ALA	C-O	5.20	1.33	1.23
1	C	140	MSE	CG-SE	5.20	2.13	1.95
1	D	200	MSE	CG-SE	5.20	2.13	1.95
1	D	14	GLU	CD-OE1	5.19	1.31	1.25
1	A	197	ARG	CD-NE	5.18	1.55	1.46
1	E	65	GLN	CD-OE1	5.18	1.35	1.24
1	H	78	SER	CB-OG	5.18	1.49	1.42
1	H	168	LYS	CB-CG	5.18	1.66	1.52
1	C	18	THR	CA-CB	5.18	1.66	1.53
1	F	218	ALA	CA-CB	5.18	1.63	1.52
1	B	236	LYS	CD-CE	5.18	1.64	1.51
1	G	134	ARG	CZ-NH2	5.17	1.39	1.33
1	E	96	ARG	CZ-NH1	5.17	1.39	1.33
1	F	6	PRO	CA-C	5.17	1.63	1.52
1	E	64	PHE	CE1-CZ	5.17	1.47	1.37
1	F	146	GLU	CD-OE2	5.17	1.31	1.25
1	E	238	ALA	CA-CB	5.17	1.63	1.52
1	C	166	SER	CB-OG	-5.16	1.35	1.42
1	J	61	TYR	CZ-OH	5.16	1.46	1.37
1	D	219	SER	CA-CB	-5.16	1.45	1.52
1	I	244	GLU	CD-OE2	5.16	1.31	1.25
1	E	200	MSE	CG-SE	5.16	2.12	1.95
1	A	119	GLU	CD-OE1	5.16	1.31	1.25
1	E	182	GLY	C-O	5.15	1.31	1.23
1	B	214	TRP	CD2-CE2	-5.15	1.35	1.41
1	F	60	ARG	CG-CD	5.14	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	118	ALA	CA-CB	5.14	1.63	1.52
1	I	10	GLU	CG-CD	5.14	1.59	1.51
1	I	168	LYS	CE-NZ	5.14	1.61	1.49
1	D	8	ILE	CB-CG1	5.14	1.68	1.54
1	F	236	LYS	CE-NZ	5.13	1.61	1.49
1	H	159	LYS	CG-CD	-5.13	1.34	1.52
1	J	190	PRO	CA-C	5.13	1.63	1.52
1	J	2	PRO	CA-C	-5.13	1.42	1.52
1	C	50	CYS	N-CA	5.13	1.56	1.46
1	G	65	GLN	N-CA	5.12	1.56	1.46
1	J	199	ARG	CG-CD	5.12	1.64	1.51
1	B	235	GLU	CD-OE1	5.12	1.31	1.25
1	A	89	ILE	CA-CB	5.11	1.66	1.54
1	E	158	VAL	CB-CG1	-5.11	1.42	1.52
1	G	96	ARG	CZ-NH1	5.11	1.39	1.33
1	D	35	LYS	CE-NZ	5.11	1.61	1.49
1	I	143	TYR	CG-CD2	5.11	1.45	1.39
1	C	205	TYR	CE1-CZ	5.11	1.45	1.38
1	J	96	ARG	CZ-NH1	5.11	1.39	1.33
1	C	142	TYR	CG-CD1	-5.11	1.32	1.39
1	A	220	ARG	CZ-NH1	5.10	1.39	1.33
1	C	199	ARG	CG-CD	-5.10	1.39	1.51
1	C	66	ARG	CG-CD	5.10	1.64	1.51
1	G	231	ARG	CZ-NH2	5.10	1.39	1.33
1	E	242	TYR	CE2-CZ	5.09	1.45	1.38
1	I	11	ARG	CZ-NH1	5.09	1.39	1.33
1	D	239	LYS	CD-CE	5.09	1.64	1.51
1	H	63	ASP	C-O	5.09	1.33	1.23
1	I	130	ILE	CB-CG2	5.09	1.68	1.52
1	I	143	TYR	CE1-CZ	5.09	1.45	1.38
1	E	95	VAL	CB-CG1	5.08	1.63	1.52
1	H	93	ILE	CA-CB	5.08	1.66	1.54
1	E	159	LYS	CG-CD	-5.08	1.35	1.52
1	H	170	ALA	CA-CB	5.08	1.63	1.52
1	G	87	GLU	CG-CD	5.08	1.59	1.51
1	D	242	TYR	CE1-CZ	5.08	1.45	1.38
1	B	197	ARG	CZ-NH1	5.07	1.39	1.33
1	F	99	PHE	CE2-CZ	5.07	1.47	1.37
1	I	11	ARG	CZ-NH2	5.07	1.39	1.33
1	E	41	SER	CB-OG	5.07	1.48	1.42
1	G	179	GLU	CD-OE1	5.07	1.31	1.25
1	C	129	PHE	CD1-CE1	5.06	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	15	MSE	CG-SE	5.06	2.12	1.95
1	H	6	PRO	CA-C	5.06	1.62	1.52
1	I	49	VAL	CB-CG2	5.06	1.63	1.52
1	F	244	GLU	CD-OE2	5.06	1.31	1.25
1	G	224	GLU	CD-OE2	5.05	1.31	1.25
1	I	15	MSE	CG-SE	5.05	2.12	1.95
1	D	195	GLN	CG-CD	5.05	1.62	1.51
1	E	8	ILE	C-O	5.05	1.32	1.23
1	I	242	TYR	CE2-CZ	5.05	1.45	1.38
1	B	79	VAL	CA-CB	5.05	1.65	1.54
1	C	112	ARG	NE-CZ	5.05	1.39	1.33
1	H	86	LYS	CE-NZ	5.05	1.61	1.49
1	H	99	PHE	CG-CD2	-5.04	1.31	1.38
1	H	143	TYR	CD1-CE1	5.04	1.47	1.39
1	I	192	THR	C-O	5.04	1.32	1.23
1	B	228	ARG	NE-CZ	5.04	1.39	1.33
1	B	142	TYR	CE1-CZ	5.03	1.45	1.38
1	A	220	ARG	NE-CZ	5.03	1.39	1.33
1	I	204	GLN	CG-CD	5.03	1.62	1.51
1	B	112	ARG	CZ-NH1	5.03	1.39	1.33
1	J	45	ASP	CB-CG	5.02	1.62	1.51
1	B	51	THR	C-O	5.02	1.32	1.23
1	A	146	GLU	CD-OE1	5.02	1.31	1.25
1	A	53	GLU	CD-OE1	5.02	1.31	1.25
1	B	153	GLU	CD-OE2	5.02	1.31	1.25
1	E	239	LYS	CA-C	5.02	1.66	1.52
1	I	80	PHE	CD2-CE2	5.01	1.49	1.39
1	B	112	ARG	CB-CG	5.01	1.66	1.52
1	G	80	PHE	CE1-CZ	5.01	1.46	1.37
1	B	74	LEU	N-CA	-5.01	1.36	1.46
1	B	99	PHE	CD1-CE1	-5.01	1.29	1.39
1	A	175	TRP	CA-C	5.01	1.66	1.52
1	I	205	TYR	CD2-CE2	-5.00	1.31	1.39
1	F	201	GLU	CD-OE1	5.00	1.31	1.25
1	I	10	GLU	CB-CG	-5.00	1.42	1.52

All (472) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	138	ARG	NE-CZ-NH2	-36.48	102.06	120.30
1	J	138	ARG	NE-CZ-NH1	34.23	137.42	120.30
1	B	104	ASP	CB-CG-OD2	-32.90	88.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	26	LEU	C-N-CD	-31.81	50.61	120.60
1	J	26	LEU	C-N-CD	-28.89	57.03	120.60
1	E	175	TRP	C-N-CD	-25.98	63.43	120.60
1	E	104	ASP	CB-CG-OD2	-24.00	96.70	118.30
1	J	104	ASP	CB-CG-OD2	-21.82	98.67	118.30
1	F	104	ASP	CB-CG-OD2	-21.61	98.85	118.30
1	B	104	ASP	CB-CG-OD1	17.91	134.42	118.30
1	J	215	ASP	CB-CG-OD1	-17.77	102.31	118.30
1	A	228	ARG	NE-CZ-NH2	-17.48	111.56	120.30
1	J	215	ASP	CB-CG-OD2	17.23	133.80	118.30
1	J	174	ASP	CB-CG-OD2	-16.32	103.61	118.30
1	E	104	ASP	CB-CG-OD1	16.23	132.91	118.30
1	F	231	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	D	138	ARG	NE-CZ-NH1	-14.95	112.83	120.30
1	J	27	PRO	CA-N-CD	-14.84	90.72	111.50
1	I	228	ARG	NE-CZ-NH1	14.49	127.55	120.30
1	F	227	ARG	NE-CZ-NH2	-14.32	113.14	120.30
1	J	27	PRO	N-CA-C	-14.23	75.10	112.10
1	J	104	ASP	CB-CG-OD1	13.19	130.17	118.30
1	H	112	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	D	67	LEU	C-N-CA	-13.01	94.97	122.30
1	F	66	ARG	NE-CZ-NH1	12.42	126.51	120.30
1	I	228	ARG	NE-CZ-NH2	-12.32	114.14	120.30
1	H	227	ARG	NE-CZ-NH1	-12.30	114.15	120.30
1	G	215	ASP	CB-CG-OD1	12.28	129.35	118.30
1	C	11	ARG	NE-CZ-NH2	-12.01	114.29	120.30
1	B	67	LEU	C-N-CA	-11.97	97.17	122.30
1	F	112	ARG	NE-CZ-NH2	11.89	126.24	120.30
1	J	138	ARG	CD-NE-CZ	11.69	139.97	123.60
1	J	28	ASP	CB-CG-OD2	-11.66	107.81	118.30
1	F	104	ASP	CB-CG-OD1	11.63	128.77	118.30
1	B	112	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	E	70	ASP	CB-CG-OD2	-11.36	108.07	118.30
1	B	199	ARG	CG-CD-NE	-11.34	87.99	111.80
1	E	228	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	F	59	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	I	231	ARG	NE-CZ-NH2	-10.97	114.81	120.30
1	C	17	VAL	CG1-CB-CG2	10.94	128.40	110.90
1	J	59	ARG	NE-CZ-NH1	-10.73	114.93	120.30
1	B	227	ARG	NE-CZ-NH1	-10.73	114.94	120.30
1	E	176	PRO	N-CA-C	-10.69	84.30	112.10
1	C	59	ARG	NE-CZ-NH2	-10.67	114.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	28	ASP	CB-CG-OD1	10.64	127.88	118.30
1	A	70	ASP	CB-CG-OD2	-10.50	108.85	118.30
1	F	227	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	C	60	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	C	206	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	G	27	PRO	CA-N-CD	-10.31	97.07	111.50
1	B	138	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	I	138	ARG	NE-CZ-NH2	10.24	125.42	120.30
1	E	138	ARG	NE-CZ-NH1	-10.11	115.25	120.30
1	F	149	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	B	96	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	G	199	ARG	NE-CZ-NH1	-9.67	115.47	120.30
1	D	239	LYS	CD-CE-NZ	9.66	133.93	111.70
1	J	158	VAL	CG1-CB-CG2	-9.62	95.50	110.90
1	C	60	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	E	227	ARG	CG-CD-NE	-9.49	91.88	111.80
1	J	199	ARG	CG-CD-NE	-9.33	92.20	111.80
1	A	231	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	C	199	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	I	126	ARG	NE-CZ-NH2	-9.21	115.70	120.30
1	A	163	LEU	CB-CG-CD1	-9.20	95.36	111.00
1	J	96	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	I	232	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	J	27	PRO	N-CA-CB	9.11	114.23	103.30
1	G	112	ARG	CG-CD-NE	-9.07	92.75	111.80
1	J	11	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	H	149	ARG	NE-CZ-NH1	-9.05	115.78	120.30
1	I	28	ASP	CB-CG-OD2	-9.04	110.17	118.30
1	J	91	ARG	NE-CZ-NH1	-9.01	115.79	120.30
1	D	163	LEU	CB-CG-CD1	-9.00	95.70	111.00
1	C	32	SER	CA-CB-OG	-8.96	87.00	111.20
1	C	232	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	D	67	LEU	O-C-N	-8.87	108.13	123.20
1	J	175	TRP	C-N-CD	-8.84	101.16	120.60
1	H	126	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	116	LEU	CB-CG-CD1	-8.77	96.09	111.00
1	J	96	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	E	138	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	G	231	ARG	NE-CZ-NH1	-8.65	115.97	120.30
1	J	104	ASP	N-CA-CB	8.60	126.08	110.60
1	I	183	GLU	CG-CD-OE2	8.58	135.45	118.30
1	F	215	ASP	CB-CG-OD2	8.55	125.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	ARG	NE-CZ-NH1	-8.54	116.03	120.30
1	E	175	TRP	O-C-N	8.49	137.23	121.10
1	H	112	ARG	CG-CD-NE	-8.48	93.98	111.80
1	J	60	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	145	MSE	CA-CB-CG	-8.39	99.03	113.30
1	B	159	LYS	CD-CE-NZ	8.36	130.92	111.70
1	H	60	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	67	LEU	O-C-N	-8.32	109.06	123.20
1	E	175	TRP	C-N-CA	8.30	156.87	122.00
1	H	60	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	C	112	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	F	111	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	I	215	ASP	CB-CG-OD2	8.23	125.71	118.30
1	E	119	GLU	OE1-CD-OE2	8.21	133.15	123.30
1	J	63	ASP	CB-CG-OD2	8.19	125.67	118.30
1	A	145	MSE	CB-CG-SE	-8.19	88.12	112.70
1	E	131	VAL	CG1-CB-CG2	-8.14	97.87	110.90
1	J	145	MSE	CG-SE-CE	-8.13	81.02	98.90
1	A	125	VAL	CG1-CB-CG2	8.12	123.89	110.90
1	J	138	ARG	CG-CD-NE	-8.12	94.75	111.80
1	G	159	LYS	CD-CE-NZ	8.10	130.33	111.70
1	D	126	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	H	145	MSE	CA-CB-CG	-8.09	99.55	113.30
1	B	149	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	I	128	VAL	CG1-CB-CG2	8.01	123.71	110.90
1	J	60	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	199	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	C	199	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	G	26	LEU	O-C-N	7.96	136.22	121.10
1	H	227	ARG	NE-CZ-NH2	7.95	124.27	120.30
1	G	27	PRO	N-CA-CB	7.93	112.82	103.30
1	I	199	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	E	175	TRP	N-CA-C	7.89	132.31	111.00
1	I	138	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	B	175	TRP	C-N-CD	-7.82	103.40	120.60
1	E	197	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	G	222	ASP	CB-CG-OD2	7.82	125.33	118.30
1	B	112	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	E	111	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	F	112	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	228	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	J	243	GLU	OE1-CD-OE2	-7.68	114.09	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ASP	CB-CG-OD1	7.66	125.19	118.30
1	G	156	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	I	145	MSE	CB-CG-SE	-7.64	89.77	112.70
1	A	112	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	C	199	ARG	CA-CB-CG	7.63	130.19	113.40
1	B	199	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	156	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	E	176	PRO	CA-N-CD	-7.56	100.91	111.50
1	E	111	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	I	116	LEU	CB-CG-CD1	-7.55	98.17	111.00
1	B	140	MSE	CA-CB-CG	-7.54	100.48	113.30
1	H	126	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	215	ASP	CB-CG-OD1	7.53	125.07	118.30
1	G	124	THR	N-CA-CB	-7.48	96.09	110.30
1	F	140	MSE	CG-SE-CE	-7.47	82.47	98.90
1	J	174	ASP	N-CA-C	7.45	131.12	111.00
1	E	227	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	F	158	VAL	CG1-CB-CG2	-7.41	99.05	110.90
1	B	221	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	E	25	LYS	CD-CE-NZ	-7.36	94.78	111.70
1	F	231	ARG	CG-CD-NE	-7.36	96.35	111.80
1	B	28	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	C	74	LEU	CD1-CG-CD2	-7.35	88.46	110.50
1	D	231	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	J	28	ASP	CB-CG-OD1	7.33	124.89	118.30
1	E	59	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	J	26	LEU	O-C-N	7.29	134.95	121.10
1	B	179	GLU	CA-CB-CG	-7.28	97.38	113.40
1	I	193	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	C	59	ARG	NH1-CZ-NH2	7.27	127.40	119.40
1	C	134	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	F	220	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	G	112	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	169	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	66	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	B	104	ASP	OD1-CG-OD2	7.15	136.89	123.30
1	I	231	ARG	CG-CD-NE	-7.15	96.79	111.80
1	B	231	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	I	70	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	F	231	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	28	ASP	CB-CG-OD1	7.02	124.62	118.30
1	D	126	ARG	NE-CZ-NH1	7.01	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	199	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	F	145	MSE	CA-CB-CG	-6.99	101.41	113.30
1	I	84	LYS	CD-CE-NZ	-6.97	95.68	111.70
1	I	2	PRO	N-CA-CB	6.96	111.65	103.30
1	J	26	LEU	CB-CA-C	-6.95	96.99	110.20
1	J	174	ASP	OD1-CG-OD2	6.95	136.50	123.30
1	D	183	GLU	CG-CD-OE1	-6.91	104.48	118.30
1	J	27	PRO	N-CD-CG	6.90	113.56	103.20
1	J	26	LEU	CA-C-N	-6.90	97.79	117.10
1	B	145	MSE	CA-CB-CG	-6.89	101.58	113.30
1	D	105	PRO	O-C-N	-6.88	111.69	122.70
1	D	199	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	E	222	ASP	CB-CG-OD1	6.86	124.47	118.30
1	D	231	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	I	59	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	C	215	ASP	CB-CG-OD2	6.74	124.36	118.30
1	J	152	ASP	CB-CG-OD2	6.72	124.35	118.30
1	F	66	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	59	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	J	231	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	C	5	ILE	CG1-CB-CG2	6.64	126.00	111.40
1	A	183	GLU	CG-CD-OE2	6.63	131.56	118.30
1	C	17	VAL	N-CA-CB	-6.63	96.92	111.50
1	H	10	GLU	OE1-CD-OE2	-6.62	115.35	123.30
1	J	141	LEU	CB-CG-CD2	-6.62	99.75	111.00
1	H	6	PRO	N-CA-C	-6.61	94.90	112.10
1	J	145	MSE	CB-CG-SE	-6.60	92.91	112.70
1	H	228	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	59	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	227	ARG	NH1-CZ-NH2	6.56	126.61	119.40
1	C	112	ARG	CG-CD-NE	6.55	125.56	111.80
1	G	17	VAL	CG1-CB-CG2	6.55	121.38	110.90
1	A	96	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	111	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	E	26	LEU	CB-CG-CD2	-6.54	99.89	111.00
1	G	124	THR	OG1-CB-CG2	6.53	125.03	110.00
1	E	191	THR	N-CA-CB	-6.52	97.90	110.30
1	I	156	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	H	11	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	D	111	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	A	70	ASP	CB-CG-OD1	6.48	124.13	118.30
1	C	126	ARG	NE-CZ-NH1	6.47	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	104	ASP	N-CA-CB	6.45	122.20	110.60
1	E	228	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	I	35	LYS	CD-CE-NZ	-6.43	96.91	111.70
1	B	243	GLU	OE1-CD-OE2	-6.40	115.61	123.30
1	C	149	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	E	105	PRO	N-CA-C	-6.39	95.48	112.10
1	G	26	LEU	CA-C-N	-6.36	99.29	117.10
1	C	199	ARG	CG-CD-NE	-6.35	98.46	111.80
1	A	183	GLU	CG-CD-OE1	-6.34	105.62	118.30
1	I	206	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	241	LEU	CB-CG-CD2	-6.33	100.24	111.00
1	J	145	MSE	CA-CB-CG	-6.33	102.54	113.30
1	E	238	ALA	O-C-N	-6.32	112.59	122.70
1	J	236	LYS	CD-CE-NZ	-6.32	97.18	111.70
1	G	115	LEU	CB-CG-CD1	-6.31	100.27	111.00
1	G	109	VAL	CG1-CB-CG2	-6.31	100.81	110.90
1	C	221	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	C	140	MSE	CA-CB-CG	-6.29	102.62	113.30
1	B	59	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	D	122	THR	OG1-CB-CG2	-6.25	95.62	110.00
1	C	199	ARG	CB-CG-CD	6.24	127.83	111.60
1	A	215	ASP	CB-CG-OD1	6.23	123.91	118.30
1	I	104	ASP	CB-CG-OD1	6.22	123.90	118.30
1	F	159	LYS	CD-CE-NZ	6.21	125.97	111.70
1	E	231	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	A	118	ALA	O-C-N	-6.20	112.77	122.70
1	D	197	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	J	61	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	E	191	THR	OG1-CB-CG2	6.17	124.20	110.00
1	D	59	ARG	CD-NE-CZ	-6.15	114.98	123.60
1	C	126	ARG	CG-CD-NE	-6.15	98.89	111.80
1	F	74	LEU	CA-CB-CG	6.15	129.44	115.30
1	E	24	ILE	CB-CG1-CD1	-6.15	96.69	113.90
1	J	134	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	J	131	VAL	CG1-CB-CG2	-6.11	101.12	110.90
1	B	239	LYS	CD-CE-NZ	-6.09	97.68	111.70
1	B	46	PHE	CZ-CE2-CD2	-6.09	112.79	120.10
1	I	6	PRO	N-CA-C	-6.08	96.28	112.10
1	J	169	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	E	175	TRP	CB-CA-C	-6.05	98.29	110.40
1	I	145	MSE	CA-CB-CG	-6.05	103.01	113.30
1	J	231	ARG	CG-CD-NE	-6.05	99.10	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	140	MSE	CA-CB-CG	-6.04	103.02	113.30
1	E	145	MSE	CB-CG-SE	-6.04	94.58	112.70
1	J	116	LEU	CA-CB-CG	-6.04	101.42	115.30
1	B	91	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	74	LEU	CA-CB-CG	6.03	129.16	115.30
1	E	134	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	59	ARG	NH1-CZ-NH2	6.02	126.02	119.40
1	F	199	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	A	201	GLU	C-N-CA	-6.00	106.71	121.70
1	H	47	THR	N-CA-C	-6.00	94.81	111.00
1	E	158	VAL	CG1-CB-CG2	-5.97	101.34	110.90
1	C	105	PRO	C-N-CA	-5.97	106.78	121.70
1	D	138	ARG	NH1-CZ-NH2	5.96	125.96	119.40
1	J	122	THR	OG1-CB-CG2	-5.95	96.33	110.00
1	B	136	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	C	228	ARG	CD-NE-CZ	5.93	131.91	123.60
1	G	145	MSE	CB-CG-SE	-5.92	94.93	112.70
1	F	39	LEU	CD1-CG-CD2	-5.92	92.75	110.50
1	I	183	GLU	CG-CD-OE1	-5.91	106.48	118.30
1	I	140	MSE	CG-SE-CE	-5.91	85.90	98.90
1	H	112	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	E	206	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	11	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	J	174	ASP	CA-C-N	-5.87	104.29	117.20
1	H	215	ASP	CB-CG-OD2	5.86	123.58	118.30
1	D	67	LEU	CA-C-N	5.85	127.91	116.20
1	D	141	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	D	156	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	E	204	GLN	CA-CB-CG	5.84	126.24	113.40
1	E	175	TRP	CA-C-O	-5.83	107.85	120.10
1	C	59	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	F	84	LYS	CD-CE-NZ	-5.83	98.30	111.70
1	F	167	LEU	CA-CB-CG	5.82	128.70	115.30
1	I	134	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	G	28	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	140	MSE	CG-SE-CE	-5.82	86.10	98.90
1	B	209	ASP	CB-CG-OD2	5.81	123.53	118.30
1	F	209	ASP	CB-CG-OD2	5.81	123.53	118.30
1	F	207	SER	N-CA-CB	-5.79	101.81	110.50
1	D	116	LEU	CA-CB-CG	-5.77	102.02	115.30
1	I	159	LYS	CD-CE-NZ	5.77	124.97	111.70
1	F	70	ASP	CB-CG-OD2	-5.75	113.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	ALA	N-CA-C	-5.75	95.49	111.00
1	J	165	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	4	SER	N-CA-CB	-5.73	101.90	110.50
1	B	126	ARG	CG-CD-NE	-5.73	99.77	111.80
1	E	222	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	E	35	LYS	CD-CE-NZ	5.73	124.87	111.70
1	D	227	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	194	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	J	81	SER	CA-CB-OG	-5.72	95.76	111.20
1	F	194	ASP	CB-CG-OD1	5.72	123.45	118.30
1	J	156	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	G	86	LYS	CB-CG-CD	5.71	126.43	111.60
1	F	161	LEU	CD1-CG-CD2	5.69	127.58	110.50
1	C	119	GLU	OE1-CD-OE2	5.69	130.12	123.30
1	E	45	ASP	CB-CG-OD1	5.68	123.41	118.30
1	I	194	ASP	CB-CG-OD1	5.68	123.42	118.30
1	J	231	ARG	CD-NE-CZ	5.68	131.55	123.60
1	J	229	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	B	74	LEU	CA-CB-CG	5.67	128.34	115.30
1	G	197	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	228	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	D	91	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	I	118	ALA	O-C-N	-5.67	113.63	122.70
1	H	116	LEU	CA-CB-CG	-5.64	102.32	115.30
1	C	228	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	39	LEU	CD1-CG-CD2	-5.63	93.61	110.50
1	D	147	LEU	CA-CB-CG	5.63	128.24	115.30
1	F	197	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	G	16	GLU	N-CA-C	-5.61	95.85	111.00
1	G	169	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	F	35	LYS	CD-CE-NZ	-5.60	98.82	111.70
1	F	185	LEU	CA-CB-CG	-5.60	102.42	115.30
1	J	167	LEU	CB-CG-CD2	5.60	120.52	111.00
1	H	194	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	D	195	GLN	CA-CB-CG	5.59	125.69	113.40
1	J	2	PRO	CA-CB-CG	-5.59	93.39	104.00
1	J	105	PRO	N-CA-C	-5.59	97.57	112.10
1	A	206	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	32	SER	CA-CB-OG	-5.58	96.13	111.20
1	G	140	MSE	CA-CB-CG	-5.58	103.82	113.30
1	E	238	ALA	C-N-CA	-5.57	107.77	121.70
1	G	24	ILE	CB-CG1-CD1	-5.57	98.30	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	LYS	CD-CE-NZ	-5.57	98.90	111.70
1	C	222	ASP	CB-CG-OD2	5.56	123.31	118.30
1	H	150	LEU	N-CA-C	-5.55	96.01	111.00
1	E	134	ARG	CG-CD-NE	-5.55	100.15	111.80
1	J	93	ILE	CG1-CB-CG2	-5.54	99.20	111.40
1	A	28	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	H	46	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	C	122	THR	OG1-CB-CG2	-5.52	97.30	110.00
1	I	149	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	G	238	ALA	N-CA-C	-5.51	96.11	111.00
1	F	126	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	213	CYS	CA-CB-SG	-5.50	104.10	114.00
1	J	134	ARG	CG-CD-NE	-5.50	100.26	111.80
1	F	102	ILE	CG1-CB-CG2	5.49	123.48	111.40
1	F	6	PRO	N-CA-C	-5.48	97.85	112.10
1	D	36	TRP	CB-CA-C	-5.48	99.44	110.40
1	I	206	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	J	63	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	D	174	ASP	CB-CG-OD2	5.47	123.22	118.30
1	J	10	GLU	CB-CA-C	-5.47	99.46	110.40
1	H	147	LEU	CA-CB-CG	5.47	127.87	115.30
1	B	15	MSE	CA-CB-CG	-5.46	104.01	113.30
1	F	28	ASP	CB-CG-OD1	5.46	123.22	118.30
1	C	156	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	91	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	227	ARG	CG-CD-NE	-5.43	100.39	111.80
1	B	207	SER	CA-CB-OG	-5.43	96.53	111.20
1	E	145	MSE	CG-SE-CE	5.43	110.84	98.90
1	B	96	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	150	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	C	236	LYS	CD-CE-NZ	-5.41	99.25	111.70
1	F	66	ARG	CD-NE-CZ	5.41	131.17	123.60
1	F	69	VAL	CA-CB-CG2	-5.41	102.79	110.90
1	J	241	LEU	CB-CG-CD2	-5.40	101.81	111.00
1	E	245	ALA	CA-C-O	-5.40	108.75	120.10
1	C	206	ARG	CG-CD-NE	-5.39	100.47	111.80
1	A	145	MSE	CB-CA-C	5.38	121.16	110.40
1	J	175	TRP	C-N-CA	5.37	144.56	122.00
1	J	20	ASP	CB-CG-OD1	5.37	123.13	118.30
1	J	111	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	C	220	ARG	CG-CD-NE	-5.37	100.53	111.80
1	B	11	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	I	206	ARG	NH1-CZ-NH2	5.36	125.30	119.40
1	C	11	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	J	227	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	H	149	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	E	57	PHE	CB-CG-CD2	-5.35	117.05	120.80
1	E	165	ASP	CB-CG-OD1	5.35	123.11	118.30
1	J	106	GLN	CA-CB-CG	5.35	125.17	113.40
1	B	168	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	C	158	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	E	223	VAL	CG1-CB-CG2	5.34	119.44	110.90
1	A	221	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	140	MSE	CG-SE-CE	5.33	110.62	98.90
1	F	140	MSE	CA-CB-CG	-5.32	104.25	113.30
1	D	134	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	D	165	ASP	CB-CG-OD1	5.32	123.08	118.30
1	G	27	PRO	N-CA-C	-5.32	98.28	112.10
1	A	231	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	F	183	GLU	CG-CD-OE1	-5.30	107.69	118.30
1	E	2	PRO	N-CA-C	5.30	125.87	112.10
1	H	153	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	J	55	VAL	CA-CB-CG2	-5.28	102.98	110.90
1	F	10	GLU	CG-CD-OE1	5.28	128.85	118.30
1	J	91	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	C	28	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	F	206	ARG	CG-CD-NE	-5.26	100.75	111.80
1	G	155	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	220	ARG	CG-CD-NE	5.25	122.83	111.80
1	B	242	TYR	CB-CG-CD1	5.25	124.15	121.00
1	D	16	GLU	OE1-CD-OE2	5.24	129.59	123.30
1	B	176	PRO	CA-N-CD	5.23	119.02	111.70
1	H	126	ARG	CG-CD-NE	-5.23	100.81	111.80
1	C	47	THR	CB-CA-C	5.22	125.71	111.60
1	J	84	LYS	CD-CE-NZ	-5.22	99.68	111.70
1	A	47	THR	N-CA-C	-5.22	96.90	111.00
1	G	27	PRO	N-CD-CG	5.22	111.03	103.20
1	G	195	GLN	CA-CB-CG	5.22	124.88	113.40
1	I	199	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	J	7	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	B	74	LEU	CD1-CG-CD2	-5.21	94.86	110.50
1	A	227	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	213	CYS	CA-CB-SG	-5.20	104.64	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	132	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	206	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	G	150	LEU	N-CA-C	-5.19	96.99	111.00
1	A	112	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	J	59	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	F	183	GLU	CG-CD-OE2	5.18	128.67	118.30
1	A	155	LEU	CA-CB-CG	-5.18	103.39	115.30
1	I	232	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	150	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	I	119	GLU	N-CA-CB	5.17	119.91	110.60
1	I	175	TRP	C-N-CD	-5.17	109.23	120.60
1	D	6	PRO	N-CA-C	-5.16	98.69	112.10
1	G	163	LEU	CB-CG-CD1	-5.16	102.24	111.00
1	C	60	ARG	CD-NE-CZ	5.15	130.81	123.60
1	A	138	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	112	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	F	152	ASP	CB-CG-OD2	5.15	122.93	118.30
1	E	60	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	I	32	SER	CB-CA-C	-5.14	100.34	110.10
1	C	136	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	D	71	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	F	2	PRO	CA-N-CD	-5.12	104.33	111.50
1	B	174	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	183	GLU	OE1-CD-OE2	5.10	129.43	123.30
1	F	145	MSE	CB-CG-SE	-5.10	97.41	112.70
1	D	145	MSE	CB-CG-SE	-5.08	97.45	112.70
1	F	71	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	J	61	TYR	CB-CG-CD2	5.08	124.05	121.00
1	J	222	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	104	ASP	N-CA-CB	5.08	119.74	110.60
1	E	61	TYR	CB-CG-CD1	5.07	124.04	121.00
1	C	200	MSE	CG-SE-CE	5.06	110.04	98.90
1	J	26	LEU	C-N-CA	5.06	143.27	122.00
1	A	239	LYS	CD-CE-NZ	-5.05	100.08	111.70
1	C	208	LEU	CA-CB-CG	5.05	126.92	115.30
1	G	145	MSE	CA-CB-CG	-5.04	104.72	113.30
1	D	67	LEU	N-CA-C	-5.04	97.40	111.00
1	F	197	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	I	48	PRO	N-CA-C	5.03	125.19	112.10
1	C	199	ARG	CD-NE-CZ	5.03	130.64	123.60
1	H	2	PRO	N-CA-CB	5.03	109.33	103.30
1	H	193	GLU	N-CA-CB	-5.03	101.55	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	240	LEU	CA-CB-CG	-5.03	103.74	115.30
1	B	149	ARG	CG-CD-NE	-5.02	101.25	111.80
1	G	206	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	I	38	VAL	CG1-CB-CG2	-5.02	102.87	110.90
1	B	87	GLU	N-CA-CB	-5.01	101.58	110.60
1	G	235	GLU	CA-CB-CG	5.01	124.41	113.40
1	J	215	ASP	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Sidechain
1	A	242	TYR	Sidechain
1	B	143	TYR	Sidechain
1	D	242	TYR	Sidechain
1	D	82	HIS	Sidechain
1	E	175	TRP	Mainchain
1	G	229	TYR	Sidechain
1	G	242	TYR	Sidechain
1	G	26	LEU	Mainchain
1	H	205	TYR	Sidechain
1	I	205	TYR	Sidechain
1	I	242	TYR	Sidechain
1	J	138	ARG	Sidechain
1	J	174	ASP	Mainchain
1	J	26	LEU	Mainchain
1	J	61	TYR	Sidechain

## 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1973	0	1959	108	0
1	B	1973	0	1959	123	0
1	C	1973	0	1959	113	0
1	D	1973	0	1959	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1973	0	1959	138	0
1	F	1973	0	1959	128	0
1	G	1973	0	1959	98	0
1	H	1973	0	1959	99	0
1	I	1973	0	1959	135	0
1	J	1973	0	1959	119	0
2	A	56	0	84	55	0
2	B	56	0	84	46	0
2	C	64	0	96	68	0
2	D	40	0	60	33	0
2	E	68	0	101	57	0
2	F	48	0	72	43	0
2	G	36	0	54	36	0
2	H	36	0	54	37	1
2	I	44	0	66	56	0
2	J	64	0	96	79	0
3	A	140	0	0	9	0
3	B	120	0	0	9	0
3	C	136	0	0	3	1
3	D	132	0	0	9	0
3	E	133	0	0	7	0
3	F	115	0	0	9	0
3	G	98	0	0	4	0
3	H	94	0	0	3	0
3	I	106	0	0	9	0
3	J	115	0	0	6	0
All	All	21431	0	20357	1196	1

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 29.

All (1196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:ILE:CG1	1:I:102:ILE:CD1	1.76	1.60
1:E:145:MSE:CB	1:E:145:MSE:CG	1.81	1.58
1:D:145:MSE:CG	1:D:145:MSE:CB	1.77	1.56
1:H:145:MSE:CB	1:H:145:MSE:CG	1.82	1.56
1:E:25:LYS:NZ	1:E:25:LYS:CE	1.67	1.56
1:F:168:LYS:CE	1:F:168:LYS:NZ	1.69	1.56
1:C:145:MSE:CB	1:C:145:MSE:CG	1.78	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ALA:CB	1:E:121:ALA:CA	1.76	1.56
1:A:225:GLU:CD	1:A:225:GLU:CG	1.75	1.54
1:G:162:LYS:CE	1:G:162:LYS:NZ	1.70	1.53
1:G:236:LYS:CE	1:G:236:LYS:NZ	1.68	1.51
1:I:145:MSE:CG	1:I:145:MSE:CB	1.89	1.50
1:H:237:PRO:CG	1:H:237:PRO:CB	1.77	1.49
1:A:145:MSE:CG	1:A:145:MSE:CB	1.88	1.48
2:A:2029:EDO:O2	2:A:2029:EDO:C2	1.63	1.46
2:E:2088:EDO:O1	2:E:2088:EDO:C1	1.64	1.46
2:J:2014:EDO:O1	2:J:2014:EDO:C1	1.64	1.46
2:D:2031:EDO:C2	2:D:2031:EDO:O2	1.64	1.46
2:A:2012:EDO:O1	2:A:2012:EDO:C1	1.63	1.45
2:J:2049:EDO:C2	2:J:2049:EDO:O2	1.64	1.45
2:B:2020:EDO:C1	2:B:2020:EDO:O1	1.64	1.45
2:J:2008:EDO:O2	2:J:2008:EDO:C2	1.63	1.45
2:J:2104:EDO:O1	2:J:2104:EDO:C1	1.63	1.44
2:A:2063:EDO:O1	2:A:2063:EDO:C1	1.64	1.44
1:F:15:MSE:SE	1:F:15:MSE:CG	2.15	1.44
2:G:2050:EDO:O2	2:G:2050:EDO:C2	1.66	1.44
2:J:2105:EDO:O2	2:J:2105:EDO:C2	1.63	1.44
2:J:2123:EDO:O1	2:J:2123:EDO:C1	1.64	1.44
2:G:2102:EDO:O2	2:G:2102:EDO:C2	1.65	1.44
2:C:2067:EDO:O2	2:C:2067:EDO:C2	1.65	1.43
2:C:2128:EDO:C2	2:C:2128:EDO:O2	1.65	1.43
1:E:145:MSE:CE	1:E:145:MSE:SE	2.15	1.43
2:B:2021:EDO:O1	2:B:2021:EDO:C1	1.65	1.43
2:J:2068:EDO:C2	2:J:2068:EDO:O2	1.64	1.43
2:E:2120:EDO:C1	2:E:2120:EDO:O1	1.64	1.43
2:C:2024:EDO:O2	2:C:2024:EDO:C2	1.65	1.43
2:H:2058:EDO:O2	2:H:2058:EDO:C2	1.64	1.43
2:E:2032:EDO:C2	2:E:2032:EDO:O2	1.66	1.42
2:I:2115:EDO:O2	2:I:2115:EDO:C2	1.67	1.42
2:D:2118:EDO:O2	2:D:2118:EDO:C2	1.66	1.42
2:F:2006:EDO:C1	2:F:2006:EDO:O1	1.68	1.41
2:B:2002:EDO:O2	2:B:2002:EDO:C2	1.69	1.41
2:B:2023:EDO:O2	2:B:2023:EDO:C2	1.67	1.41
2:G:2056:EDO:C2	2:G:2056:EDO:O2	1.65	1.41
2:J:2053:EDO:C2	2:J:2053:EDO:O2	1.63	1.41
2:C:2004:EDO:O1	2:C:2004:EDO:C1	1.67	1.41
2:F:2043:EDO:O2	2:F:2043:EDO:C2	1.65	1.41
2:G:2093:EDO:C2	2:G:2093:EDO:O2	1.64	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:MSE:SE	1:A:145:MSE:CE	2.19	1.40
2:A:2124:EDO:O1	2:A:2124:EDO:C1	1.69	1.40
2:C:2085:EDO:O2	2:C:2085:EDO:C2	1.66	1.40
1:I:140:MSE:SE	1:I:140:MSE:CG	2.18	1.40
1:J:237:PRO:CB	1:J:237:PRO:CG	1.74	1.40
2:J:2104:EDO:O2	2:J:2104:EDO:C2	1.66	1.40
2:C:2126:EDO:C2	2:C:2126:EDO:O2	1.65	1.40
2:E:2089:EDO:C2	2:E:2089:EDO:O2	1.68	1.40
2:H:2010:EDO:O2	2:H:2010:EDO:C2	1.70	1.40
2:B:2021:EDO:O2	2:B:2021:EDO:C2	1.68	1.40
2:D:2074:EDO:O1	2:D:2074:EDO:C1	1.70	1.40
2:G:2009:EDO:O1	2:G:2009:EDO:C1	1.67	1.40
1:B:140:MSE:CG	1:B:140:MSE:SE	2.19	1.40
1:H:145:MSE:SE	1:H:145:MSE:CE	2.17	1.39
2:C:2082:EDO:C2	2:C:2082:EDO:O2	1.68	1.39
2:A:2012:EDO:O2	2:A:2012:EDO:C2	1.70	1.39
2:A:2124:EDO:O2	2:A:2124:EDO:C2	1.69	1.39
2:A:2122:EDO:O2	2:A:2122:EDO:C2	1.69	1.38
2:F:2098:EDO:O2	2:F:2098:EDO:C2	1.72	1.38
1:G:145:MSE:SE	1:G:145:MSE:CE	2.19	1.38
2:I:2007:EDO:O1	2:I:2007:EDO:C1	1.68	1.38
1:B:162:LYS:CE	1:B:162:LYS:NZ	1.84	1.38
2:B:2002:EDO:O1	2:B:2002:EDO:C1	1.71	1.38
1:C:145:MSE:SE	1:C:145:MSE:CE	2.20	1.38
2:C:2085:EDO:O1	2:C:2085:EDO:C1	1.68	1.38
2:H:2059:EDO:C2	2:H:2059:EDO:O2	1.71	1.37
2:C:2004:EDO:O2	2:C:2004:EDO:C2	1.73	1.36
2:E:2005:EDO:C2	2:E:2005:EDO:O2	1.75	1.34
2:J:2008:EDO:O1	2:J:2008:EDO:C1	1.80	1.30
1:I:228:ARG:HD2	2:I:2107:EDO:C2	1.65	1.26
1:E:214:TRP:HH2	1:F:242:TYR:CD1	1.56	1.23
1:I:228:ARG:CD	2:I:2107:EDO:H22	1.69	1.22
1:B:220:ARG:HG3	1:B:224:GLU:OE2	1.32	1.22
1:F:145:MSE:HE3	2:F:2086:EDO:O2	1.40	1.21
1:J:199:ARG:HH21	2:J:2104:EDO:H22	1.10	1.14
1:E:241:LEU:HD23	1:E:244:GLU:OE1	1.45	1.14
2:C:2075:EDO:H11	2:E:2127:EDO:H22	1.17	1.12
1:F:14:GLU:HG2	1:F:25:LYS:NZ	1.62	1.12
1:C:129:PHE:CE2	1:C:140:MSE:HE3	1.84	1.12
1:J:215:ASP:HB3	1:J:217:PRO:HD3	1.17	1.11
1:B:205:TYR:H	2:B:2030:EDO:H22	1.01	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:TYR:H	2:D:2035:EDO:H22	1.02	1.10
1:E:129:PHE:CE2	1:E:140:MSE:HE3	1.86	1.10
1:C:48:PRO:HD2	2:C:2024:EDO:H11	1.28	1.09
1:C:108:THR:HG22	2:C:2117:EDO:H22	1.34	1.09
1:A:118:ALA:O	1:A:119:GLU:HB2	1.44	1.09
1:G:105:PRO:O	1:G:106:GLN:HB2	1.47	1.09
2:C:2075:EDO:C1	2:E:2127:EDO:H22	1.83	1.06
1:E:236:LYS:HZ1	2:F:2043:EDO:H22	1.16	1.06
1:G:49:VAL:H	2:G:2056:EDO:H12	1.19	1.06
1:C:108:THR:CG2	2:C:2117:EDO:H22	1.85	1.05
1:C:59:ARG:HB3	2:C:2128:EDO:H21	1.06	1.05
2:F:2095:EDO:H22	3:F:553:HOH:O	1.55	1.05
1:J:97:ILE:H	2:J:2109:EDO:H12	1.21	1.05
1:D:145:MSE:HE3	2:D:2118:EDO:H21	1.09	1.04
1:E:199:ARG:HE	2:E:2091:EDO:H12	1.21	1.04
1:E:214:TRP:CH2	1:F:242:TYR:CD1	2.45	1.03
1:I:228:ARG:NE	2:I:2107:EDO:H11	1.75	1.01
1:J:105:PRO:O	1:J:106:GLN:CB	2.07	1.01
1:I:134:ARG:NH1	3:I:2137:HOH:O	1.91	1.01
1:J:105:PRO:O	1:J:106:GLN:HB2	1.19	1.01
2:I:2121:EDO:H21	3:I:2181:HOH:O	1.61	1.00
1:D:205:TYR:N	2:D:2035:EDO:H22	1.77	1.00
1:J:162:LYS:HE3	3:J:2146:HOH:O	1.62	1.00
1:B:111:ARG:HH22	1:C:111:ARG:HH22	1.08	1.00
1:A:235:GLU:HB3	2:A:2001:EDO:H21	1.38	0.99
1:B:205:TYR:N	2:B:2030:EDO:H22	1.76	0.99
1:B:49:VAL:H	2:B:2028:EDO:C1	1.74	0.99
1:J:97:ILE:N	2:J:2109:EDO:H12	1.77	0.98
1:A:145:MSE:CB	1:A:145:MSE:SE	2.61	0.98
1:D:235:GLU:HB3	2:D:2003:EDO:H11	1.44	0.98
1:I:108:THR:HG22	2:I:2046:EDO:H22	1.44	0.97
1:J:86:LYS:HB3	2:J:2109:EDO:H21	1.44	0.97
1:B:65:GLN:HG2	3:B:2233:HOH:O	1.65	0.97
1:C:183:GLU:HG2	2:C:2085:EDO:H12	1.43	0.97
1:D:47:THR:HG23	3:D:2211:HOH:O	1.65	0.97
1:G:183:GLU:HG2	2:G:2057:EDO:O2	1.64	0.97
1:A:48:PRO:HD2	2:A:2012:EDO:H22	1.48	0.96
1:J:199:ARG:HE	2:J:2104:EDO:H12	1.27	0.96
1:I:228:ARG:HD2	2:I:2107:EDO:H22	0.98	0.96
1:I:150:LEU:HD12	1:J:174:ASP:HB3	1.47	0.96
1:B:220:ARG:CG	1:B:224:GLU:OE2	2.14	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:ARG:HG3	1:H:59:ARG:HH11	1.28	0.95
1:C:117:HIS:HD2	1:D:8:ILE:H	1.14	0.95
3:B:2191:HOH:O	1:D:200:MSE:HG3	1.65	0.95
1:F:14:GLU:HG2	1:F:25:LYS:HZ1	1.19	0.95
1:B:48:PRO:HD2	2:B:2028:EDO:H21	1.48	0.94
1:C:183:GLU:H	2:C:2085:EDO:H11	1.32	0.94
1:G:169:ARG:O	2:G:2112:EDO:H11	1.66	0.94
1:G:8:ILE:H	1:H:117:HIS:HD2	0.94	0.94
1:J:97:ILE:H	2:J:2109:EDO:C1	1.81	0.94
1:G:8:ILE:H	1:H:117:HIS:CD2	1.85	0.94
1:I:117:HIS:HD2	1:J:8:ILE:H	1.16	0.94
1:B:105:PRO:O	1:B:106:GLN:HB2	1.69	0.93
1:D:239:LYS:HE3	1:D:244:GLU:OE2	1.69	0.93
1:E:236:LYS:NZ	2:F:2043:EDO:H22	1.84	0.93
1:A:145:MSE:CE	1:A:145:MSE:HB3	2.00	0.92
1:I:118:ALA:O	1:I:119:GLU:HB2	1.69	0.92
1:B:49:VAL:H	2:B:2028:EDO:H11	1.33	0.92
1:E:214:TRP:HH2	1:F:242:TYR:CE1	1.87	0.92
1:E:8:ILE:H	1:F:117:HIS:HD2	1.16	0.92
1:I:59:ARG:HH11	1:I:59:ARG:CG	1.82	0.92
2:C:2075:EDO:H11	2:E:2127:EDO:C2	1.98	0.91
1:D:69:VAL:HG21	1:D:158:VAL:HG11	1.51	0.91
1:B:150:LEU:HD22	3:B:2151:HOH:O	1.71	0.91
1:E:225:GLU:HG3	1:E:228:ARG:HH21	1.36	0.90
1:E:145:MSE:CB	1:E:145:MSE:SE	2.69	0.90
1:D:145:MSE:HE3	2:D:2118:EDO:C2	2.01	0.90
1:E:59:ARG:HB3	2:E:2040:EDO:H11	1.50	0.90
1:C:59:ARG:HB3	2:C:2128:EDO:C2	2.00	0.89
1:C:228:ARG:HD3	3:C:2171:HOH:O	1.71	0.89
1:E:2:PRO:HB2	1:F:10:GLU:OE2	1.71	0.89
1:I:145:MSE:CB	1:I:145:MSE:SE	2.71	0.89
1:I:62:GLU:HB2	3:I:2223:HOH:O	1.71	0.89
1:F:129:PHE:CE2	1:F:140:MSE:HE3	2.07	0.89
1:F:145:MSE:CE	2:F:2086:EDO:O2	2.20	0.89
1:A:145:MSE:CB	1:A:145:MSE:CE	2.50	0.88
1:J:16:GLU:O	2:J:2123:EDO:H21	1.73	0.88
1:E:117:HIS:HD2	1:F:8:ILE:H	1.18	0.88
1:E:225:GLU:HG3	1:E:228:ARG:NH2	1.89	0.88
1:I:59:ARG:HH11	1:I:59:ARG:HG3	1.38	0.88
1:G:105:PRO:O	1:G:106:GLN:CB	2.20	0.88
1:D:145:MSE:CE	2:D:2118:EDO:H21	2.00	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:ILE:HG12	2:J:2109:EDO:H11	1.53	0.87
1:I:8:ILE:HG22	1:J:119:GLU:HG3	1.55	0.87
2:A:2029:EDO:C2	2:B:2125:EDO:H11	2.03	0.87
1:C:48:PRO:CD	2:C:2024:EDO:H11	2.04	0.86
1:D:190:PRO:HA	1:D:195:GLN:HE21	1.37	0.86
1:E:239:LYS:HE2	1:E:244:GLU:HG2	1.56	0.86
1:C:8:ILE:H	1:D:117:HIS:HD2	1.21	0.86
1:I:66:ARG:HB3	1:I:66:ARG:NH1	1.91	0.86
1:B:49:VAL:HB	2:B:2028:EDO:H12	1.55	0.86
1:D:145:MSE:CB	1:D:145:MSE:SE	2.73	0.86
1:J:206:ARG:HA	2:J:2106:EDO:H22	1.55	0.85
1:A:8:ILE:H	1:B:117:HIS:HD2	1.21	0.85
1:E:25:LYS:NZ	1:E:25:LYS:CD	2.39	0.85
1:E:241:LEU:HA	1:E:244:GLU:OE1	1.74	0.85
1:I:8:ILE:H	1:J:117:HIS:HD2	1.25	0.85
1:I:129:PHE:CE2	1:I:140:MSE:HE3	2.11	0.85
1:J:96:ARG:HG3	2:J:2109:EDO:O2	1.75	0.85
1:H:14:GLU:HG2	1:H:25:LYS:HZ1	1.40	0.85
1:G:21:HIS:ND1	2:G:2093:EDO:H11	1.91	0.85
1:B:106:GLN:HE22	1:C:107:GLY:HA3	1.42	0.84
1:H:145:MSE:CB	1:H:145:MSE:SE	2.75	0.84
1:A:49:VAL:H	2:A:2012:EDO:H21	1.42	0.84
1:D:191:THR:H	1:D:195:GLN:NE2	1.76	0.84
2:A:2029:EDO:H21	2:B:2125:EDO:H11	1.58	0.84
1:C:197:ARG:HH22	1:E:96:ARG:HH21	1.26	0.84
1:A:193:GLU:OE1	3:A:2222:HOH:O	1.95	0.83
1:J:207:SER:H	2:J:2106:EDO:H12	1.43	0.83
1:C:129:PHE:HE2	1:C:140:MSE:HE3	1.43	0.83
1:I:205:TYR:H	2:I:2051:EDO:H22	1.42	0.83
1:D:129:PHE:CE2	1:D:140:MSE:HE3	2.13	0.83
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.14	0.83
1:I:5:ILE:HD13	1:J:5:ILE:HD13	1.59	0.83
1:C:197:ARG:HH22	1:E:96:ARG:NH2	1.77	0.83
1:F:105:PRO:O	1:F:106:GLN:HB2	1.79	0.83
1:H:55:VAL:O	1:H:59:ARG:HG2	1.77	0.83
1:H:105:PRO:O	1:H:106:GLN:HB2	1.78	0.83
1:A:122:THR:HG23	1:A:123:HIS:CD2	2.13	0.83
1:B:244:GLU:N	1:B:244:GLU:OE1	2.12	0.83
1:D:205:TYR:H	2:D:2035:EDO:C2	1.89	0.82
1:G:69:VAL:HG21	1:G:158:VAL:HG11	1.61	0.82
1:G:48:PRO:HD2	2:G:2056:EDO:H11	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:112:ARG:HD3	2:I:2046:EDO:H11	1.62	0.82
1:C:8:ILE:HG22	1:D:119:GLU:HG3	1.62	0.82
1:C:193:GLU:OE1	2:E:2127:EDO:H21	1.79	0.82
1:J:228:ARG:NH2	2:J:2049:EDO:H22	1.94	0.82
1:I:228:ARG:CD	2:I:2107:EDO:C2	2.43	0.81
1:H:145:MSE:CG	1:H:145:MSE:CA	2.57	0.81
1:G:183:GLU:N	2:G:2057:EDO:O2	2.12	0.81
1:F:90:GLU:HG3	3:F:572:HOH:O	1.80	0.80
1:A:239:LYS:CE	1:A:244:GLU:HG2	2.10	0.80
1:G:8:ILE:N	1:H:117:HIS:HD2	1.77	0.80
1:I:36:TRP:NE1	1:I:162:LYS:NZ	2.29	0.80
1:A:167:LEU:O	2:A:2124:EDO:H22	1.81	0.80
2:I:2121:EDO:C2	3:I:2181:HOH:O	2.24	0.80
1:J:199:ARG:NH2	2:J:2104:EDO:H22	1.92	0.80
1:B:205:TYR:H	2:B:2030:EDO:C2	1.88	0.80
1:C:117:HIS:CD2	1:D:8:ILE:H	1.99	0.80
1:A:242:TYR:CD1	1:B:214:TRP:HH2	2.00	0.80
1:B:92:HIS:NE2	2:B:2125:EDO:H12	1.97	0.80
1:C:59:ARG:CB	2:C:2128:EDO:H21	2.02	0.80
1:C:47:THR:HG23	2:C:2024:EDO:O1	1.82	0.80
1:A:117:HIS:HD2	1:B:8:ILE:H	1.26	0.79
1:H:70:ASP:HB3	2:H:2113:EDO:H12	1.63	0.79
1:A:235:GLU:HB3	2:A:2001:EDO:C2	2.12	0.79
1:A:218:ALA:O	2:A:2063:EDO:H12	1.83	0.79
1:C:197:ARG:HD3	2:C:2075:EDO:O1	1.82	0.79
1:E:122:THR:HG21	3:E:938:HOH:O	1.81	0.79
1:H:14:GLU:HG2	1:H:25:LYS:NZ	1.98	0.79
1:C:122:THR:HG23	1:C:123:HIS:CD2	2.17	0.79
1:D:235:GLU:O	2:D:2003:EDO:C1	2.31	0.79
1:G:96:ARG:HG3	1:G:96:ARG:HH11	1.48	0.79
1:G:179:GLU:HG2	1:H:59:ARG:HH12	1.46	0.79
1:A:47:THR:HG23	2:A:2012:EDO:O2	1.83	0.79
1:H:183:GLU:HG2	2:H:2058:EDO:H12	1.63	0.78
2:E:2120:EDO:H22	1:F:88:TRP:HE1	1.49	0.78
1:I:225:GLU:HG3	1:I:228:ARG:HH11	1.47	0.78
1:F:145:MSE:HE3	2:F:2086:EDO:HO2	1.48	0.78
1:I:188:PRO:O	1:I:199:ARG:NH2	2.16	0.78
1:D:235:GLU:O	2:D:2003:EDO:H12	1.84	0.78
1:D:112:ARG:CG	1:D:112:ARG:HH11	1.96	0.78
2:I:2099:EDO:H12	1:J:191:THR:CG2	2.14	0.77
1:E:8:ILE:H	1:F:117:HIS:CD2	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:7:LEU:HA	1:J:140:MSE:HE1	1.67	0.77
1:B:111:ARG:NH2	1:C:111:ARG:HH22	1.81	0.77
1:E:169:ARG:HH12	2:E:2089:EDO:H22	1.48	0.77
2:H:2058:EDO:O2	2:H:2058:EDO:C1	2.31	0.77
1:A:5:ILE:HD13	1:B:5:ILE:HD13	1.65	0.77
1:B:49:VAL:N	2:B:2028:EDO:H11	2.00	0.77
1:I:140:MSE:CG	1:I:140:MSE:CE	2.63	0.77
1:C:193:GLU:OE2	3:C:2223:HOH:O	2.02	0.77
1:H:70:ASP:CB	2:H:2113:EDO:H12	2.13	0.77
1:I:203:GLY:CA	2:I:2051:EDO:H21	2.15	0.77
1:E:203:GLY:HA2	2:E:2042:EDO:O2	1.85	0.77
1:F:112:ARG:HH11	1:F:112:ARG:HB3	1.48	0.77
1:F:112:ARG:HB3	1:F:112:ARG:NH1	2.01	0.76
1:C:145:MSE:CB	1:C:145:MSE:SE	2.83	0.76
1:B:49:VAL:CB	2:B:2028:EDO:H12	2.15	0.76
1:E:117:HIS:CD2	1:F:8:ILE:H	2.02	0.76
1:D:203:GLY:HA2	2:D:2035:EDO:H11	1.67	0.76
3:A:2228:HOH:O	1:J:122:THR:HG21	1.85	0.76
1:E:214:TRP:CH2	1:F:242:TYR:CE1	2.71	0.76
1:H:106:GLN:O	1:H:111:ARG:NH2	2.19	0.76
1:I:117:HIS:CD2	1:J:8:ILE:H	2.03	0.76
1:I:200:MSE:HE2	1:I:200:MSE:HA	1.68	0.76
1:I:118:ALA:O	1:I:119:GLU:CB	2.24	0.76
1:D:145:MSE:CG	1:D:145:MSE:CA	2.64	0.76
1:A:216:THR:HB	2:A:2063:EDO:H11	1.69	0.75
1:I:140:MSE:HB3	1:I:140:MSE:HE2	1.67	0.75
1:C:129:PHE:CE2	1:C:140:MSE:CE	2.66	0.75
1:I:102:ILE:CD1	1:I:102:ILE:CB	2.64	0.75
1:B:106:GLN:O	1:B:111:ARG:NH2	2.19	0.75
1:D:15:MSE:CE	1:D:112:ARG:HD3	2.17	0.75
1:A:122:THR:HG23	1:A:123:HIS:HD2	1.52	0.74
1:I:10:GLU:OE2	1:J:2:PRO:HB2	1.87	0.74
1:I:108:THR:CG2	2:I:2046:EDO:H22	2.15	0.74
1:G:236:LYS:HE3	3:G:1166:HOH:O	1.86	0.74
2:C:2085:EDO:O2	2:C:2085:EDO:C1	2.34	0.74
1:D:200:MSE:HE2	1:D:200:MSE:HA	1.70	0.74
2:F:2043:EDO:O2	2:F:2043:EDO:C1	2.36	0.74
1:G:49:VAL:H	2:G:2056:EDO:C1	1.98	0.74
1:I:228:ARG:NE	2:I:2107:EDO:C1	2.51	0.74
1:A:145:MSE:CG	1:A:145:MSE:CA	2.65	0.74
1:B:49:VAL:N	2:B:2028:EDO:C1	2.50	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:MSE:CG	1:E:145:MSE:CA	2.66	0.73
1:I:181:ILE:O	2:I:2103:EDO:H21	1.88	0.73
1:A:163:LEU:HD22	1:A:167:LEU:HD22	1.70	0.73
1:I:66:ARG:CG	1:I:66:ARG:HH11	2.01	0.73
1:B:239:LYS:HE2	1:B:244:GLU:CD	2.08	0.73
1:J:97:ILE:H	2:J:2109:EDO:C2	2.01	0.73
1:F:222:ASP:OD2	2:F:2097:EDO:H22	1.88	0.73
1:I:145:MSE:CG	1:I:145:MSE:CA	2.67	0.73
1:I:228:ARG:HE	2:I:2107:EDO:H11	1.52	0.73
1:C:108:THR:HG21	2:C:2117:EDO:H22	1.70	0.73
1:A:118:ALA:O	1:A:119:GLU:CB	2.18	0.72
1:B:122:THR:HG23	1:B:123:HIS:CD2	2.24	0.72
1:I:192:THR:OG1	2:I:2115:EDO:H11	1.88	0.72
1:A:11:ARG:NH1	1:A:14:GLU:OE2	2.22	0.72
1:D:111:ARG:HH22	1:E:111:ARG:HH22	1.38	0.72
1:E:17:VAL:HA	2:E:2078:EDO:H21	1.71	0.72
1:I:36:TRP:CD1	1:I:162:LYS:NZ	2.58	0.72
1:F:107:GLY:HA3	1:G:106:GLN:HE22	1.55	0.71
1:B:49:VAL:H	2:B:2028:EDO:H12	1.53	0.71
1:F:74:LEU:HD23	1:F:102:ILE:HB	1.73	0.71
1:I:228:ARG:HD2	2:I:2107:EDO:H21	1.69	0.71
1:C:145:MSE:CG	1:C:145:MSE:CA	2.66	0.71
1:A:145:MSE:HB3	1:A:145:MSE:HE3	1.70	0.71
1:G:48:PRO:CD	2:G:2056:EDO:H11	2.20	0.71
1:C:67:LEU:O	1:C:162:LYS:HE2	1.90	0.71
1:F:14:GLU:CG	1:F:25:LYS:NZ	2.48	0.71
1:J:199:ARG:HH21	2:J:2104:EDO:C2	1.97	0.71
1:H:18:THR:H	2:H:2044:EDO:C2	2.04	0.71
1:J:21:HIS:ND1	2:J:2068:EDO:H21	2.06	0.71
1:J:199:ARG:HE	2:J:2104:EDO:C1	2.04	0.71
1:I:140:MSE:SE	1:I:140:MSE:CB	2.90	0.70
1:J:199:ARG:NE	2:J:2104:EDO:H12	2.04	0.70
1:J:215:ASP:HB3	1:J:217:PRO:CD	2.10	0.70
1:J:228:ARG:HH21	2:J:2049:EDO:H22	1.53	0.70
1:B:239:LYS:HE2	1:B:244:GLU:OE2	1.90	0.70
1:C:91:ARG:HD2	2:C:2126:EDO:O1	1.91	0.70
1:A:203:GLY:HA2	2:A:2065:EDO:O2	1.92	0.70
1:G:49:VAL:N	2:G:2056:EDO:H12	2.02	0.70
1:I:49:VAL:H	2:I:2121:EDO:HO2	1.39	0.70
1:G:235:GLU:HB2	2:G:2009:EDO:H11	1.72	0.70
1:B:140:MSE:HE3	1:B:142:TYR:OH	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:ARG:HG3	1:G:96:ARG:NH1	2.03	0.70
1:I:200:MSE:HE1	1:I:213:CYS:SG	2.31	0.70
1:I:232:ARG:O	2:I:2007:EDO:O1	2.10	0.70
1:J:215:ASP:CB	1:J:217:PRO:HD3	2.10	0.70
2:C:2075:EDO:C1	2:E:2127:EDO:C2	2.65	0.69
3:C:2186:HOH:O	1:D:231:ARG:HD3	1.91	0.69
1:E:206:ARG:HA	2:E:2090:EDO:H22	1.72	0.69
1:I:8:ILE:H	1:J:117:HIS:CD2	2.09	0.69
1:I:183:GLU:H	2:I:2103:EDO:C2	2.05	0.69
1:J:203:GLY:HA2	2:J:2055:EDO:O2	1.92	0.69
1:A:106:GLN:O	1:A:111:ARG:NH2	2.25	0.69
1:C:8:ILE:H	1:D:117:HIS:CD2	2.08	0.69
1:E:199:ARG:HH21	2:E:2091:EDO:H22	1.55	0.69
1:F:24:ILE:HD11	1:F:26:LEU:HD21	1.75	0.69
1:F:111:ARG:NH2	1:G:106:GLN:HE21	1.91	0.69
1:C:59:ARG:HD3	2:C:2128:EDO:H22	1.75	0.69
1:H:70:ASP:CG	2:H:2113:EDO:H12	2.13	0.69
1:H:183:GLU:H	2:H:2058:EDO:C1	2.05	0.69
1:A:232:ARG:O	2:A:2001:EDO:H22	1.92	0.69
2:A:2124:EDO:O2	3:A:2197:HOH:O	2.06	0.69
1:D:112:ARG:HH11	1:D:112:ARG:HG2	1.56	0.69
1:D:228:ARG:HG3	2:D:2072:EDO:H11	1.75	0.69
1:E:5:ILE:HD13	1:F:5:ILE:HD13	1.74	0.69
1:C:183:GLU:HG2	2:C:2085:EDO:C1	2.20	0.69
2:A:2029:EDO:H21	2:B:2125:EDO:C1	2.23	0.68
1:H:105:PRO:O	1:H:106:GLN:CB	2.39	0.68
1:A:63:ASP:OD2	1:A:228:ARG:NH2	2.26	0.68
1:J:21:HIS:ND1	2:J:2068:EDO:C2	2.57	0.68
2:G:2057:EDO:H12	1:H:240:LEU:HD11	1.76	0.68
1:H:122:THR:HG23	1:H:123:HIS:CD2	2.29	0.68
1:I:66:ARG:HH11	1:I:66:ARG:CB	2.05	0.68
1:I:112:ARG:HD3	2:I:2046:EDO:C1	2.23	0.68
1:A:21:HIS:ND1	2:A:2011:EDO:H22	2.07	0.67
1:B:232:ARG:HG3	2:B:2002:EDO:H11	1.76	0.67
2:I:2099:EDO:H12	1:J:191:THR:HG21	1.74	0.67
1:B:91:ARG:NH2	2:B:2125:EDO:O2	2.28	0.67
1:E:10:GLU:OE2	1:F:2:PRO:HB2	1.94	0.67
1:A:231:ARG:HG2	2:A:2017:EDO:H22	1.76	0.67
1:E:122:THR:HG23	1:E:123:HIS:CD2	2.29	0.67
1:H:232:ARG:HG3	2:H:2010:EDO:H22	1.77	0.67
1:C:224:GLU:OE1	1:C:231:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ARG:HE	2:E:2091:EDO:C1	2.05	0.67
2:J:2104:EDO:O1	2:J:2104:EDO:O2	2.12	0.67
1:D:43:PRO:HB2	2:D:2118:EDO:H22	1.75	0.66
1:F:168:LYS:NZ	1:F:168:LYS:CD	2.58	0.66
1:E:207:SER:H	2:E:2090:EDO:H22	1.61	0.66
1:H:190:PRO:HG2	1:H:210:TRP:HE3	1.61	0.66
1:G:145:MSE:HE2	3:G:1000:HOH:O	1.95	0.66
1:I:105:PRO:O	1:I:106:GLN:HB2	1.96	0.66
1:A:239:LYS:HD3	1:A:244:GLU:CG	2.26	0.66
1:B:140:MSE:SE	1:B:140:MSE:CB	2.92	0.66
1:E:199:ARG:NE	2:E:2091:EDO:H12	2.04	0.66
1:D:47:THR:CG2	3:D:2211:HOH:O	2.33	0.66
1:B:242:TYR:CE2	1:B:243:GLU:HG3	2.29	0.66
1:E:67:LEU:O	1:E:162:LYS:HE3	1.95	0.66
1:G:200:MSE:HG3	2:G:2050:EDO:O2	1.96	0.66
1:G:239:LYS:NZ	1:G:244:GLU:HG2	2.11	0.66
2:J:2104:EDO:C1	2:J:2104:EDO:HO1	2.07	0.66
2:J:2104:EDO:C1	2:J:2104:EDO:O2	2.42	0.66
1:H:183:GLU:H	2:H:2058:EDO:H11	1.61	0.65
1:J:16:GLU:C	2:J:2123:EDO:H21	2.16	0.65
1:I:43:PRO:HG3	1:I:145:MSE:HG2	1.77	0.65
1:A:8:ILE:H	1:B:117:HIS:CD2	2.11	0.65
2:H:2058:EDO:C2	2:H:2058:EDO:HO2	2.08	0.65
1:A:239:LYS:HE2	1:A:244:GLU:HG2	1.77	0.65
1:E:129:PHE:HE2	1:E:140:MSE:HE3	1.52	0.65
1:F:183:GLU:HG2	2:F:2043:EDO:C1	2.26	0.65
2:J:2104:EDO:O1	2:J:2104:EDO:C2	2.44	0.65
1:A:8:ILE:HG13	1:A:140:MSE:HE2	1.77	0.65
2:B:2020:EDO:C1	2:B:2020:EDO:HO1	2.07	0.65
1:C:91:ARG:HH11	2:C:2126:EDO:H12	1.61	0.65
1:F:222:ASP:OD2	2:F:2097:EDO:C2	2.44	0.65
2:E:2092:EDO:O1	1:G:87:GLU:OE1	2.15	0.65
1:G:113:LEU:HB3	1:G:129:PHE:CZ	2.30	0.65
1:A:235:GLU:CB	2:A:2001:EDO:H21	2.19	0.65
1:F:105:PRO:O	1:F:106:GLN:CB	2.44	0.65
1:J:232:ARG:O	2:J:2008:EDO:O1	2.15	0.65
1:A:20:ASP:OD2	1:A:86:LYS:NZ	2.28	0.65
1:B:48:PRO:HD2	2:B:2028:EDO:C2	2.27	0.65
1:J:104:ASP:HB2	3:J:2130:HOH:O	1.97	0.65
1:J:205:TYR:O	2:J:2055:EDO:H12	1.95	0.65
1:B:35:LYS:HE3	3:B:2231:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:CD	2:A:2012:EDO:H22	2.25	0.64
1:A:232:ARG:O	2:A:2001:EDO:C2	2.45	0.64
1:J:42:HIS:CE1	1:J:75:SER:HB3	2.33	0.64
1:F:15:MSE:SE	1:F:15:MSE:CB	2.93	0.64
1:J:97:ILE:HG12	2:J:2109:EDO:C1	2.27	0.64
1:C:112:ARG:CB	1:C:112:ARG:HH11	2.10	0.64
1:E:42:HIS:CE1	1:E:75:SER:HB3	2.32	0.64
1:F:221:ASP:OD2	3:F:543:HOH:O	2.15	0.64
2:J:2008:EDO:C2	2:J:2008:EDO:HO2	2.07	0.64
2:A:2029:EDO:O2	2:B:2125:EDO:H11	1.97	0.64
2:B:2021:EDO:C1	2:B:2021:EDO:HO1	2.08	0.64
1:D:77:ASP:OD2	3:D:2244:HOH:O	2.14	0.64
2:G:2102:EDO:C2	2:G:2102:EDO:HO2	2.09	0.64
1:H:87:GLU:OE2	2:H:2054:EDO:H22	1.97	0.64
1:I:126:ARG:HH22	2:I:2121:EDO:H11	1.62	0.64
1:B:105:PRO:O	1:B:106:GLN:CB	2.44	0.64
1:H:159:LYS:NZ	1:H:225:GLU:OE2	2.30	0.64
2:E:2088:EDO:C1	2:E:2088:EDO:HO1	2.07	0.64
1:B:43:PRO:HG3	1:B:145:MSE:HG2	1.80	0.64
2:J:2068:EDO:C2	2:J:2068:EDO:HO2	2.08	0.64
2:G:2093:EDO:O2	2:G:2093:EDO:C1	2.42	0.64
1:H:182:GLY:HA3	2:H:2058:EDO:H11	1.80	0.64
1:A:145:MSE:CB	1:A:145:MSE:HE2	2.27	0.63
1:A:239:LYS:HD3	1:A:244:GLU:HG2	1.80	0.63
2:A:2029:EDO:C2	2:A:2029:EDO:HO2	2.07	0.63
1:C:183:GLU:N	2:C:2085:EDO:H11	2.10	0.63
1:G:35:LYS:HD2	1:G:70:ASP:OD2	1.97	0.63
1:I:17:VAL:HA	2:I:2100:EDO:H12	1.80	0.63
2:J:2008:EDO:O2	2:J:2008:EDO:C1	2.46	0.63
1:D:105:PRO:HG2	1:E:122:THR:OG1	1.98	0.63
2:E:2120:EDO:H22	1:F:88:TRP:NE1	2.13	0.63
1:I:66:ARG:HB3	1:I:66:ARG:HH11	1.61	0.63
1:I:228:ARG:CZ	2:I:2107:EDO:H11	2.27	0.63
1:E:176:PRO:HD2	1:E:177:ASN:N	2.13	0.63
1:I:59:ARG:HH12	1:J:179:GLU:CD	2.02	0.63
1:I:66:ARG:NH1	1:I:66:ARG:CB	2.62	0.63
2:E:2120:EDO:C2	1:F:88:TRP:HE1	2.10	0.63
1:J:5:ILE:HG22	1:J:114:GLY:HA3	1.80	0.63
1:I:66:ARG:HH11	1:I:66:ARG:HG2	1.63	0.63
1:A:200:MSE:CE	2:A:2065:EDO:H11	2.28	0.63
2:E:2120:EDO:C1	2:E:2120:EDO:HO1	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:LEU:HD22	3:H:785:HOH:O	1.97	0.63
1:J:16:GLU:O	2:J:2123:EDO:C2	2.46	0.63
1:C:183:GLU:H	2:C:2085:EDO:C1	2.09	0.62
1:D:91:ARG:NH1	3:D:2175:HOH:O	2.32	0.62
1:F:104:ASP:HB3	2:F:2087:EDO:H22	1.81	0.62
1:G:239:LYS:CE	1:G:244:GLU:HG2	2.29	0.62
1:J:244:GLU:O	1:J:244:GLU:CD	2.37	0.62
1:B:207:SER:HB2	2:B:2030:EDO:H12	1.80	0.62
1:F:39:LEU:HD13	1:F:72:ILE:HG23	1.81	0.62
1:A:200:MSE:HE2	1:A:200:MSE:HA	1.80	0.62
1:F:123:HIS:CD2	2:F:2086:EDO:C2	2.82	0.62
1:F:200:MSE:HE1	1:F:213:CYS:SG	2.39	0.62
1:H:38:VAL:HB	1:H:71:LEU:HD23	1.82	0.62
1:A:239:LYS:CD	1:A:244:GLU:HG2	2.30	0.62
1:B:239:LYS:HG2	1:B:243:GLU:OE1	1.99	0.62
1:I:48:PRO:HD2	2:I:2121:EDO:O2	2.00	0.62
1:B:243:GLU:HB2	1:B:244:GLU:OE1	2.00	0.62
2:C:2024:EDO:C2	2:C:2024:EDO:HO2	2.09	0.62
1:D:204:GLN:N	2:D:2035:EDO:C2	2.63	0.62
1:E:176:PRO:HD2	1:E:177:ASN:H	1.65	0.62
2:G:2093:EDO:C2	2:G:2093:EDO:HO2	2.08	0.62
1:I:49:VAL:N	2:I:2121:EDO:O2	2.26	0.62
1:I:191:THR:H	1:I:195:GLN:NE2	1.97	0.62
2:J:2053:EDO:C2	2:J:2053:EDO:HO2	2.07	0.62
1:D:204:GLN:N	2:D:2035:EDO:H21	2.15	0.61
2:A:2022:EDO:C2	1:B:236:LYS:HZ1	2.12	0.61
2:D:2031:EDO:C2	2:D:2031:EDO:HO2	2.08	0.61
1:I:228:ARG:NE	2:I:2107:EDO:C2	2.62	0.61
1:D:42:HIS:CE1	1:D:75:SER:HB3	2.35	0.61
1:F:200:MSE:HE2	1:F:200:MSE:HA	1.81	0.61
1:I:140:MSE:HE2	1:I:140:MSE:CB	2.30	0.61
1:G:6:PRO:HG2	1:G:129:PHE:HE2	1.65	0.61
1:G:7:LEU:HA	1:G:140:MSE:HE1	1.83	0.61
2:A:2012:EDO:C1	2:A:2012:EDO:HO1	2.07	0.61
1:F:111:ARG:HH21	1:G:106:GLN:HE21	1.47	0.61
1:H:18:THR:H	2:H:2044:EDO:H21	1.64	0.61
1:I:99:PHE:HB2	1:I:100:PRO:HD2	1.82	0.61
1:G:183:GLU:H	2:G:2057:EDO:HO2	1.46	0.61
3:I:2182:HOH:O	1:J:138:ARG:HD2	2.00	0.61
1:J:32:SER:HA	2:J:2108:EDO:H21	1.82	0.61
1:B:140:MSE:CE	1:B:142:TYR:OH	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:ARG:HH11	1:H:59:ARG:CG	2.08	0.61
1:I:59:ARG:HG3	1:I:59:ARG:NH1	2.13	0.61
1:E:104:ASP:OD2	1:E:104:ASP:N	2.31	0.61
1:E:121:ALA:CB	1:E:121:ALA:C	2.66	0.61
1:J:200:MSE:HE1	1:J:213:CYS:SG	2.40	0.61
1:B:203:GLY:CA	2:B:2030:EDO:H21	2.31	0.60
1:D:62:GLU:HG2	1:D:66:ARG:NH1	2.16	0.60
1:F:200:MSE:CE	2:F:2034:EDO:H21	2.30	0.60
1:G:67:LEU:O	1:G:162:LYS:HE3	2.01	0.60
1:A:216:THR:O	2:A:2063:EDO:H11	2.01	0.60
2:G:2056:EDO:C2	2:G:2056:EDO:HO2	2.09	0.60
1:D:111:ARG:NH2	1:E:111:ARG:HH22	1.98	0.60
1:I:225:GLU:CG	1:I:228:ARG:HH11	2.13	0.60
1:C:191:THR:H	1:C:195:GLN:NE2	2.00	0.60
1:I:50:CYS:SG	2:I:2121:EDO:O1	2.57	0.60
1:E:39:LEU:HD13	1:E:72:ILE:HG23	1.84	0.60
1:A:200:MSE:HE1	2:A:2065:EDO:H11	1.84	0.60
2:I:2115:EDO:C2	2:I:2115:EDO:HO2	2.10	0.60
1:H:145:MSE:CB	1:H:145:MSE:CE	2.79	0.60
2:C:2004:EDO:C1	2:C:2004:EDO:HO1	2.10	0.60
1:D:235:GLU:HA	2:D:2119:EDO:H12	1.82	0.60
1:I:182:GLY:HA3	2:I:2103:EDO:H21	1.84	0.60
1:A:47:THR:CG2	2:A:2012:EDO:O2	2.50	0.59
1:B:197:ARG:O	1:B:201:GLU:HG2	2.02	0.59
1:H:69:VAL:HG21	1:H:158:VAL:HG11	1.83	0.59
1:C:43:PRO:HG3	1:C:145:MSE:HG2	1.84	0.59
1:E:236:LYS:HE2	3:E:536:HOH:O	2.00	0.59
1:G:74:LEU:HD23	1:G:102:ILE:HB	1.83	0.59
1:H:17:VAL:HA	2:H:2044:EDO:H21	1.85	0.59
1:H:106:GLN:O	1:H:111:ARG:CZ	2.49	0.59
1:D:107:GLY:HA3	1:E:106:GLN:HE22	1.68	0.59
1:F:14:GLU:HG2	1:F:25:LYS:HZ3	1.60	0.59
1:I:48:PRO:CD	2:I:2121:EDO:O2	2.50	0.59
1:B:190:PRO:HB3	1:B:195:GLN:HB3	1.84	0.59
1:F:183:GLU:H	2:F:2043:EDO:H11	1.68	0.59
2:A:2063:EDO:C1	2:A:2063:EDO:HO1	2.07	0.59
1:C:59:ARG:HD3	2:C:2128:EDO:C2	2.33	0.59
1:C:200:MSE:HA	1:C:200:MSE:HE2	1.84	0.59
2:I:2099:EDO:H12	1:J:191:THR:HG22	1.84	0.59
1:B:205:TYR:O	2:B:2030:EDO:H11	2.03	0.59
2:C:2128:EDO:C2	2:C:2128:EDO:HO2	2.08	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:222:ASP:OD2	2:J:2110:EDO:O1	2.18	0.59
1:C:112:ARG:HH11	1:C:112:ARG:HB3	1.67	0.59
2:C:2067:EDO:C2	2:C:2067:EDO:HO2	2.09	0.59
2:F:2006:EDO:C1	2:F:2006:EDO:HO1	2.11	0.59
1:A:228:ARG:HH22	1:A:232:ARG:HH12	1.49	0.59
1:I:203:GLY:HA2	2:I:2051:EDO:H21	1.85	0.59
1:C:5:ILE:HG23	1:C:6:PRO:O	2.03	0.59
2:E:2032:EDO:C2	2:E:2032:EDO:HO2	2.10	0.59
1:H:18:THR:HB	2:H:2044:EDO:O2	2.03	0.59
1:B:49:VAL:N	2:B:2028:EDO:H12	2.16	0.58
1:A:145:MSE:HE2	1:A:145:MSE:HB2	1.85	0.58
1:A:44:ALA:O	1:A:47:THR:HB	2.03	0.58
1:C:179:GLU:CD	1:D:59:ARG:NH1	2.57	0.58
1:J:106:GLN:O	1:J:111:ARG:NH2	2.37	0.58
1:A:228:ARG:HH22	1:A:232:ARG:NH1	2.02	0.58
1:B:35:LYS:CE	3:B:2231:HOH:O	2.51	0.58
1:J:35:LYS:HD3	1:J:70:ASP:OD2	2.03	0.58
1:D:106:GLN:O	1:D:111:ARG:NH2	2.36	0.58
1:E:176:PRO:CD	1:E:177:ASN:N	2.63	0.58
1:D:68:GLY:H	1:D:162:LYS:HE3	1.67	0.58
1:B:35:LYS:HD3	1:B:70:ASP:OD2	2.03	0.58
2:H:2059:EDO:H22	3:H:1074:HOH:O	2.04	0.58
1:E:92:HIS:NE2	2:E:2076:EDO:H21	2.18	0.57
1:H:190:PRO:HG2	1:H:210:TRP:CE3	2.39	0.57
1:I:48:PRO:HG2	1:J:186:ILE:HG21	1.86	0.57
3:B:2225:HOH:O	1:C:122:THR:HG21	2.03	0.57
2:J:2049:EDO:O2	2:J:2049:EDO:C1	2.47	0.57
1:F:105:PRO:HG2	1:G:122:THR:HB	1.87	0.57
1:B:106:GLN:NE2	1:C:107:GLY:HA3	2.17	0.57
1:B:163:LEU:O	1:B:167:LEU:HB2	2.04	0.57
1:C:193:GLU:OE1	2:E:2127:EDO:C2	2.52	0.57
1:E:176:PRO:CD	1:E:177:ASN:H	2.15	0.57
1:E:232:ARG:O	2:E:2005:EDO:O2	2.23	0.57
1:G:124:THR:HG23	1:G:125:VAL:O	2.03	0.57
1:G:162:LYS:NZ	1:G:162:LYS:CD	2.65	0.57
1:B:205:TYR:O	2:B:2030:EDO:C1	2.52	0.57
2:C:2085:EDO:C2	2:C:2085:EDO:HO2	2.10	0.57
1:D:106:GLN:O	1:D:111:ARG:CZ	2.53	0.57
1:A:198:ALA:O	1:A:202:SER:HB3	2.05	0.57
1:C:49:VAL:H	2:C:2024:EDO:H12	1.70	0.57
1:E:5:ILE:HG22	1:E:114:GLY:HA3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ALA:O	1:E:239:LYS:CB	2.50	0.57
1:H:191:THR:H	1:H:195:GLN:NE2	2.02	0.57
1:H:200:MSE:CE	2:H:2060:EDO:H22	2.34	0.57
1:I:126:ARG:NH2	2:I:2121:EDO:H11	2.19	0.57
1:B:203:GLY:C	2:B:2030:EDO:H21	2.25	0.56
1:C:5:ILE:HG12	1:C:142:TYR:OH	2.05	0.56
1:E:132:ASP:CG	2:E:2039:EDO:H12	2.25	0.56
1:J:97:ILE:CG1	2:J:2109:EDO:H11	2.32	0.56
1:A:243:GLU:CD	3:A:2163:HOH:O	2.42	0.56
2:J:2049:EDO:C2	2:J:2049:EDO:HO2	2.08	0.56
1:A:171:VAL:HB	1:B:147:LEU:HD23	1.88	0.56
1:C:104:ASP:N	1:C:105:PRO:HD3	2.20	0.56
1:E:105:PRO:O	1:E:106:GLN:HB2	2.05	0.56
1:E:105:PRO:O	1:E:106:GLN:CB	2.52	0.56
1:F:104:ASP:HB2	3:F:467:HOH:O	2.03	0.56
1:H:126:ARG:HB3	1:H:149:ARG:CZ	2.35	0.56
1:I:50:CYS:HG	2:I:2121:EDO:HO1	1.49	0.56
1:C:235:GLU:OE1	2:C:2080:EDO:H21	2.04	0.56
2:J:2104:EDO:C2	2:J:2104:EDO:HO2	2.10	0.56
1:E:169:ARG:HH12	2:E:2089:EDO:C2	2.17	0.56
1:E:235:GLU:O	2:E:2005:EDO:O2	2.17	0.56
1:A:218:ALA:O	2:A:2063:EDO:C1	2.51	0.56
2:B:2002:EDO:C2	2:B:2002:EDO:HO2	2.12	0.56
1:D:47:THR:HG22	1:D:50:CYS:SG	2.45	0.56
2:J:2014:EDO:C1	2:J:2014:EDO:HO1	2.07	0.56
2:C:2085:EDO:C1	2:C:2085:EDO:HO1	2.11	0.56
1:G:39:LEU:C	1:G:39:LEU:HD23	2.26	0.56
1:I:200:MSE:HA	1:I:200:MSE:CE	2.36	0.56
1:J:87:GLU:HB3	2:J:2014:EDO:H11	1.88	0.56
2:E:2005:EDO:H21	1:F:179:GLU:OE2	2.05	0.55
1:F:84:LYS:HD2	1:F:87:GLU:OE1	2.06	0.55
1:I:132:ASP:CG	2:I:2045:EDO:H21	2.26	0.55
1:J:90:GLU:OE2	1:J:96:ARG:HG3	2.06	0.55
2:J:2105:EDO:C2	2:J:2105:EDO:HO2	2.07	0.55
1:C:44:ALA:O	1:C:47:THR:HB	2.06	0.55
1:I:39:LEU:HD12	1:I:40:PHE:N	2.21	0.55
2:E:2079:EDO:H22	3:E:337:HOH:O	2.07	0.55
2:A:2122:EDO:C2	2:A:2122:EDO:HO2	2.13	0.55
1:B:134:ARG:HG3	2:B:2025:EDO:H22	1.87	0.55
1:D:232:ARG:N	2:D:2072:EDO:H22	2.20	0.55
1:F:104:ASP:OD2	1:F:104:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:ASP:OD1	2:H:2113:EDO:H12	2.07	0.55
2:A:2122:EDO:O2	2:A:2122:EDO:O1	2.21	0.55
1:J:228:ARG:CZ	2:J:2049:EDO:H22	2.36	0.55
2:A:2022:EDO:C2	1:B:236:LYS:NZ	2.71	0.54
1:C:49:VAL:H	2:C:2024:EDO:C1	2.20	0.54
1:E:200:MSE:HE3	1:E:210:TRP:HA	1.89	0.54
1:F:204:GLN:NE2	3:F:1120:HOH:O	2.40	0.54
1:G:203:GLY:HA2	2:G:2047:EDO:O2	2.07	0.54
1:J:197:ARG:O	1:J:201:GLU:HG3	2.07	0.54
1:F:42:HIS:CE1	1:F:75:SER:HB3	2.43	0.54
1:E:119:GLU:HG3	1:F:8:ILE:HG22	1.89	0.54
1:D:112:ARG:CG	1:D:112:ARG:NH1	2.69	0.54
1:E:207:SER:N	2:E:2090:EDO:H22	2.23	0.54
1:F:126:ARG:HB3	1:F:149:ARG:CZ	2.37	0.54
1:I:59:ARG:NH1	1:J:179:GLU:CD	2.60	0.54
2:B:2002:EDO:O2	2:B:2002:EDO:C1	2.51	0.54
1:D:112:ARG:HG2	1:D:112:ARG:NH1	2.22	0.54
1:C:49:VAL:HG23	2:C:2024:EDO:H12	1.90	0.54
1:E:47:THR:HB	1:E:48:PRO:HD2	1.90	0.54
1:G:96:ARG:HD2	3:G:780:HOH:O	2.08	0.54
1:G:183:GLU:N	2:G:2057:EDO:HO2	2.04	0.54
1:C:235:GLU:OE1	2:C:2004:EDO:C2	2.56	0.54
2:C:2075:EDO:H12	2:E:2127:EDO:H22	1.82	0.54
2:C:2126:EDO:C2	2:C:2126:EDO:HO2	2.08	0.54
1:F:123:HIS:CD2	2:F:2086:EDO:H22	2.43	0.54
1:I:105:PRO:O	1:I:106:GLN:CB	2.55	0.54
1:G:86:LYS:HD2	1:G:97:ILE:HB	1.88	0.54
1:E:5:ILE:CD1	1:F:5:ILE:HG21	2.38	0.54
1:C:39:LEU:HD13	1:C:72:ILE:HG23	1.89	0.54
1:I:49:VAL:N	2:I:2121:EDO:HO2	2.03	0.54
1:A:147:LEU:HD23	1:B:171:VAL:HB	1.90	0.53
1:D:43:PRO:HB2	2:D:2118:EDO:C2	2.38	0.53
1:D:44:ALA:O	1:D:47:THR:HB	2.08	0.53
1:F:169:ARG:HB3	1:F:185:LEU:HB3	1.90	0.53
1:H:43:PRO:HG3	1:H:145:MSE:HG2	1.90	0.53
1:I:192:THR:HG1	2:I:2115:EDO:H11	1.73	0.53
1:D:111:ARG:HH21	1:E:106:GLN:HE21	1.56	0.53
1:G:90:GLU:OE2	1:G:96:ARG:HG2	2.09	0.53
1:I:67:LEU:O	1:I:162:LYS:HE2	2.08	0.53
1:A:105:PRO:O	1:A:106:GLN:CB	2.56	0.53
1:A:216:THR:C	2:A:2063:EDO:H11	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:GLU:HG3	3:F:516:HOH:O	2.08	0.53
1:G:145:MSE:CE	1:G:145:MSE:CB	2.86	0.53
1:I:59:ARG:HH11	1:I:59:ARG:CB	2.20	0.53
1:I:206:ARG:HD2	1:I:214:TRP:CZ2	2.44	0.53
1:D:114:GLY:O	1:D:117:HIS:HE1	1.92	0.53
1:C:48:PRO:HG2	1:D:186:ILE:HG21	1.89	0.53
1:D:112:ARG:HH11	1:D:112:ARG:CB	2.21	0.53
1:F:200:MSE:HE1	2:F:2034:EDO:H21	1.91	0.53
1:G:158:VAL:HG12	1:G:162:LYS:HD2	1.90	0.53
1:A:47:THR:HG22	1:A:50:CYS:SG	2.49	0.53
1:D:204:GLN:N	2:D:2035:EDO:H22	2.24	0.53
1:A:130:ILE:HD12	1:A:157:ILE:HG21	1.91	0.53
1:B:62:GLU:O	1:B:66:ARG:HG3	2.08	0.53
1:C:169:ARG:HB3	1:C:185:LEU:HB3	1.91	0.53
1:F:205:TYR:HB2	2:F:2034:EDO:H12	1.89	0.53
1:J:222:ASP:OD2	2:J:2110:EDO:C1	2.56	0.53
1:B:126:ARG:HB3	1:B:149:ARG:CZ	2.39	0.53
1:C:145:MSE:HE3	2:C:2067:EDO:H22	1.91	0.53
1:A:10:GLU:OE2	1:B:2:PRO:N	2.42	0.53
1:A:200:MSE:C	1:A:202:SER:H	2.11	0.53
1:B:111:ARG:HH22	1:C:111:ARG:NH2	1.91	0.53
1:B:243:GLU:CB	1:B:244:GLU:OE1	2.56	0.53
1:F:96:ARG:O	2:F:2095:EDO:H11	2.09	0.53
1:G:228:ARG:NH2	3:G:767:HOH:O	2.41	0.53
1:F:163:LEU:HD22	1:F:167:LEU:HD22	1.91	0.52
2:G:2009:EDO:C1	2:G:2009:EDO:HO1	2.10	0.52
1:F:200:MSE:HA	1:F:200:MSE:CE	2.40	0.52
1:F:205:TYR:H	2:F:2034:EDO:H12	1.73	0.52
1:A:231:ARG:NH1	2:A:2017:EDO:H11	2.24	0.52
2:B:2021:EDO:C2	2:B:2021:EDO:HO2	2.12	0.52
1:F:183:GLU:HG2	2:F:2043:EDO:H11	1.90	0.52
1:C:21:HIS:CB	2:C:2064:EDO:H22	2.40	0.52
1:C:174:ASP:HB3	3:D:2163:HOH:O	2.09	0.52
1:H:59:ARG:HG3	1:H:59:ARG:NH1	2.07	0.52
1:H:129:PHE:CE2	1:H:140:MSE:HE3	2.45	0.52
1:H:145:MSE:CB	1:H:145:MSE:HE2	2.40	0.52
1:I:5:ILE:HG22	1:I:114:GLY:HA3	1.91	0.52
2:A:2124:EDO:C1	2:A:2124:EDO:O2	2.50	0.52
1:J:84:LYS:HD2	1:J:87:GLU:OE2	2.09	0.52
1:J:200:MSE:HA	1:J:200:MSE:HE2	1.91	0.52
1:E:91:ARG:HD3	2:E:2076:EDO:H11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:GLU:CG	1:F:25:LYS:CE	2.88	0.52
1:F:24:ILE:HD11	1:F:26:LEU:CD2	2.39	0.52
1:F:69:VAL:HG21	1:F:158:VAL:HG21	1.92	0.52
2:F:2043:EDO:C2	2:F:2043:EDO:HO2	2.08	0.52
1:J:240:LEU:N	1:J:243:GLU:OE1	2.38	0.52
1:B:99:PHE:HB2	1:B:100:PRO:HD2	1.92	0.52
1:C:126:ARG:HB3	1:C:149:ARG:CZ	2.39	0.52
1:J:185:LEU:O	1:J:214:TRP:HB2	2.10	0.52
1:D:15:MSE:SE	1:D:109:VAL:HG13	2.60	0.51
1:A:134:ARG:HA	2:A:2116:EDO:H21	1.92	0.51
2:G:2102:EDO:O2	2:G:2102:EDO:C1	2.51	0.51
1:C:47:THR:HG22	1:C:50:CYS:SG	2.50	0.51
1:I:228:ARG:NE	2:I:2107:EDO:H22	2.22	0.51
2:F:2038:EDO:H11	1:H:191:THR:CG2	2.40	0.51
1:H:42:HIS:CE1	1:H:75:SER:HB3	2.46	0.51
2:J:2105:EDO:O2	2:J:2105:EDO:C1	2.50	0.51
1:E:207:SER:HB3	1:E:213:CYS:SG	2.51	0.51
2:E:2032:EDO:O2	2:E:2032:EDO:C1	2.53	0.51
1:I:140:MSE:CE	1:I:140:MSE:CB	2.88	0.51
1:J:222:ASP:OD2	2:J:2110:EDO:H11	2.09	0.51
2:B:2023:EDO:C2	2:B:2023:EDO:HO2	2.11	0.51
1:D:203:GLY:N	2:D:2035:EDO:H21	2.26	0.51
2:D:2074:EDO:C1	2:D:2074:EDO:HO1	2.13	0.51
1:E:238:ALA:O	1:E:239:LYS:HB3	2.10	0.51
1:E:62:GLU:HG2	1:E:66:ARG:HE	1.76	0.51
1:J:97:ILE:H	2:J:2109:EDO:H22	1.75	0.51
2:C:2128:EDO:O2	2:C:2128:EDO:C1	2.55	0.51
1:E:206:ARG:CA	2:E:2090:EDO:H22	2.40	0.51
1:F:191:THR:H	1:F:195:GLN:NE2	2.09	0.51
1:B:50:CYS:HG	2:B:2028:EDO:HO1	1.56	0.50
1:D:200:MSE:HA	1:D:200:MSE:CE	2.33	0.50
1:D:205:TYR:O	2:D:2035:EDO:H12	2.12	0.50
1:G:130:ILE:HD12	1:G:157:ILE:HG21	1.93	0.50
1:H:183:GLU:N	2:H:2058:EDO:H11	2.24	0.50
1:I:225:GLU:CB	1:I:228:ARG:HH11	2.24	0.50
1:J:112:ARG:NH1	2:J:2053:EDO:O2	2.44	0.50
1:A:118:ALA:O	1:A:120:SER:N	2.43	0.50
1:A:239:LYS:HD3	1:A:244:GLU:OE2	2.11	0.50
1:C:153:GLU:OE1	1:D:150:LEU:HD22	2.11	0.50
1:G:75:SER:OG	1:G:82:HIS:HE1	1.93	0.50
1:E:7:LEU:HD21	1:F:3:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:PRO:CG	1:J:186:ILE:HG21	2.42	0.50
1:E:126:ARG:HB3	1:E:149:ARG:CZ	2.41	0.50
1:G:126:ARG:HB3	1:G:149:ARG:CZ	2.41	0.50
1:B:132:ASP:CG	2:B:2025:EDO:H21	2.32	0.50
1:B:238:ALA:O	1:B:239:LYS:CB	2.58	0.50
1:B:239:LYS:CG	1:B:243:GLU:OE1	2.59	0.50
1:I:90:GLU:OE1	1:I:96:ARG:HG3	2.11	0.50
1:G:99:PHE:HB2	1:G:100:PRO:HD2	1.94	0.50
1:G:145:MSE:CE	1:G:145:MSE:HB3	2.41	0.50
1:J:228:ARG:HE	2:J:2049:EDO:H11	1.76	0.50
2:C:2082:EDO:C2	2:C:2082:EDO:HO2	2.12	0.50
1:D:203:GLY:CA	2:D:2035:EDO:H21	2.42	0.50
1:E:215:ASP:OD2	1:E:217:PRO:HD3	2.12	0.50
1:H:140:MSE:CE	1:H:142:TYR:OH	2.60	0.50
2:D:2118:EDO:C2	2:D:2118:EDO:HO2	2.10	0.50
1:G:2:PRO:N	1:H:10:GLU:OE2	2.44	0.50
1:B:92:HIS:NE2	2:B:2125:EDO:C1	2.72	0.49
1:B:200:MSE:HE2	1:B:200:MSE:HA	1.92	0.49
1:H:169:ARG:O	2:H:2111:EDO:H11	2.12	0.49
1:C:48:PRO:HD2	2:C:2024:EDO:C1	2.20	0.49
1:F:239:LYS:HG3	1:F:244:GLU:OE2	2.13	0.49
1:G:42:HIS:HB2	1:G:50:CYS:SG	2.52	0.49
2:A:2122:EDO:O2	2:A:2122:EDO:C1	2.53	0.49
1:D:122:THR:OG1	1:E:105:PRO:HG2	2.12	0.49
1:E:90:GLU:OE2	2:E:2127:EDO:O1	2.25	0.49
1:E:209:ASP:OD2	2:E:2120:EDO:H21	2.12	0.49
2:G:2057:EDO:H12	1:H:240:LEU:CD1	2.41	0.49
1:I:134:ARG:HG3	2:I:2045:EDO:H22	1.94	0.49
1:A:147:LEU:HG	1:B:161:LEU:HD13	1.94	0.49
1:A:207:SER:HB3	2:A:2065:EDO:H22	1.95	0.49
1:E:240:LEU:O	1:E:244:GLU:HG3	2.12	0.49
1:I:59:ARG:NH1	1:J:179:GLU:OE1	2.45	0.49
1:C:235:GLU:HB3	2:C:2004:EDO:C2	2.43	0.49
1:E:242:TYR:OH	1:F:206:ARG:HG2	2.13	0.49
1:G:11:ARG:NH1	1:G:14:GLU:OE2	2.43	0.49
1:H:200:MSE:HE2	2:H:2060:EDO:H22	1.95	0.49
1:G:74:LEU:HD13	1:G:74:LEU:C	2.32	0.49
1:F:107:GLY:HA3	1:G:106:GLN:NE2	2.26	0.49
1:F:222:ASP:OD2	2:F:2097:EDO:O2	2.30	0.49
1:I:128:VAL:HG13	1:I:141:LEU:HB2	1.93	0.49
1:B:5:ILE:HG22	1:B:114:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLY:HA2	2:B:2030:EDO:H21	1.95	0.49
1:C:42:HIS:CE1	1:C:75:SER:HB3	2.47	0.49
1:F:183:GLU:HG2	2:F:2043:EDO:H12	1.95	0.49
1:G:197:ARG:HA	2:G:2050:EDO:C2	2.43	0.49
1:D:199:ARG:NH1	3:D:2192:HOH:O	2.33	0.49
1:E:241:LEU:CD2	1:E:244:GLU:OE1	2.38	0.49
1:J:122:THR:HG23	1:J:123:HIS:CD2	2.48	0.49
1:C:186:ILE:HG21	1:D:48:PRO:HG2	1.95	0.48
1:F:25:LYS:NZ	3:F:556:HOH:O	2.41	0.48
1:F:199:ARG:HG2	1:F:200:MSE:CE	2.43	0.48
1:D:32:SER:O	3:D:2214:HOH:O	2.20	0.48
1:F:67:LEU:O	1:F:162:LYS:HE3	2.13	0.48
1:G:169:ARG:O	2:G:2112:EDO:C1	2.51	0.48
1:H:235:GLU:OE1	2:H:2010:EDO:H21	2.13	0.48
1:A:105:PRO:O	1:A:106:GLN:HB2	2.13	0.48
1:A:200:MSE:C	1:A:202:SER:N	2.66	0.48
1:A:119:GLU:HG3	1:B:8:ILE:HG22	1.94	0.48
1:A:183:GLU:HG2	2:A:2022:EDO:O2	2.14	0.48
1:E:199:ARG:HH21	2:E:2091:EDO:C2	2.22	0.48
1:C:167:LEU:HD11	2:C:2036:EDO:H21	1.95	0.48
1:E:67:LEU:HD13	1:E:158:VAL:HG23	1.95	0.48
1:E:90:GLU:OE2	2:E:2127:EDO:C1	2.62	0.48
1:H:59:ARG:CG	1:H:59:ARG:NH1	2.73	0.48
2:E:2005:EDO:C2	3:E:513:HOH:O	2.62	0.48
1:A:243:GLU:C	1:A:245:ALA:N	2.65	0.48
1:I:84:LYS:HD2	1:I:87:GLU:OE1	2.14	0.48
2:J:2123:EDO:O1	2:J:2123:EDO:O2	2.23	0.48
1:E:240:LEU:HD11	2:F:2043:EDO:H21	1.94	0.48
1:F:14:GLU:HG3	1:F:25:LYS:CE	2.44	0.48
1:I:66:ARG:HB3	1:I:66:ARG:CZ	2.44	0.48
1:I:205:TYR:H	2:I:2051:EDO:C2	2.20	0.48
1:A:117:HIS:CD2	1:B:8:ILE:H	2.16	0.48
1:A:214:TRP:CH2	3:A:2219:HOH:O	2.55	0.48
1:F:163:LEU:O	1:F:167:LEU:HB2	2.14	0.48
1:I:126:ARG:HH22	2:I:2121:EDO:C1	2.26	0.48
1:A:174:ASP:HB3	3:B:2222:HOH:O	2.13	0.47
1:A:200:MSE:HE2	2:A:2065:EDO:H11	1.95	0.47
1:B:5:ILE:HB	1:B:140:MSE:HE1	1.96	0.47
1:C:235:GLU:O	2:C:2004:EDO:O2	2.32	0.47
1:D:111:ARG:HH22	1:E:111:ARG:NH2	2.10	0.47
1:H:117:HIS:HB2	1:H:125:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:200:MSE:HE1	2:H:2060:EDO:H22	1.96	0.47
1:A:159:LYS:HE2	1:A:225:GLU:OE2	2.15	0.47
1:C:178:ASN:HD21	1:D:52:THR:HB	1.79	0.47
1:F:123:HIS:HD2	2:F:2086:EDO:H22	1.80	0.47
2:F:2098:EDO:C2	2:F:2098:EDO:HO2	2.15	0.47
2:G:2050:EDO:C2	2:G:2050:EDO:HO2	2.09	0.47
1:H:74:LEU:HD13	1:H:75:SER:N	2.28	0.47
1:H:232:ARG:O	2:H:2010:EDO:O2	2.31	0.47
1:C:92:HIS:O	1:C:245:ALA:HB1	2.14	0.47
1:F:199:ARG:HG2	1:F:200:MSE:HE3	1.96	0.47
1:H:235:GLU:HB3	2:H:2010:EDO:H21	1.97	0.47
1:I:163:LEU:O	1:I:167:LEU:HB2	2.15	0.47
2:I:2103:EDO:HO2	1:J:236:LYS:HZ1	1.54	0.47
1:B:67:LEU:HB2	1:B:69:VAL:HG23	1.96	0.47
1:C:215:ASP:OD2	1:C:217:PRO:HD3	2.13	0.47
1:D:159:LYS:HE2	1:D:225:GLU:OE2	2.15	0.47
1:E:3:GLY:HA3	1:F:7:LEU:HD21	1.96	0.47
1:E:121:ALA:CB	1:E:121:ALA:N	2.67	0.47
1:C:36:TRP:CD1	1:C:162:LYS:NZ	2.82	0.47
1:E:10:GLU:OE2	1:F:2:PRO:CB	2.62	0.47
1:G:197:ARG:HA	2:G:2050:EDO:H22	1.95	0.47
1:H:69:VAL:CG2	1:H:158:VAL:HG11	2.43	0.47
1:H:215:ASP:OD2	1:H:217:PRO:HD3	2.15	0.47
1:B:7:LEU:O	1:B:10:GLU:HB2	2.14	0.47
1:B:54:PHE:HE2	1:B:101:ILE:HG12	1.80	0.47
1:C:91:ARG:NH1	2:C:2126:EDO:H12	2.30	0.47
1:D:96:ARG:HH12	1:F:197:ARG:NH1	2.13	0.47
3:E:290:HOH:O	1:F:174:ASP:HB3	2.13	0.47
1:G:100:PRO:HD3	2:G:2093:EDO:H21	1.96	0.47
1:G:175:TRP:CG	1:G:176:PRO:HA	2.49	0.47
1:A:105:PRO:HG2	1:J:122:THR:OG1	2.14	0.47
1:C:219:SER:HB3	1:C:222:ASP:H	1.79	0.47
1:D:189:PRO:HA	1:D:190:PRO:HD3	1.72	0.47
1:J:199:ARG:HG2	2:J:2104:EDO:H12	1.97	0.47
1:I:5:ILE:CD1	1:J:5:ILE:HD13	2.38	0.47
1:B:86:LYS:HE3	1:B:101:ILE:CD1	2.45	0.47
1:I:92:HIS:O	1:I:245:ALA:HB1	2.15	0.47
1:J:86:LYS:HB3	2:J:2109:EDO:C2	2.31	0.47
2:B:2023:EDO:O2	2:B:2023:EDO:C1	2.55	0.46
1:C:193:GLU:O	2:C:2075:EDO:O1	2.33	0.46
2:C:2024:EDO:O2	2:C:2024:EDO:C1	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2031:EDO:O2	2:D:2031:EDO:C1	2.57	0.46
1:F:123:HIS:CD2	2:F:2086:EDO:H21	2.48	0.46
1:G:202:SER:OG	1:G:204:GLN:HG2	2.15	0.46
1:I:144:PRO:HD3	1:J:139:THR:OG1	2.14	0.46
1:C:186:ILE:HG21	1:D:48:PRO:CG	2.45	0.46
1:A:49:VAL:H	2:A:2012:EDO:C2	2.22	0.46
2:C:2004:EDO:O1	2:C:2004:EDO:C2	2.56	0.46
1:H:48:PRO:O	1:H:52:THR:HG23	2.15	0.46
1:H:79:VAL:O	1:H:83:ILE:HG13	2.15	0.46
1:J:228:ARG:HE	2:J:2049:EDO:C1	2.27	0.46
2:A:2012:EDO:C2	2:A:2012:EDO:HO2	2.13	0.46
1:C:235:GLU:OE1	2:C:2080:EDO:C2	2.63	0.46
1:D:191:THR:H	1:D:195:GLN:HE22	1.59	0.46
1:E:236:LYS:NZ	2:F:2043:EDO:C2	2.69	0.46
1:H:207:SER:HB2	2:H:2060:EDO:H11	1.97	0.46
2:I:2007:EDO:C1	2:I:2007:EDO:HO1	2.11	0.46
1:J:86:LYS:O	2:J:2109:EDO:O1	2.16	0.46
1:A:214:TRP:HH2	3:A:2219:HOH:O	1.94	0.46
1:C:129:PHE:HE2	1:C:140:MSE:CE	2.16	0.46
1:C:145:MSE:CB	1:C:145:MSE:CE	2.93	0.46
1:C:224:GLU:CD	1:C:231:ARG:HH22	2.19	0.46
1:F:90:GLU:HG2	1:F:96:ARG:HA	1.97	0.46
1:J:109:VAL:HG21	2:J:2061:EDO:H22	1.98	0.46
1:A:47:THR:HG23	2:A:2012:EDO:C2	2.45	0.46
1:B:65:GLN:HA	1:B:65:GLN:HE21	1.81	0.46
1:H:183:GLU:HG2	2:H:2058:EDO:C1	2.39	0.46
2:H:2058:EDO:O2	2:H:2058:EDO:O1	2.33	0.46
1:I:128:VAL:O	1:I:140:MSE:HA	2.16	0.46
1:D:74:LEU:HD13	1:D:74:LEU:C	2.36	0.46
1:G:236:LYS:NZ	1:G:236:LYS:CD	2.68	0.46
1:I:238:ALA:C	1:I:239:LYS:HD2	2.36	0.46
1:B:222:ASP:OD2	2:B:2018:EDO:H11	2.16	0.46
1:D:204:GLN:H	2:D:2035:EDO:H21	1.81	0.46
1:F:106:GLN:H	1:G:106:GLN:H	1.64	0.46
1:F:239:LYS:HD2	1:F:244:GLU:OE2	2.16	0.46
2:J:2123:EDO:O1	2:J:2123:EDO:C2	2.58	0.46
1:D:153:GLU:OE1	1:D:153:GLU:HA	2.16	0.46
1:H:74:LEU:HD13	1:H:74:LEU:C	2.36	0.46
1:A:47:THR:CG2	1:A:50:CYS:SG	3.04	0.46
1:B:96:ARG:O	1:B:98:PRO:HD3	2.15	0.46
1:C:232:ARG:O	2:C:2004:EDO:O2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:TRP:HA	2:E:2076:EDO:C1	2.46	0.46
1:E:194:ASP:OD1	1:E:194:ASP:C	2.54	0.46
1:H:36:TRP:CD2	1:H:132:ASP:HA	2.52	0.46
1:I:69:VAL:HG21	1:I:158:VAL:HG21	1.98	0.46
1:E:159:LYS:HZ2	2:E:2088:EDO:C2	2.28	0.45
1:J:208:LEU:HA	1:J:208:LEU:HD12	1.74	0.45
1:C:55:VAL:O	1:C:59:ARG:HG3	2.16	0.45
1:E:185:LEU:O	1:E:214:TRP:HB2	2.16	0.45
1:E:186:ILE:HG21	1:F:48:PRO:HG2	1.97	0.45
1:G:5:ILE:HG21	1:H:5:ILE:HD13	1.98	0.45
1:I:5:ILE:HD11	1:J:5:ILE:HG21	1.98	0.45
1:C:48:PRO:CG	2:C:2024:EDO:H11	2.45	0.45
1:C:91:ARG:CD	2:C:2126:EDO:O1	2.62	0.45
1:C:235:GLU:OE1	2:C:2004:EDO:H22	2.15	0.45
1:E:18:THR:HG21	2:E:2077:EDO:H12	1.97	0.45
1:A:214:TRP:CZ3	3:A:2219:HOH:O	2.68	0.45
2:A:2124:EDO:C1	2:A:2124:EDO:HO1	2.13	0.45
1:B:243:GLU:C	1:B:244:GLU:OE1	2.55	0.45
2:I:2007:EDO:H12	3:I:2207:HOH:O	2.17	0.45
1:J:228:ARG:HH21	2:J:2049:EDO:C2	2.26	0.45
1:F:207:SER:HB2	2:F:2034:EDO:H22	1.98	0.45
1:F:208:LEU:HD12	1:F:208:LEU:HA	1.83	0.45
1:G:74:LEU:HD13	1:G:75:SER:N	2.31	0.45
1:A:59:ARG:HH11	1:A:59:ARG:HD3	1.62	0.45
1:A:186:ILE:HG21	1:B:48:PRO:HG2	1.98	0.45
1:B:67:LEU:HD13	1:B:158:VAL:HG23	1.99	0.45
1:B:104:ASP:N	1:B:104:ASP:OD2	2.37	0.45
1:B:106:GLN:HG2	1:C:122:THR:HA	1.99	0.45
1:E:205:TYR:O	2:E:2042:EDO:H12	2.16	0.45
2:F:2038:EDO:H11	1:H:191:THR:HG22	1.98	0.45
1:G:10:GLU:OE2	1:H:2:PRO:N	2.49	0.45
1:H:215:ASP:C	1:H:217:PRO:HD3	2.37	0.45
1:H:235:GLU:O	2:H:2010:EDO:O2	2.33	0.45
1:I:84:LYS:HD2	1:I:84:LYS:HA	1.83	0.45
1:J:200:MSE:SE	2:J:2105:EDO:H21	2.66	0.45
1:C:235:GLU:HB3	2:C:2004:EDO:H21	1.99	0.45
1:E:159:LYS:NZ	1:E:225:GLU:OE2	2.50	0.45
1:J:169:ARG:HE	1:J:215:ASP:HB2	1.81	0.45
1:B:220:ARG:CD	1:B:224:GLU:OE2	2.65	0.45
1:D:134:ARG:HG3	2:D:2031:EDO:H11	1.99	0.45
1:B:111:ARG:HH21	1:C:106:GLN:NE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:LYS:NZ	1:F:244:GLU:OE1	2.47	0.45
1:G:189:PRO:HA	1:G:190:PRO:HD3	1.82	0.45
1:I:203:GLY:C	2:I:2051:EDO:H21	2.37	0.45
1:C:189:PRO:HA	1:C:190:PRO:HD3	1.83	0.45
1:F:203:GLY:O	2:F:2098:EDO:H12	2.16	0.45
1:F:206:ARG:NH1	1:F:214:TRP:CH2	2.85	0.45
1:I:174:ASP:HB3	3:J:2219:HOH:O	2.16	0.45
1:I:184:GLY:HA2	1:I:216:THR:HG22	1.99	0.45
1:J:15:MSE:O	1:J:15:MSE:HG3	2.17	0.45
1:C:47:THR:HA	1:C:48:PRO:HD3	1.89	0.44
1:F:218:ALA:HA	2:F:2097:EDO:O2	2.18	0.44
1:A:5:ILE:HG22	1:A:114:GLY:HA3	1.98	0.44
1:D:114:GLY:O	1:D:117:HIS:CE1	2.70	0.44
1:F:114:GLY:O	1:F:117:HIS:HE1	1.99	0.44
1:I:19:THR:HG22	1:I:102:ILE:HG12	2.00	0.44
1:B:130:ILE:HD13	1:B:157:ILE:HG21	1.98	0.44
1:B:244:GLU:N	1:B:244:GLU:CD	2.71	0.44
1:D:163:LEU:HD21	1:D:222:ASP:CG	2.38	0.44
1:E:92:HIS:NE2	2:E:2076:EDO:C2	2.80	0.44
1:F:239:LYS:CE	1:F:244:GLU:OE1	2.65	0.44
1:G:41:SER:HB2	1:G:124:THR:HG21	1.99	0.44
1:G:106:GLN:O	1:G:111:ARG:NH2	2.50	0.44
1:J:157:ILE:HG22	1:J:161:LEU:HD22	1.98	0.44
2:J:2108:EDO:C1	3:J:2191:HOH:O	2.65	0.44
1:A:33:GLN:HB2	1:A:35:LYS:HG3	1.99	0.44
1:A:126:ARG:HB3	1:A:149:ARG:CZ	2.47	0.44
2:C:2004:EDO:C2	2:C:2004:EDO:HO2	2.16	0.44
1:D:215:ASP:OD2	1:D:217:PRO:HD3	2.17	0.44
1:A:174:ASP:HA	1:B:150:LEU:HD23	1.98	0.44
1:D:126:ARG:HB3	1:D:149:ARG:CZ	2.47	0.44
1:B:239:LYS:HA	1:B:243:GLU:OE1	2.16	0.44
1:D:244:GLU:H	1:D:244:GLU:HG3	1.64	0.44
1:E:171:VAL:HB	1:F:147:LEU:HD12	2.00	0.44
1:G:239:LYS:HG2	1:G:244:GLU:CG	2.47	0.44
1:I:140:MSE:CE	1:I:142:TYR:OH	2.65	0.44
1:I:157:ILE:HG23	1:J:147:LEU:CD1	2.47	0.44
1:J:21:HIS:CB	2:J:2068:EDO:H21	2.47	0.44
1:J:48:PRO:O	1:J:52:THR:HG23	2.17	0.44
1:A:232:ARG:O	2:A:2001:EDO:O2	2.35	0.44
1:E:206:ARG:HA	2:E:2090:EDO:C2	2.44	0.44
1:I:17:VAL:HA	2:I:2100:EDO:C1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.72	0.44
1:D:39:LEU:HD12	1:D:40:PHE:N	2.33	0.44
1:I:42:HIS:CE1	1:I:75:SER:HB3	2.53	0.44
2:I:2115:EDO:O2	2:I:2115:EDO:C1	2.55	0.44
1:J:114:GLY:O	1:J:117:HIS:HE1	2.00	0.44
1:J:169:ARG:HB3	1:J:185:LEU:HB3	1.99	0.44
1:A:242:TYR:CE1	1:B:214:TRP:HH2	2.35	0.44
1:B:65:GLN:O	1:B:67:LEU:O	2.36	0.44
1:D:129:PHE:CZ	1:D:140:MSE:HE3	2.50	0.44
1:E:53:GLU:HG2	1:F:173:ALA:HB2	2.00	0.44
1:E:236:LYS:NZ	1:F:183:GLU:OE2	2.50	0.44
1:G:186:ILE:HG21	1:H:48:PRO:HG2	2.00	0.44
1:G:205:TYR:H	2:G:2047:EDO:C1	2.31	0.44
1:H:200:MSE:HE1	1:H:213:CYS:SG	2.58	0.44
1:J:109:VAL:CG2	2:J:2061:EDO:H22	2.47	0.44
1:A:163:LEU:HD22	1:A:167:LEU:CD2	2.44	0.43
1:E:112:ARG:HH11	2:E:2079:EDO:H12	1.83	0.43
1:I:199:ARG:HD3	3:I:2153:HOH:O	2.17	0.43
1:C:112:ARG:HH11	1:C:112:ARG:CA	2.31	0.43
2:D:2119:EDO:H22	3:D:2205:HOH:O	2.17	0.43
1:E:5:ILE:HD11	1:F:5:ILE:HG21	2.00	0.43
1:E:24:ILE:HG21	1:E:24:ILE:HD13	1.62	0.43
1:F:182:GLY:HA3	2:F:2043:EDO:H21	1.98	0.43
1:I:150:LEU:HD12	1:J:174:ASP:CB	2.33	0.43
1:C:36:TRP:CD2	1:C:132:ASP:HA	2.52	0.43
1:E:147:LEU:HD23	1:F:171:VAL:HB	2.00	0.43
2:I:2007:EDO:C1	3:I:2207:HOH:O	2.65	0.43
1:A:157:ILE:HG22	1:A:161:LEU:HD22	2.01	0.43
1:A:207:SER:HB2	1:A:213:CYS:SG	2.58	0.43
1:B:28:ASP:O	1:B:32:SER:HB2	2.18	0.43
1:F:237:PRO:HG2	1:F:240:LEU:HD21	2.00	0.43
1:H:5:ILE:HG13	1:H:6:PRO:O	2.19	0.43
1:I:163:LEU:HD22	1:I:167:LEU:HD22	2.00	0.43
1:J:76:VAL:O	1:J:105:PRO:HA	2.19	0.43
1:B:24:ILE:HD13	1:B:24:ILE:HG21	1.75	0.43
1:C:103:ALA:C	1:C:105:PRO:HD3	2.37	0.43
1:I:122:THR:HG23	1:I:123:HIS:CD2	2.53	0.43
1:I:203:GLY:N	2:I:2051:EDO:H21	2.33	0.43
1:B:240:LEU:HA	1:B:240:LEU:HD23	1.75	0.43
1:H:183:GLU:H	2:H:2058:EDO:H12	1.82	0.43
1:H:235:GLU:CG	2:H:2010:EDO:H21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:LEU:HD12	1:I:39:LEU:C	2.38	0.43
1:I:192:THR:HG21	2:I:2115:EDO:C2	2.49	0.43
1:J:67:LEU:CD2	1:J:159:LYS:HD3	2.49	0.43
1:J:235:GLU:O	2:J:2008:EDO:O1	2.37	0.43
1:D:47:THR:CG2	1:D:50:CYS:SG	3.06	0.43
1:D:143:TYR:HD2	1:D:147:LEU:HD13	1.84	0.43
2:E:2089:EDO:C2	2:E:2089:EDO:HO2	2.12	0.43
1:G:179:GLU:HG2	1:H:59:ARG:NH1	2.23	0.43
2:G:2093:EDO:O2	2:G:2093:EDO:O1	2.34	0.43
1:J:21:HIS:CG	2:J:2068:EDO:H21	2.54	0.43
1:J:157:ILE:CG2	1:J:161:LEU:HD22	2.49	0.43
1:C:21:HIS:HB2	2:C:2064:EDO:H22	2.00	0.43
1:D:112:ARG:HD2	3:D:2218:HOH:O	2.18	0.43
1:D:175:TRP:CG	1:D:176:PRO:HA	2.54	0.43
1:G:139:THR:OG1	1:H:144:PRO:HD3	2.19	0.43
1:C:188:PRO:HA	1:C:189:PRO:HD3	1.94	0.43
1:D:228:ARG:HG3	2:D:2072:EDO:C1	2.47	0.43
1:G:146:GLU:HB3	2:H:2111:EDO:H21	2.01	0.43
1:H:76:VAL:HG11	1:I:106:GLN:NE2	2.34	0.43
1:H:117:HIS:HB2	1:H:125:VAL:CG1	2.48	0.43
1:D:111:ARG:NH2	1:E:106:GLN:HE21	2.16	0.42
1:E:88:TRP:HA	2:E:2076:EDO:H12	2.01	0.42
1:G:8:ILE:N	1:H:117:HIS:CD2	2.66	0.42
1:G:235:GLU:HB2	2:G:2009:EDO:C1	2.46	0.42
1:A:14:GLU:O	1:A:112:ARG:NH2	2.51	0.42
1:B:189:PRO:HA	1:B:190:PRO:HD3	1.94	0.42
1:D:239:LYS:CE	1:D:244:GLU:OE2	2.55	0.42
1:E:15:MSE:CE	1:E:112:ARG:HG2	2.49	0.42
1:F:36:TRP:CD2	1:F:132:ASP:HA	2.54	0.42
1:F:111:ARG:NH2	1:G:106:GLN:NE2	2.64	0.42
1:H:12:PHE:CZ	1:H:39:LEU:HD23	2.54	0.42
1:H:200:MSE:HE2	1:H:200:MSE:HA	2.01	0.42
1:J:42:HIS:HB2	1:J:50:CYS:SG	2.58	0.42
1:B:210:TRP:CZ3	1:B:211:TRP:HB3	2.54	0.42
1:D:104:ASP:N	1:D:105:PRO:CD	2.82	0.42
1:D:191:THR:N	1:D:195:GLN:NE2	2.57	0.42
1:E:106:GLN:O	1:E:111:ARG:NH2	2.53	0.42
1:G:132:ASP:OD1	1:G:132:ASP:C	2.58	0.42
2:J:2008:EDO:C1	2:J:2008:EDO:HO2	2.31	0.42
2:A:2029:EDO:O2	2:A:2029:EDO:C1	2.54	0.42
2:C:2024:EDO:H21	2:C:2067:EDO:O1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:THR:HG23	1:E:123:HIS:HD2	1.83	0.42
1:H:145:MSE:CE	1:H:145:MSE:HB3	2.48	0.42
1:A:7:LEU:HA	1:A:140:MSE:HE1	2.00	0.42
1:C:67:LEU:O	1:C:162:LYS:CE	2.62	0.42
1:E:174:ASP:HB3	3:E:505:HOH:O	2.19	0.42
1:H:76:VAL:HG11	1:I:106:GLN:HE22	1.83	0.42
1:I:180:ILE:HA	1:J:241:LEU:HB2	2.01	0.42
1:I:199:ARG:HD2	1:I:205:TYR:CE1	2.55	0.42
1:J:5:ILE:HB	1:J:6:PRO:HD2	2.02	0.42
1:A:61:TYR:HD1	1:A:71:LEU:HD12	1.85	0.42
1:C:139:THR:OG1	1:D:144:PRO:HD3	2.19	0.42
1:E:200:MSE:HE1	1:E:213:CYS:SG	2.59	0.42
1:G:5:ILE:HD13	1:H:5:ILE:HD13	2.00	0.42
1:G:146:GLU:CB	2:H:2111:EDO:H21	2.49	0.42
1:H:132:ASP:C	1:H:132:ASP:OD1	2.58	0.42
1:J:190:PRO:HG3	1:J:199:ARG:HG3	2.01	0.42
1:D:235:GLU:CB	2:D:2003:EDO:H11	2.31	0.42
1:E:91:ARG:NH1	2:E:2076:EDO:O2	2.53	0.42
1:F:140:MSE:HB3	1:F:140:MSE:HE2	1.71	0.42
1:F:204:GLN:HE21	1:F:204:GLN:HB2	1.42	0.42
1:E:134:ARG:HG3	2:E:2039:EDO:H11	2.01	0.42
1:G:242:TYR:CD2	1:G:243:GLU:HG3	2.55	0.42
1:I:146:GLU:HG3	3:J:2159:HOH:O	2.20	0.42
2:A:2124:EDO:C2	2:A:2124:EDO:HO2	2.13	0.42
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.54	0.42
1:E:25:LYS:NZ	1:E:25:LYS:HD2	2.28	0.42
1:E:208:LEU:HD13	1:F:242:TYR:CD1	2.55	0.42
1:E:214:TRP:CH2	1:F:242:TYR:CG	3.04	0.42
1:F:79:VAL:HG22	2:F:2038:EDO:H12	2.02	0.42
1:F:185:LEU:HD23	1:F:185:LEU:HA	1.87	0.42
1:A:189:PRO:HA	1:A:190:PRO:HD3	1.78	0.42
1:E:139:THR:C	1:E:140:MSE:HG3	2.40	0.42
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.78	0.42
1:F:79:VAL:CG2	2:F:2038:EDO:H12	2.50	0.42
1:J:97:ILE:N	2:J:2109:EDO:C1	2.55	0.42
1:F:99:PHE:HB2	1:F:100:PRO:HD2	2.01	0.41
1:F:106:GLN:HG2	1:G:122:THR:HA	2.02	0.41
2:F:2087:EDO:H11	3:F:998:HOH:O	2.20	0.41
1:G:8:ILE:HG13	1:H:117:HIS:CD2	2.55	0.41
1:I:157:ILE:HG23	1:J:147:LEU:HD11	2.01	0.41
1:J:67:LEU:HD21	1:J:159:LYS:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:163:LEU:HD22	1:J:167:LEU:HD22	2.00	0.41
1:A:242:TYR:HD1	1:B:208:LEU:CD1	2.33	0.41
1:B:105:PRO:HG2	1:C:122:THR:OG1	2.21	0.41
1:F:42:HIS:HB2	1:F:50:CYS:SG	2.60	0.41
1:A:45:ASP:O	1:A:46:PHE:HB2	2.20	0.41
1:B:204:GLN:N	2:B:2030:EDO:H21	2.35	0.41
1:C:14:GLU:OE1	1:C:25:LYS:HE2	2.20	0.41
1:C:111:ARG:HG3	1:C:116:LEU:HD12	2.02	0.41
1:E:91:ARG:HD3	2:E:2076:EDO:C1	2.50	0.41
1:I:192:THR:CG2	2:I:2115:EDO:H22	2.50	0.41
1:J:96:ARG:CG	2:J:2109:EDO:O2	2.59	0.41
1:J:225:GLU:HG3	2:J:2049:EDO:C2	2.50	0.41
2:J:2108:EDO:H11	3:J:2191:HOH:O	2.20	0.41
1:B:87:GLU:HG2	1:B:91:ARG:NH2	2.35	0.41
1:B:185:LEU:O	1:B:214:TRP:HB2	2.21	0.41
1:B:231:ARG:HH11	1:B:231:ARG:HD2	1.62	0.41
1:F:41:SER:HA	1:F:74:LEU:O	2.20	0.41
1:G:42:HIS:CE1	1:G:75:SER:HB3	2.55	0.41
1:I:86:LYS:HE3	1:I:101:ILE:CD1	2.50	0.41
1:A:91:ARG:HG2	1:A:92:HIS:CD2	2.54	0.41
1:B:91:ARG:NE	2:B:2125:EDO:O2	2.53	0.41
1:B:173:ALA:O	1:B:174:ASP:HB2	2.19	0.41
1:G:19:THR:HG22	1:G:102:ILE:HG12	2.02	0.41
1:I:19:THR:HA	1:I:102:ILE:HA	2.02	0.41
1:F:128:VAL:O	1:F:140:MSE:HA	2.20	0.41
1:J:35:LYS:CD	1:J:70:ASP:OD2	2.67	0.41
1:C:179:GLU:CD	1:D:59:ARG:HH12	2.24	0.41
1:F:13:PRO:O	1:F:15:MSE:HG2	2.21	0.41
1:H:35:LYS:NZ	1:H:65:GLN:HE22	2.19	0.41
1:I:11:ARG:HD3	3:I:2167:HOH:O	2.20	0.41
1:E:36:TRP:CD1	1:E:162:LYS:HE2	2.56	0.41
1:G:145:MSE:HE2	1:G:145:MSE:CB	2.51	0.41
1:I:242:TYR:HA	1:I:245:ALA:HB3	2.03	0.41
1:B:67:LEU:CB	1:B:69:VAL:HG23	2.51	0.41
1:B:227:ARG:HH11	1:B:227:ARG:HD2	1.62	0.41
1:E:15:MSE:SE	1:E:109:VAL:HG13	2.71	0.41
1:E:15:MSE:HE1	1:E:112:ARG:HG2	2.02	0.41
1:E:128:VAL:O	1:E:140:MSE:HA	2.21	0.41
1:E:150:LEU:HD12	1:E:150:LEU:HA	1.86	0.41
1:G:5:ILE:O	1:H:2:PRO:HB3	2.21	0.41
1:G:183:GLU:HG2	2:G:2057:EDO:C2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:LYS:HG2	1:G:244:GLU:OE2	2.20	0.41
1:H:235:GLU:OE1	2:H:2010:EDO:C2	2.69	0.41
1:A:244:GLU:OE2	2:A:2066:EDO:H22	2.21	0.41
1:E:236:LYS:CE	2:F:2043:EDO:H22	2.50	0.41
1:B:216:THR:HA	3:B:2200:HOH:O	2.20	0.40
1:C:15:MSE:O	1:C:15:MSE:HG3	2.21	0.40
1:C:36:TRP:HB2	1:C:69:VAL:HG22	2.04	0.40
1:D:5:ILE:HG22	1:D:114:GLY:HA3	2.03	0.40
1:E:191:THR:H	1:E:195:GLN:NE2	2.18	0.40
1:F:112:ARG:NH1	1:F:112:ARG:CB	2.79	0.40
1:J:183:GLU:H	1:J:183:GLU:HG2	1.45	0.40
3:A:2219:HOH:O	1:B:242:TYR:HB2	2.21	0.40
1:B:68:GLY:HA3	3:B:2242:HOH:O	2.21	0.40
1:B:169:ARG:HB3	1:B:185:LEU:HB3	2.03	0.40
1:C:35:LYS:HG3	2:C:2084:EDO:H11	2.02	0.40
1:D:43:PRO:HG3	1:D:145:MSE:HG2	2.01	0.40
1:E:52:THR:HB	1:F:178:ASN:HD21	1.85	0.40
1:F:168:LYS:HE3	3:F:1011:HOH:O	2.20	0.40
1:H:132:ASP:OD2	1:H:138:ARG:HD3	2.21	0.40
1:H:227:ARG:HH11	1:H:227:ARG:HD2	1.55	0.40
1:B:104:ASP:OD1	1:B:107:GLY:HA2	2.22	0.40
1:D:74:LEU:HD23	1:D:102:ILE:HB	2.03	0.40
1:D:106:GLN:O	1:D:111:ARG:NH1	2.54	0.40
1:D:231:ARG:HH11	1:D:231:ARG:HD2	1.56	0.40
1:E:5:ILE:HD13	1:F:5:ILE:HG21	2.03	0.40
1:G:199:ARG:HH11	1:G:199:ARG:HD2	1.56	0.40
1:J:189:PRO:HA	1:J:190:PRO:HD3	1.73	0.40
1:A:171:VAL:HA	1:A:172:PRO:HD2	1.88	0.40
1:A:231:ARG:NH2	3:A:2260:HOH:O	2.28	0.40
1:B:187:VAL:O	1:B:188:PRO:C	2.60	0.40
1:E:52:THR:HG22	1:F:180:ILE:HD12	2.03	0.40
1:E:104:ASP:HB2	3:E:336:HOH:O	2.22	0.40
1:G:240:LEU:HD23	1:G:240:LEU:HA	1.88	0.40
1:J:240:LEU:H	1:J:243:GLU:CD	2.22	0.40
1:B:244:GLU:CD	1:B:244:GLU:H	2.25	0.40
1:E:84:LYS:HA	1:E:84:LYS:HD2	1.94	0.40
1:F:219:SER:N	2:F:2097:EDO:O2	2.36	0.40
1:H:42:HIS:HB2	1:H:50:CYS:SG	2.62	0.40
1:H:231:ARG:NH2	3:H:1081:HOH:O	2.50	0.40
1:I:143:TYR:CD2	1:I:147:LEU:HD13	2.57	0.40
1:J:216:THR:N	1:J:217:PRO:CD	2.85	0.40



All (1) 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)
2:H:2114:EDO:O1	3:C:2190:HOH:O[1_556]	2.16	0.04

## 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	242/249 (97%)	229 (95%)	10 (4%)	3 (1%)	13	7
1	B	242/249 (97%)	234 (97%)	6 (2%)	2 (1%)	19	13
1	C	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	34	30
1	D	242/249 (97%)	231 (96%)	9 (4%)	2 (1%)	19	13
1	E	242/249 (97%)	233 (96%)	6 (2%)	3 (1%)	13	7
1	F	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	34	30
1	G	242/249 (97%)	232 (96%)	7 (3%)	3 (1%)	13	7
1	H	242/249 (97%)	233 (96%)	7 (3%)	2 (1%)	19	13
1	I	242/249 (97%)	234 (97%)	7 (3%)	1 (0%)	34	30
1	J	242/249 (97%)	236 (98%)	3 (1%)	3 (1%)	13	7
All	All	2420/2490 (97%)	2332 (96%)	67 (3%)	21 (1%)	17	11

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	176	PRO
1	G	27	PRO
1	J	27	PRO
1	A	106	GLN
1	A	244	GLU
1	B	106	GLN
1	E	106	GLN

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Mol	Chain	Res	Type
1	H	106	GLN
1	J	106	GLN
1	G	106	GLN
1	I	119	GLU
1	D	105	PRO
1	E	239	LYS
1	G	239	LYS
1	F	106	GLN
1	C	125	VAL
1	H	125	VAL
1	A	203	GLY
1	B	125	VAL
1	D	125	VAL
1	J	125	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/211 (100%)	190 (90%)	20 (10%)	8	5
1	B	210/211 (100%)	193 (92%)	17 (8%)	11	7
1	C	210/211 (100%)	189 (90%)	21 (10%)	7	4
1	D	210/211 (100%)	193 (92%)	17 (8%)	11	7
1	E	210/211 (100%)	197 (94%)	13 (6%)	18	13
1	F	210/211 (100%)	193 (92%)	17 (8%)	11	7
1	G	210/211 (100%)	195 (93%)	15 (7%)	14	10
1	H	210/211 (100%)	197 (94%)	13 (6%)	18	13
1	I	210/211 (100%)	190 (90%)	20 (10%)	8	5
1	J	210/211 (100%)	190 (90%)	20 (10%)	8	5
All	All	2100/2110 (100%)	1927 (92%)	173 (8%)	11	7

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	14	GLU
1	A	16	GLU
1	A	28	ASP
1	A	47	THR
1	A	147	LEU
1	A	159	LYS
1	A	161	LEU
1	A	162	LYS
1	A	166	SER
1	A	167	LEU
1	A	176	PRO
1	A	194	ASP
1	A	197	ARG
1	A	202	SER
1	A	207	SER
1	A	208	LEU
1	A	212	PHE
1	A	214	TRP
1	A	244	GLU
1	B	4	SER
1	B	11	ARG
1	B	39	LEU
1	B	59	ARG
1	B	65	GLN
1	B	112	ARG
1	B	147	LEU
1	B	150	LEU
1	B	159	LYS
1	B	161	LEU
1	B	162	LYS
1	B	167	LEU
1	B	199	ARG
1	B	208	LEU
1	B	212	PHE
1	B	228	ARG
1	B	244	GLU
1	C	5	ILE
1	C	11	ARG
1	C	17	VAL
1	C	28	ASP
1	C	39	LEU
1	C	47	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	66	ARG
1	C	74	LEU
1	C	112	ARG
1	C	147	LEU
1	C	161	LEU
1	C	167	LEU
1	C	199	ARG
1	C	204	GLN
1	C	208	LEU
1	C	212	PHE
1	C	217	PRO
1	C	219	SER
1	C	220	ARG
1	C	224	GLU
1	C	239	LYS
1	D	28	ASP
1	D	47	THR
1	D	48	PRO
1	D	96	ARG
1	D	112	ARG
1	D	122	THR
1	D	147	LEU
1	D	161	LEU
1	D	163	LEU
1	D	167	LEU
1	D	197	ARG
1	D	208	LEU
1	D	212	PHE
1	D	217	PRO
1	D	225	GLU
1	D	242	TYR
1	D	244	GLU
1	E	2	PRO
1	E	11	ARG
1	E	28	ASP
1	E	70	ASP
1	E	112	ARG
1	E	147	LEU
1	E	159	LYS
1	E	167	LEU
1	E	191	THR
1	E	194	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	201	GLU
1	E	208	LEU
1	E	212	PHE
1	F	2	PRO
1	F	11	ARG
1	F	24	ILE
1	F	28	ASP
1	F	95	VAL
1	F	112	ARG
1	F	119	GLU
1	F	159	LYS
1	F	161	LEU
1	F	167	LEU
1	F	197	ARG
1	F	204	GLN
1	F	208	LEU
1	F	212	PHE
1	F	217	PRO
1	F	220	ARG
1	F	239	LYS
1	G	11	ARG
1	G	17	VAL
1	G	28	ASP
1	G	96	ARG
1	G	106	GLN
1	G	112	ARG
1	G	124	THR
1	G	144	PRO
1	G	147	LEU
1	G	150	LEU
1	G	161	LEU
1	G	167	LEU
1	G	199	ARG
1	G	208	LEU
1	G	242	TYR
1	H	28	ASP
1	H	39	LEU
1	H	59	ARG
1	H	93	ILE
1	H	119	GLU
1	H	144	PRO
1	H	147	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	159	LYS
1	H	161	LEU
1	H	167	LEU
1	H	201	GLU
1	H	204	GLN
1	H	208	LEU
1	I	4	SER
1	I	11	ARG
1	I	28	ASP
1	I	39	LEU
1	I	59	ARG
1	I	62	GLU
1	I	66	ARG
1	I	112	ARG
1	I	119	GLU
1	I	125	VAL
1	I	128	VAL
1	I	144	PRO
1	I	147	LEU
1	I	158	VAL
1	I	167	LEU
1	I	199	ARG
1	I	212	PHE
1	I	235	GLU
1	I	239	LYS
1	I	244	GLU
1	J	2	PRO
1	J	28	ASP
1	J	48	PRO
1	J	70	ASP
1	J	74	LEU
1	J	106	GLN
1	J	122	THR
1	J	147	LEU
1	J	161	LEU
1	J	162	LYS
1	J	166	SER
1	J	167	LEU
1	J	174	ASP
1	J	183	GLU
1	J	199	ARG
1	J	208	LEU

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Mol	Chain	Res	Type
1	J	212	PHE
1	J	215	ASP
1	J	228	ARG
1	J	244	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	117	HIS
1	A	123	HIS
1	A	204	GLN
1	B	65	GLN
1	B	106	GLN
1	B	117	HIS
1	C	106	GLN
1	C	117	HIS
1	C	195	GLN
1	C	204	GLN
1	D	106	GLN
1	D	117	HIS
1	D	195	GLN
1	E	65	GLN
1	E	106	GLN
1	E	117	HIS
1	E	123	HIS
1	E	195	GLN
1	F	117	HIS
1	F	123	HIS
1	F	195	GLN
1	F	204	GLN
1	G	92	HIS
1	G	106	GLN
1	H	65	GLN
1	H	117	HIS
1	H	195	GLN
1	I	92	HIS
1	I	117	HIS
1	I	195	GLN
1	J	92	HIS
1	J	117	HIS
1	J	195	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

128 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	EDO	J	2061	-	3,3,3	2.22	1 (33%)	2,2,2	0.97	0
2	EDO	J	2068	-	3,3,3	2.88	2 (66%)	2,2,2	0.03	0
2	EDO	E	2077	-	3,3,3	2.72	2 (66%)	2,2,2	0.92	0
2	EDO	C	2024	-	3,3,3	3.42	2 (66%)	2,2,2	0.85	0
2	EDO	C	2126	-	3,3,3	3.29	3 (100%)	2,2,2	0.67	0
2	EDO	C	2084	-	3,3,3	3.15	2 (66%)	2,2,2	1.25	0
2	EDO	B	2021	-	3,3,3	4.02	2 (66%)	2,2,2	0.18	0
2	EDO	H	2114	-	3,3,3	3.17	2 (66%)	2,2,2	0.93	0
2	EDO	H	2054	-	3,3,3	2.25	2 (66%)	2,2,2	0.93	0
2	EDO	D	2003	-	3,3,3	2.78	2 (66%)	2,2,2	0.95	0
2	EDO	C	2075	-	3,3,3	2.17	2 (66%)	2,2,2	1.28	0
2	EDO	A	2011	-	3,3,3	2.69	2 (66%)	2,2,2	1.30	0
2	EDO	G	2056	-	3,3,3	3.16	2 (66%)	2,2,2	0.99	0
2	EDO	A	2066	-	3,3,3	2.99	2 (66%)	2,2,2	0.45	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	C	2128	-	3,3,3	3.40	2 (66%)	2,2,2	0.99	0
2	EDO	I	2100	-	3,3,3	1.81	1 (33%)	2,2,2	0.77	0
2	EDO	J	2069	-	3,3,3	2.85	2 (66%)	2,2,2	0.48	0
2	EDO	H	2010	-	3,3,3	3.96	2 (66%)	2,2,2	0.44	0
2	EDO	B	2023	-	3,3,3	3.23	2 (66%)	2,2,2	0.97	0
2	EDO	E	2120	-	3,3,3	2.97	2 (66%)	2,2,2	0.73	0
2	EDO	F	2043	-	3,3,3	3.04	2 (66%)	2,2,2	1.37	0
2	EDO	D	2118	-	3,3,3	3.17	2 (66%)	2,2,2	0.22	0
2	EDO	E	2041	-	3,3,3	1.70	1 (33%)	2,2,2	1.07	0
2	EDO	H	2059	-	3,3,3	4.05	3 (100%)	2,2,2	0.61	0
2	EDO	A	2065	-	3,3,3	2.60	2 (66%)	2,2,2	0.73	0
2	EDO	E	2032	-	3,3,3	3.05	1 (33%)	2,2,2	0.82	0
2	EDO	F	2086	-	3,3,3	2.48	2 (66%)	2,2,2	1.45	1 (50%)
2	EDO	J	2108	-	3,3,3	1.62	1 (33%)	2,2,2	0.79	0
2	EDO	I	2007	-	3,3,3	3.79	2 (66%)	2,2,2	1.45	0
2	EDO	C	2083	-	3,3,3	2.77	2 (66%)	2,2,2	1.24	0
2	EDO	J	2049	-	3,3,3	2.94	2 (66%)	2,2,2	0.86	0
2	EDO	F	2034	-	3,3,3	2.19	1 (33%)	2,2,2	0.23	0
2	EDO	A	2022	-	3,3,3	2.05	1 (33%)	2,2,2	1.05	0
2	EDO	A	2012	-	3,3,3	4.02	2 (66%)	2,2,2	0.32	0
2	EDO	B	2070	-	3,3,3	2.82	2 (66%)	2,2,2	0.91	0
2	EDO	E	2076	-	3,3,3	2.57	2 (66%)	2,2,2	0.96	0
2	EDO	I	2121	-	3,3,3	1.25	0	2,2,2	0.77	0
2	EDO	B	2015	-	3,3,3	2.37	2 (66%)	2,2,2	0.70	0
2	EDO	D	2074	-	3,3,3	3.75	2 (66%)	2,2,2	1.47	0
2	EDO	F	2038	-	3,3,3	2.47	2 (66%)	2,2,2	0.73	0
2	EDO	E	2079	-	3,3,3	2.70	2 (66%)	2,2,2	1.14	0
2	EDO	C	2064	-	3,3,3	2.71	2 (66%)	2,2,2	0.57	0
2	EDO	F	2097	-	3,3,3	2.96	2 (66%)	2,2,2	0.13	0
2	EDO	C	2004	-	3,3,3	4.46	2 (66%)	2,2,2	0.47	0
2	EDO	C	2081	-	3,3,3	2.85	3 (100%)	2,2,2	0.88	0
2	EDO	I	2099	-	3,3,3	2.50	2 (66%)	2,2,2	1.85	1 (50%)
2	EDO	G	2093	-	3,3,3	3.03	2 (66%)	2,2,2	1.15	0
2	EDO	J	2106	-	3,3,3	2.38	1 (33%)	2,2,2	0.96	0
2	EDO	B	2027	-	3,3,3	1.71	1 (33%)	2,2,2	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	B	2020	-	3,3,3	2.97	2 (66%)	2,2,2	0.76	0
2	EDO	I	2103	-	3,3,3	2.84	2 (66%)	2,2,2	1.87	1 (50%)
2	EDO	H	2044	-	3,3,3	2.20	2 (66%)	2,2,2	0.29	0
2	EDO	J	2008	-	3,3,3	4.96	2 (66%)	2,2,2	1.21	0
2	EDO	A	2017	-	3,3,3	2.04	2 (66%)	2,2,2	0.96	0
2	EDO	A	2116	-	3,3,3	3.05	2 (66%)	2,2,2	0.54	0
2	EDO	I	2052	-	3,3,3	2.60	2 (66%)	2,2,2	1.01	0
2	EDO	D	2073	-	3,3,3	2.08	2 (66%)	2,2,2	0.63	0
2	EDO	D	2033	-	3,3,3	2.31	2 (66%)	2,2,2	0.99	0
2	EDO	C	2085	-	3,3,3	4.02	2 (66%)	2,2,2	1.39	0
2	EDO	E	2040	-	3,3,3	2.64	2 (66%)	2,2,2	0.85	0
2	EDO	D	2072	-	3,3,3	2.66	2 (66%)	2,2,2	0.58	0
2	EDO	I	2107	-	3,3,3	1.52	1 (33%)	2,2,2	0.68	0
2	EDO	D	2119	-	3,3,3	2.58	2 (66%)	2,2,2	1.04	0
2	EDO	C	2082	-	3,3,3	3.27	1 (33%)	2,2,2	0.58	0
2	EDO	A	2019	-	3,3,3	2.71	2 (66%)	2,2,2	0.75	0
2	EDO	F	2095	-	3,3,3	3.06	2 (66%)	2,2,2	0.97	0
2	EDO	J	2105	-	3,3,3	3.02	2 (66%)	2,2,2	0.52	0
2	EDO	B	2002	-	3,3,3	4.61	2 (66%)	2,2,2	1.21	0
2	EDO	I	2045	-	3,3,3	2.97	2 (66%)	2,2,2	0.49	0
2	EDO	D	2035	-	3,3,3	1.27	0	2,2,2	0.26	0
2	EDO	C	2026	-	3,3,3	1.07	0	2,2,2	0.75	0
2	EDO	C	2080	-	3,3,3	2.74	2 (66%)	2,2,2	0.53	0
2	EDO	E	2078	-	3,3,3	2.42	1 (33%)	2,2,2	1.34	0
2	EDO	E	2088	-	3,3,3	2.84	2 (66%)	2,2,2	1.20	0
2	EDO	E	2042	-	3,3,3	2.18	2 (66%)	2,2,2	0.85	0
2	EDO	A	2063	-	3,3,3	3.38	2 (66%)	2,2,2	1.09	0
2	EDO	J	2055	-	3,3,3	2.11	1 (33%)	2,2,2	0.83	0
2	EDO	E	2092	-	3,3,3	1.82	2 (66%)	2,2,2	1.24	0
2	EDO	E	2039	-	3,3,3	2.11	2 (66%)	2,2,2	0.34	0
2	EDO	J	2053	-	3,3,3	3.37	2 (66%)	2,2,2	0.38	0
2	EDO	B	2025	-	3,3,3	2.92	2 (66%)	2,2,2	0.69	0
2	EDO	E	2089	-	3,3,3	3.48	2 (66%)	2,2,2	0.29	0
2	EDO	F	2037	-	3,3,3	2.49	2 (66%)	2,2,2	1.04	0
2	EDO	A	2124	-	3,3,3	4.40	2 (66%)	2,2,2	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	G	2047	-	3,3,3	2.81	2 (66%)	2,2,2	0.79	0
2	EDO	C	2117	-	3,3,3	2.40	2 (66%)	2,2,2	0.46	0
2	EDO	D	2071	-	3,3,3	2.92	2 (66%)	2,2,2	0.52	0
2	EDO	J	2104	-	3,3,3	3.79	2 (66%)	2,2,2	2.05	1 (50%)
2	EDO	J	2123	-	3,3,3	3.44	2 (66%)	2,2,2	1.95	1 (50%)
2	EDO	B	2018	-	3,3,3	2.14	2 (66%)	2,2,2	0.88	0
2	EDO	I	2051	-	3,3,3	2.00	1 (33%)	2,2,2	1.09	0
2	EDO	H	2113	-	3,3,3	2.50	1 (33%)	2,2,2	0.89	0
2	EDO	J	2048	-	3,3,3	3.06	2 (66%)	2,2,2	0.90	0
2	EDO	J	2109	-	3,3,3	1.29	1 (33%)	2,2,2	1.17	0
2	EDO	G	2102	-	3,3,3	3.07	2 (66%)	2,2,2	0.74	0
2	EDO	H	2058	-	3,3,3	3.32	2 (66%)	2,2,2	1.51	1 (50%)
2	EDO	E	2090	-	3,3,3	2.68	2 (66%)	2,2,2	0.59	0
2	EDO	A	2029	-	3,3,3	3.24	2 (66%)	2,2,2	0.76	0
2	EDO	B	2062	-	3,3,3	1.86	1 (33%)	2,2,2	1.06	0
2	EDO	I	2046	-	3,3,3	2.23	1 (33%)	2,2,2	1.02	0
2	EDO	E	2127	-	3,3,3	2.61	2 (66%)	2,2,2	1.49	1 (50%)
2	EDO	B	2030	-	3,3,3	1.03	0	2,2,2	0.35	0
2	EDO	C	2036	-	3,3,3	2.69	2 (66%)	2,2,2	1.10	0
2	EDO	F	2006	-	3,3,3	3.55	3 (100%)	2,2,2	0.92	0
2	EDO	D	2031	-	3,3,3	2.99	2 (66%)	2,2,2	0.58	0
2	EDO	F	2094	-	3,3,3	3.00	2 (66%)	2,2,2	1.42	0
2	EDO	H	2060	-	3,3,3	1.01	0	2,2,2	0.22	0
2	EDO	G	2050	-	3,3,3	2.97	2 (66%)	2,2,2	0.38	0
2	EDO	G	2057	-	3,3,3	1.45	1 (33%)	2,2,2	0.90	0
2	EDO	C	2067	-	3,3,3	2.83	1 (33%)	2,2,2	0.40	0
2	EDO	F	2098	-	3,3,3	4.16	2 (66%)	2,2,2	0.77	0
2	EDO	G	2009	-	3,3,3	3.73	2 (66%)	2,2,2	1.28	0
2	EDO	H	2111	-	3,3,3	2.55	3 (100%)	2,2,2	1.09	0
2	EDO	G	2112	-	3,3,3	2.66	2 (66%)	2,2,2	0.50	0
2	EDO	I	2115	-	3,3,3	3.67	2 (66%)	2,2,2	0.93	0
2	EDO	J	2014	-	3,3,3	3.41	2 (66%)	2,2,2	0.74	0
2	EDO	A	2001	-	3,3,3	2.53	2 (66%)	2,2,2	0.27	0
2	EDO	B	2028	-	3,3,3	2.31	2 (66%)	2,2,2	1.26	0
2	EDO	B	2125	-	3,3,3	2.80	3 (100%)	2,2,2	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	J	2110	-	3,3,3	2.49	2 (66%)	2,2,2	1.07	0
2	EDO	G	2101	-	3,3,3	2.27	2 (66%)	2,2,2	1.88	1 (50%)
2	EDO	B	2013	-	3,3,3	2.44	2 (66%)	2,2,2	0.71	0
2	EDO	A	2122	-	3,3,3	3.12	1 (33%)	2,2,2	1.27	0
2	EDO	E	2091	-	3,3,3	3.28	2 (66%)	2,2,2	1.25	0
2	EDO	F	2096	-	3,3,3	2.40	2 (66%)	2,2,2	0.95	0
2	EDO	F	2087	-	3,3,3	1.66	1 (33%)	2,2,2	0.80	0
2	EDO	A	2016	-	3,3,3	2.17	2 (66%)	2,2,2	0.55	0
2	EDO	E	2005	-	3,3,3	4.47	2 (66%)	2,2,2	0.46	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	EDO	J	2061	-	-	1/1/1/1	-
2	EDO	J	2068	-	-	1/1/1/1	-
2	EDO	E	2077	-	-	1/1/1/1	-
2	EDO	C	2024	-	-	1/1/1/1	-
2	EDO	C	2126	-	-	1/1/1/1	-
2	EDO	C	2084	-	-	0/1/1/1	-
2	EDO	B	2021	-	-	0/1/1/1	-
2	EDO	H	2114	-	-	0/1/1/1	-
2	EDO	H	2054	-	-	0/1/1/1	-
2	EDO	D	2003	-	-	1/1/1/1	-
2	EDO	C	2075	-	-	1/1/1/1	-
2	EDO	A	2011	-	-	0/1/1/1	-
2	EDO	G	2056	-	-	1/1/1/1	-
2	EDO	A	2066	-	-	0/1/1/1	-
2	EDO	C	2128	-	-	1/1/1/1	-
2	EDO	I	2100	-	-	1/1/1/1	-
2	EDO	J	2069	-	-	1/1/1/1	-
2	EDO	H	2010	-	-	1/1/1/1	-
2	EDO	B	2023	-	-	0/1/1/1	-
2	EDO	E	2120	-	-	1/1/1/1	-
2	EDO	F	2043	-	-	0/1/1/1	-
2	EDO	D	2118	-	-	1/1/1/1	-
2	EDO	E	2041	-	-	1/1/1/1	-
2	EDO	H	2059	-	-	1/1/1/1	-
2	EDO	A	2065	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	E	2032	-	-	1/1/1/1	-
2	EDO	F	2086	-	-	1/1/1/1	-
2	EDO	J	2108	-	-	1/1/1/1	-
2	EDO	I	2007	-	-	1/1/1/1	-
2	EDO	C	2083	-	-	1/1/1/1	-
2	EDO	J	2049	-	-	0/1/1/1	-
2	EDO	F	2034	-	-	1/1/1/1	-
2	EDO	A	2022	-	-	1/1/1/1	-
2	EDO	A	2012	-	-	1/1/1/1	-
2	EDO	B	2070	-	-	1/1/1/1	-
2	EDO	E	2076	-	-	1/1/1/1	-
2	EDO	I	2121	-	-	1/1/1/1	-
2	EDO	B	2015	-	-	0/1/1/1	-
2	EDO	D	2074	-	-	1/1/1/1	-
2	EDO	F	2038	-	-	0/1/1/1	-
2	EDO	E	2079	-	-	1/1/1/1	-
2	EDO	C	2064	-	-	1/1/1/1	-
2	EDO	F	2097	-	-	1/1/1/1	-
2	EDO	C	2004	-	-	1/1/1/1	-
2	EDO	C	2081	-	-	0/1/1/1	-
2	EDO	I	2099	-	-	1/1/1/1	-
2	EDO	G	2093	-	-	1/1/1/1	-
2	EDO	J	2106	-	-	0/1/1/1	-
2	EDO	B	2027	-	-	0/1/1/1	-
2	EDO	B	2020	-	-	0/1/1/1	-
2	EDO	I	2103	-	-	1/1/1/1	-
2	EDO	H	2044	-	-	0/1/1/1	-
2	EDO	J	2008	-	-	1/1/1/1	-
2	EDO	A	2017	-	-	1/1/1/1	-
2	EDO	A	2116	-	-	1/1/1/1	-
2	EDO	I	2052	-	-	1/1/1/1	-
2	EDO	D	2073	-	-	1/1/1/1	-
2	EDO	D	2033	-	-	1/1/1/1	-
2	EDO	C	2085	-	-	1/1/1/1	-
2	EDO	E	2040	-	-	0/1/1/1	-
2	EDO	D	2072	-	-	1/1/1/1	-
2	EDO	I	2107	-	-	0/1/1/1	-
2	EDO	D	2119	-	-	1/1/1/1	-
2	EDO	C	2082	-	-	0/1/1/1	-
2	EDO	A	2019	-	-	0/1/1/1	-
2	EDO	F	2095	-	-	0/1/1/1	-
2	EDO	J	2105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	2002	-	-	1/1/1/1	-
2	EDO	I	2045	-	-	1/1/1/1	-
2	EDO	D	2035	-	-	1/1/1/1	-
2	EDO	C	2026	-	-	1/1/1/1	-
2	EDO	C	2080	-	-	1/1/1/1	-
2	EDO	E	2078	-	-	0/1/1/1	-
2	EDO	E	2088	-	-	1/1/1/1	-
2	EDO	E	2042	-	-	1/1/1/1	-
2	EDO	A	2063	-	-	1/1/1/1	-
2	EDO	J	2055	-	-	1/1/1/1	-
2	EDO	E	2092	-	-	1/1/1/1	-
2	EDO	E	2039	-	-	1/1/1/1	-
2	EDO	J	2053	-	-	1/1/1/1	-
2	EDO	B	2025	-	-	1/1/1/1	-
2	EDO	E	2089	-	-	1/1/1/1	-
2	EDO	F	2037	-	-	1/1/1/1	-
2	EDO	A	2124	-	-	1/1/1/1	-
2	EDO	G	2047	-	-	0/1/1/1	-
2	EDO	C	2117	-	-	0/1/1/1	-
2	EDO	D	2071	-	-	1/1/1/1	-
2	EDO	J	2104	-	-	1/1/1/1	-
2	EDO	J	2123	-	-	1/1/1/1	-
2	EDO	B	2018	-	-	1/1/1/1	-
2	EDO	I	2051	-	-	1/1/1/1	-
2	EDO	H	2113	-	-	0/1/1/1	-
2	EDO	J	2048	-	-	1/1/1/1	-
2	EDO	J	2109	-	-	0/1/1/1	-
2	EDO	G	2102	-	-	0/1/1/1	-
2	EDO	H	2058	-	-	1/1/1/1	-
2	EDO	E	2090	-	-	1/1/1/1	-
2	EDO	A	2029	-	-	1/1/1/1	-
2	EDO	B	2062	-	-	0/1/1/1	-
2	EDO	I	2046	-	-	0/1/1/1	-
2	EDO	E	2127	-	-	0/1/1/1	-
2	EDO	B	2030	-	-	0/1/1/1	-
2	EDO	C	2036	-	-	1/1/1/1	-
2	EDO	F	2006	-	-	1/1/1/1	-
2	EDO	D	2031	-	-	1/1/1/1	-
2	EDO	F	2094	-	-	1/1/1/1	-
2	EDO	H	2060	-	-	1/1/1/1	-
2	EDO	G	2050	-	-	0/1/1/1	-
2	EDO	G	2057	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	2067	-	-	1/1/1/1	-
2	EDO	F	2098	-	-	1/1/1/1	-
2	EDO	G	2009	-	-	1/1/1/1	-
2	EDO	H	2111	-	-	0/1/1/1	-
2	EDO	G	2112	-	-	0/1/1/1	-
2	EDO	I	2115	-	-	0/1/1/1	-
2	EDO	J	2014	-	-	0/1/1/1	-
2	EDO	A	2001	-	-	1/1/1/1	-
2	EDO	B	2028	-	-	1/1/1/1	-
2	EDO	B	2125	-	-	1/1/1/1	-
2	EDO	J	2110	-	-	0/1/1/1	-
2	EDO	G	2101	-	-	1/1/1/1	-
2	EDO	B	2013	-	-	1/1/1/1	-
2	EDO	A	2122	-	-	1/1/1/1	-
2	EDO	E	2091	-	-	1/1/1/1	-
2	EDO	F	2096	-	-	1/1/1/1	-
2	EDO	F	2087	-	-	1/1/1/1	-
2	EDO	A	2016	-	-	1/1/1/1	-
2	EDO	E	2005	-	-	1/1/1/1	-

All (230) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2008	EDO	O1-C1	7.34	1.80	1.42
2	E	2005	EDO	O2-C2	6.46	1.75	1.42
2	C	2004	EDO	O2-C2	5.99	1.73	1.42
2	F	2098	EDO	O2-C2	5.81	1.72	1.42
2	B	2002	EDO	O1-C1	5.75	1.71	1.42
2	H	2059	EDO	O2-C2	5.75	1.71	1.42
2	A	2012	EDO	O2-C2	5.49	1.70	1.42
2	D	2074	EDO	O1-C1	5.48	1.70	1.42
2	H	2010	EDO	O2-C2	5.48	1.70	1.42
2	A	2124	EDO	O1-C1	5.37	1.69	1.42
2	A	2124	EDO	O2-C2	5.36	1.69	1.42
2	A	2122	EDO	O2-C2	5.34	1.69	1.42
2	B	2002	EDO	O2-C2	5.28	1.69	1.42
2	B	2021	EDO	O2-C2	5.18	1.68	1.42
2	C	2082	EDO	O2-C2	5.15	1.68	1.42
2	E	2089	EDO	O2-C2	5.13	1.68	1.42
2	I	2007	EDO	O1-C1	5.12	1.68	1.42
2	F	2006	EDO	O1-C1	5.09	1.68	1.42
2	C	2085	EDO	O1-C1	5.04	1.68	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2023	EDO	O2-C2	4.98	1.67	1.42
2	G	2009	EDO	O1-C1	4.91	1.67	1.42
2	C	2004	EDO	O1-C1	4.84	1.67	1.42
2	I	2115	EDO	O2-C2	4.83	1.67	1.42
2	D	2118	EDO	O2-C2	4.80	1.66	1.42
2	J	2104	EDO	O2-C2	4.78	1.66	1.42
2	E	2032	EDO	O2-C2	4.77	1.66	1.42
2	C	2085	EDO	O2-C2	4.74	1.66	1.42
2	G	2050	EDO	O2-C2	4.63	1.66	1.42
2	G	2056	EDO	O2-C2	4.59	1.65	1.42
2	G	2102	EDO	O2-C2	4.57	1.65	1.42
2	C	2024	EDO	O2-C2	4.54	1.65	1.42
2	C	2067	EDO	O2-C2	4.50	1.65	1.42
2	F	2043	EDO	O2-C2	4.48	1.65	1.42
2	C	2128	EDO	O2-C2	4.45	1.65	1.42
2	C	2126	EDO	O2-C2	4.43	1.65	1.42
2	B	2021	EDO	O1-C1	4.43	1.65	1.42
2	D	2031	EDO	O2-C2	4.36	1.64	1.42
2	J	2068	EDO	O2-C2	4.35	1.64	1.42
2	G	2093	EDO	O2-C2	4.35	1.64	1.42
2	J	2049	EDO	O2-C2	4.32	1.64	1.42
2	H	2058	EDO	O2-C2	4.29	1.64	1.42
2	J	2014	EDO	O1-C1	4.28	1.64	1.42
2	E	2120	EDO	O1-C1	4.28	1.64	1.42
2	J	2123	EDO	O1-C1	4.26	1.64	1.42
2	B	2020	EDO	O1-C1	4.26	1.64	1.42
2	A	2063	EDO	O1-C1	4.25	1.64	1.42
2	E	2088	EDO	O1-C1	4.25	1.64	1.42
2	J	2105	EDO	O2-C2	4.20	1.63	1.42
2	A	2012	EDO	O1-C1	4.18	1.63	1.42
2	J	2008	EDO	O2-C2	4.17	1.63	1.42
2	J	2053	EDO	O2-C2	4.17	1.63	1.42
2	J	2104	EDO	O1-C1	4.16	1.63	1.42
2	A	2029	EDO	O2-C2	4.15	1.63	1.42
2	H	2114	EDO	O1-C1	4.13	1.63	1.42
2	E	2091	EDO	O2-C2	4.10	1.63	1.42
2	D	2071	EDO	O2-C2	4.10	1.63	1.42
2	J	2048	EDO	O2-C2	4.09	1.63	1.42
2	H	2010	EDO	O1-C1	4.04	1.62	1.42
2	A	2063	EDO	O2-C2	4.03	1.62	1.42
2	D	2072	EDO	O2-C2	4.02	1.62	1.42
2	D	2003	EDO	O2-C2	4.00	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2014	EDO	O2-C2	3.99	1.62	1.42
2	C	2084	EDO	O2-C2	3.98	1.62	1.42
2	I	2045	EDO	O1-C1	3.97	1.62	1.42
2	E	2091	EDO	O1-C1	3.93	1.62	1.42
2	I	2007	EDO	O2-C2	3.92	1.62	1.42
2	I	2103	EDO	O1-C1	3.92	1.62	1.42
2	A	2065	EDO	O1-C1	3.91	1.62	1.42
2	G	2009	EDO	O2-C2	3.90	1.62	1.42
2	E	2078	EDO	O1-C1	3.89	1.62	1.42
2	F	2098	EDO	O1-C1	3.87	1.62	1.42
2	J	2053	EDO	O1-C1	3.86	1.62	1.42
2	E	2005	EDO	O1-C1	3.86	1.62	1.42
2	A	2116	EDO	O2-C2	3.85	1.62	1.42
2	C	2036	EDO	O1-C1	3.84	1.61	1.42
2	H	2058	EDO	O1-C1	3.82	1.61	1.42
2	A	2011	EDO	O2-C2	3.82	1.61	1.42
2	B	2025	EDO	O1-C1	3.80	1.61	1.42
2	C	2084	EDO	O1-C1	3.74	1.61	1.42
2	J	2061	EDO	O1-C1	3.73	1.61	1.42
2	I	2115	EDO	O1-C1	3.73	1.61	1.42
2	A	2029	EDO	O1-C1	3.72	1.61	1.42
2	J	2123	EDO	O2-C2	3.72	1.61	1.42
2	F	2095	EDO	O1-C1	3.71	1.61	1.42
2	A	2066	EDO	O2-C2	3.70	1.61	1.42
2	F	2034	EDO	O2-C2	3.70	1.61	1.42
2	F	2095	EDO	O2-C2	3.69	1.61	1.42
2	H	2113	EDO	O1-C1	3.69	1.61	1.42
2	F	2094	EDO	O1-C1	3.68	1.61	1.42
2	J	2106	EDO	O1-C1	3.66	1.61	1.42
2	F	2097	EDO	O1-C1	3.66	1.61	1.42
2	C	2081	EDO	O2-C2	3.65	1.60	1.42
2	F	2086	EDO	O1-C1	3.62	1.60	1.42
2	C	2064	EDO	O1-C1	3.62	1.60	1.42
2	F	2094	EDO	O2-C2	3.61	1.60	1.42
2	F	2097	EDO	O2-C2	3.59	1.60	1.42
2	G	2047	EDO	O2-C2	3.59	1.60	1.42
2	E	2079	EDO	O2-C2	3.57	1.60	1.42
2	C	2024	EDO	O1-C1	3.57	1.60	1.42
2	A	2019	EDO	O1-C1	3.55	1.60	1.42
2	B	2070	EDO	O1-C1	3.53	1.60	1.42
2	C	2083	EDO	O2-C2	3.51	1.60	1.42
2	J	2069	EDO	O2-C2	3.51	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2127	EDO	O2-C2	3.51	1.60	1.42
2	C	2080	EDO	O2-C2	3.50	1.60	1.42
2	F	2037	EDO	O2-C2	3.50	1.60	1.42
2	F	2096	EDO	O2-C2	3.46	1.59	1.42
2	J	2110	EDO	O2-C2	3.46	1.59	1.42
2	J	2055	EDO	O2-C2	3.43	1.59	1.42
2	A	2116	EDO	O1-C1	3.40	1.59	1.42
2	I	2052	EDO	O1-C1	3.36	1.59	1.42
2	C	2128	EDO	O1-C1	3.36	1.59	1.42
2	A	2066	EDO	O1-C1	3.35	1.59	1.42
2	J	2069	EDO	O1-C1	3.35	1.59	1.42
2	E	2090	EDO	O2-C2	3.34	1.59	1.42
2	E	2077	EDO	O1-C1	3.34	1.59	1.42
2	B	2028	EDO	O2-C2	3.32	1.59	1.42
2	D	2033	EDO	O2-C2	3.31	1.59	1.42
2	E	2077	EDO	O2-C2	3.31	1.59	1.42
2	I	2046	EDO	O2-C2	3.31	1.59	1.42
2	H	2114	EDO	O2-C2	3.27	1.59	1.42
2	D	2119	EDO	O2-C2	3.26	1.58	1.42
2	G	2112	EDO	O1-C1	3.26	1.58	1.42
2	G	2047	EDO	O1-C1	3.25	1.58	1.42
2	C	2083	EDO	O1-C1	3.23	1.58	1.42
2	J	2048	EDO	O1-C1	3.23	1.58	1.42
2	E	2040	EDO	O1-C1	3.22	1.58	1.42
2	B	2025	EDO	O2-C2	3.22	1.58	1.42
2	E	2076	EDO	O2-C2	3.20	1.58	1.42
2	E	2090	EDO	O1-C1	3.19	1.58	1.42
2	F	2038	EDO	O1-C1	3.17	1.58	1.42
2	H	2044	EDO	O1-C1	3.17	1.58	1.42
2	B	2015	EDO	O1-C1	3.16	1.58	1.42
2	H	2059	EDO	O1-C1	3.14	1.58	1.42
2	J	2105	EDO	O1-C1	3.13	1.58	1.42
2	I	2099	EDO	O2-C2	3.10	1.58	1.42
2	H	2111	EDO	O2-C2	3.08	1.58	1.42
2	G	2112	EDO	O2-C2	3.06	1.57	1.42
2	D	2119	EDO	O1-C1	3.05	1.57	1.42
2	A	2022	EDO	O1-C1	3.05	1.57	1.42
2	A	2001	EDO	O1-C1	3.04	1.57	1.42
2	B	2070	EDO	O2-C2	3.03	1.57	1.42
2	C	2075	EDO	O1-C1	3.03	1.57	1.42
2	C	2080	EDO	O1-C1	3.02	1.57	1.42
2	B	2125	EDO	O1-C1	3.02	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2040	EDO	O2-C2	3.01	1.57	1.42
2	A	2019	EDO	O2-C2	3.00	1.57	1.42
2	B	2013	EDO	O2-C2	3.00	1.57	1.42
2	I	2052	EDO	O2-C2	2.99	1.57	1.42
2	D	2074	EDO	O2-C2	2.99	1.57	1.42
2	C	2064	EDO	O2-C2	2.98	1.57	1.42
2	C	2117	EDO	O2-C2	2.97	1.57	1.42
2	B	2062	EDO	O1-C1	2.96	1.57	1.42
2	I	2099	EDO	O1-C1	2.95	1.57	1.42
2	G	2101	EDO	O2-C2	2.93	1.57	1.42
2	E	2089	EDO	O1-C1	2.93	1.57	1.42
2	B	2125	EDO	O2-C2	2.93	1.57	1.42
2	H	2054	EDO	O2-C2	2.93	1.57	1.42
2	B	2013	EDO	O1-C1	2.91	1.57	1.42
2	G	2093	EDO	O1-C1	2.90	1.57	1.42
2	E	2079	EDO	O1-C1	2.88	1.57	1.42
2	I	2100	EDO	O2-C2	2.87	1.56	1.42
2	E	2041	EDO	O1-C1	2.87	1.56	1.42
2	F	2087	EDO	O1-C1	2.86	1.56	1.42
2	I	2045	EDO	O2-C2	2.84	1.56	1.42
2	C	2126	EDO	O1-C1	2.82	1.56	1.42
2	F	2006	EDO	O2-C2	2.79	1.56	1.42
2	I	2051	EDO	O2-C2	2.79	1.56	1.42
2	F	2043	EDO	O1-C1	2.78	1.56	1.42
2	C	2117	EDO	O1-C1	2.78	1.56	1.42
2	A	2001	EDO	O2-C2	2.78	1.56	1.42
2	E	2120	EDO	O2-C2	2.76	1.56	1.42
2	B	2020	EDO	O2-C2	2.73	1.56	1.42
2	I	2103	EDO	O2-C2	2.73	1.56	1.42
2	G	2102	EDO	O1-C1	2.69	1.56	1.42
2	F	2038	EDO	O2-C2	2.69	1.56	1.42
2	J	2049	EDO	O1-C1	2.68	1.55	1.42
2	A	2016	EDO	O1-C1	2.68	1.55	1.42
2	E	2042	EDO	O2-C2	2.65	1.55	1.42
2	D	2118	EDO	O1-C1	2.65	1.55	1.42
2	C	2036	EDO	O2-C2	2.60	1.55	1.42
2	A	2011	EDO	O1-C1	2.59	1.55	1.42
2	H	2054	EDO	O1-C1	2.57	1.55	1.42
2	J	2110	EDO	O1-C1	2.57	1.55	1.42
2	D	2071	EDO	O1-C1	2.54	1.55	1.42
2	E	2039	EDO	O2-C2	2.54	1.55	1.42
2	E	2042	EDO	O1-C1	2.53	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2017	EDO	O2-C2	2.53	1.55	1.42
2	J	2108	EDO	O2-C2	2.52	1.55	1.42
2	G	2101	EDO	O1-C1	2.52	1.55	1.42
2	E	2076	EDO	O1-C1	2.52	1.55	1.42
2	A	2016	EDO	O2-C2	2.52	1.55	1.42
2	D	2073	EDO	O1-C1	2.50	1.55	1.42
2	G	2056	EDO	O1-C1	2.50	1.55	1.42
2	D	2003	EDO	O1-C1	2.50	1.55	1.42
2	H	2059	EDO	C2-C1	2.50	1.65	1.48
2	D	2073	EDO	O2-C2	2.49	1.54	1.42
2	B	2015	EDO	O2-C2	2.47	1.54	1.42
2	F	2037	EDO	O1-C1	2.47	1.54	1.42
2	B	2018	EDO	O2-C2	2.47	1.54	1.42
2	E	2088	EDO	O2-C2	2.47	1.54	1.42
2	D	2031	EDO	O1-C1	2.46	1.54	1.42
2	E	2127	EDO	O1-C1	2.44	1.54	1.42
2	J	2068	EDO	O1-C1	2.44	1.54	1.42
2	A	2017	EDO	O1-C1	2.44	1.54	1.42
2	C	2081	EDO	O1-C1	2.43	1.54	1.42
2	E	2092	EDO	O1-C1	2.42	1.54	1.42
2	E	2039	EDO	O1-C1	2.40	1.54	1.42
2	B	2125	EDO	C2-C1	2.40	1.64	1.48
2	F	2086	EDO	O2-C2	2.30	1.54	1.42
2	G	2057	EDO	O1-C1	2.29	1.53	1.42
2	H	2111	EDO	C2-C1	2.28	1.64	1.48
2	C	2081	EDO	C2-C1	2.28	1.64	1.48
2	B	2018	EDO	O1-C1	2.26	1.53	1.42
2	D	2072	EDO	O1-C1	2.22	1.53	1.42
2	B	2028	EDO	O1-C1	2.20	1.53	1.42
2	C	2126	EDO	C2-C1	2.20	1.63	1.48
2	H	2111	EDO	O1-C1	2.20	1.53	1.42
2	D	2033	EDO	O1-C1	2.19	1.53	1.42
2	F	2096	EDO	O1-C1	2.18	1.53	1.42
2	C	2075	EDO	O2-C2	2.15	1.53	1.42
2	J	2109	EDO	O2-C2	2.15	1.53	1.42
2	B	2027	EDO	O1-C1	2.15	1.53	1.42
2	I	2107	EDO	O1-C1	2.12	1.53	1.42
2	B	2023	EDO	O1-C1	2.11	1.53	1.42
2	A	2065	EDO	O2-C2	2.09	1.52	1.42
2	F	2006	EDO	C2-C1	2.03	1.62	1.48
2	E	2092	EDO	O2-C2	2.02	1.52	1.42
2	G	2050	EDO	O1-C1	2.01	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2044	EDO	O2-C2	2.00	1.52	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2101	EDO	O2-C2-C1	-2.64	92.91	111.91
2	J	2123	EDO	O2-C2-C1	-2.60	93.21	111.91
2	I	2099	EDO	O2-C2-C1	-2.55	93.54	111.91
2	J	2104	EDO	O2-C2-C1	-2.20	96.06	111.91
2	H	2058	EDO	O2-C2-C1	-2.14	96.52	111.91
2	I	2103	EDO	O1-C1-C2	-2.08	96.97	111.91
2	E	2127	EDO	O1-C1-C2	-2.01	97.45	111.91
2	F	2086	EDO	O2-C2-C1	-2.00	97.49	111.91

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	EDO	O1-C1-C2-O2
2	A	2012	EDO	O1-C1-C2-O2
2	A	2122	EDO	O1-C1-C2-O2
2	B	2025	EDO	O1-C1-C2-O2
2	E	2039	EDO	O1-C1-C2-O2
2	E	2042	EDO	O1-C1-C2-O2
2	I	2103	EDO	O1-C1-C2-O2
2	J	2008	EDO	O1-C1-C2-O2
2	A	2029	EDO	O1-C1-C2-O2
2	D	2031	EDO	O1-C1-C2-O2
2	D	2035	EDO	O1-C1-C2-O2
2	E	2041	EDO	O1-C1-C2-O2
2	E	2076	EDO	O1-C1-C2-O2
2	E	2077	EDO	O1-C1-C2-O2
2	F	2087	EDO	O1-C1-C2-O2
2	G	2093	EDO	O1-C1-C2-O2
2	H	2059	EDO	O1-C1-C2-O2
2	H	2060	EDO	O1-C1-C2-O2
2	I	2007	EDO	O1-C1-C2-O2
2	I	2121	EDO	O1-C1-C2-O2
2	J	2068	EDO	O1-C1-C2-O2
2	A	2022	EDO	O1-C1-C2-O2
2	C	2004	EDO	O1-C1-C2-O2
2	E	2005	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	E	2091	EDO	O1-C1-C2-O2
2	G	2101	EDO	O1-C1-C2-O2
2	J	2053	EDO	O1-C1-C2-O2
2	B	2013	EDO	O1-C1-C2-O2
2	B	2070	EDO	O1-C1-C2-O2
2	C	2085	EDO	O1-C1-C2-O2
2	E	2090	EDO	O1-C1-C2-O2
2	F	2034	EDO	O1-C1-C2-O2
2	F	2098	EDO	O1-C1-C2-O2
2	G	2009	EDO	O1-C1-C2-O2
2	I	2100	EDO	O1-C1-C2-O2
2	J	2055	EDO	O1-C1-C2-O2
2	A	2065	EDO	O1-C1-C2-O2
2	B	2002	EDO	O1-C1-C2-O2
2	C	2024	EDO	O1-C1-C2-O2
2	C	2036	EDO	O1-C1-C2-O2
2	C	2064	EDO	O1-C1-C2-O2
2	C	2075	EDO	O1-C1-C2-O2
2	C	2083	EDO	O1-C1-C2-O2
2	D	2033	EDO	O1-C1-C2-O2
2	D	2071	EDO	O1-C1-C2-O2
2	D	2072	EDO	O1-C1-C2-O2
2	D	2074	EDO	O1-C1-C2-O2
2	E	2032	EDO	O1-C1-C2-O2
2	E	2089	EDO	O1-C1-C2-O2
2	F	2006	EDO	O1-C1-C2-O2
2	F	2037	EDO	O1-C1-C2-O2
2	F	2096	EDO	O1-C1-C2-O2
2	H	2058	EDO	O1-C1-C2-O2
2	I	2045	EDO	O1-C1-C2-O2
2	I	2051	EDO	O1-C1-C2-O2
2	I	2099	EDO	O1-C1-C2-O2
2	A	2116	EDO	O1-C1-C2-O2
2	E	2079	EDO	O1-C1-C2-O2
2	J	2069	EDO	O1-C1-C2-O2
2	J	2104	EDO	O1-C1-C2-O2
2	J	2123	EDO	O1-C1-C2-O2
2	A	2016	EDO	O1-C1-C2-O2
2	B	2125	EDO	O1-C1-C2-O2
2	D	2003	EDO	O1-C1-C2-O2
2	E	2088	EDO	O1-C1-C2-O2
2	F	2094	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	F	2097	EDO	O1-C1-C2-O2
2	G	2057	EDO	O1-C1-C2-O2
2	I	2052	EDO	O1-C1-C2-O2
2	J	2048	EDO	O1-C1-C2-O2
2	J	2061	EDO	O1-C1-C2-O2
2	J	2108	EDO	O1-C1-C2-O2
2	A	2063	EDO	O1-C1-C2-O2
2	A	2124	EDO	O1-C1-C2-O2
2	B	2018	EDO	O1-C1-C2-O2
2	C	2026	EDO	O1-C1-C2-O2
2	C	2128	EDO	O1-C1-C2-O2
2	D	2118	EDO	O1-C1-C2-O2
2	E	2120	EDO	O1-C1-C2-O2
2	A	2017	EDO	O1-C1-C2-O2
2	B	2028	EDO	O1-C1-C2-O2
2	C	2067	EDO	O1-C1-C2-O2
2	C	2080	EDO	O1-C1-C2-O2
2	C	2126	EDO	O1-C1-C2-O2
2	D	2073	EDO	O1-C1-C2-O2
2	D	2119	EDO	O1-C1-C2-O2
2	E	2092	EDO	O1-C1-C2-O2
2	F	2086	EDO	O1-C1-C2-O2
2	G	2056	EDO	O1-C1-C2-O2
2	H	2010	EDO	O1-C1-C2-O2

There are no ring outliers.

107 monomers are involved in 502 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2061	EDO	2	0
2	J	2068	EDO	6	0
2	E	2077	EDO	1	0
2	C	2024	EDO	12	0
2	C	2126	EDO	6	0
2	C	2084	EDO	1	0
2	B	2021	EDO	4	0
2	H	2114	EDO	0	1
2	H	2054	EDO	1	0
2	D	2003	EDO	4	0
2	C	2075	EDO	7	0
2	A	2011	EDO	1	0
2	G	2056	EDO	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2066	EDO	1	0
2	C	2128	EDO	8	0
2	I	2100	EDO	2	0
2	H	2010	EDO	8	0
2	B	2023	EDO	3	0
2	E	2120	EDO	6	0
2	F	2043	EDO	13	0
2	D	2118	EDO	7	0
2	H	2059	EDO	2	0
2	A	2065	EDO	5	0
2	E	2032	EDO	3	0
2	F	2086	EDO	7	0
2	J	2108	EDO	3	0
2	I	2007	EDO	5	0
2	J	2049	EDO	10	0
2	F	2034	EDO	5	0
2	A	2022	EDO	3	0
2	A	2012	EDO	11	0
2	E	2076	EDO	7	0
2	I	2121	EDO	12	0
2	D	2074	EDO	2	0
2	F	2038	EDO	4	0
2	E	2079	EDO	2	0
2	C	2064	EDO	2	0
2	F	2097	EDO	5	0
2	C	2004	EDO	11	0
2	I	2099	EDO	3	0
2	G	2093	EDO	6	0
2	J	2106	EDO	2	0
2	B	2020	EDO	2	0
2	I	2103	EDO	4	0
2	H	2044	EDO	4	0
2	J	2008	EDO	7	0
2	A	2017	EDO	2	0
2	A	2116	EDO	1	0
2	C	2085	EDO	10	0
2	E	2040	EDO	1	0
2	D	2072	EDO	3	0
2	I	2107	EDO	11	0
2	D	2119	EDO	2	0
2	C	2082	EDO	2	0
2	F	2095	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2105	EDO	4	0
2	B	2002	EDO	5	0
2	I	2045	EDO	2	0
2	D	2035	EDO	11	0
2	C	2080	EDO	2	0
2	E	2078	EDO	1	0
2	E	2088	EDO	3	0
2	E	2042	EDO	2	0
2	A	2063	EDO	7	0
2	J	2055	EDO	2	0
2	E	2092	EDO	1	0
2	E	2039	EDO	2	0
2	J	2053	EDO	3	0
2	B	2025	EDO	2	0
2	E	2089	EDO	4	0
2	A	2124	EDO	7	0
2	G	2047	EDO	2	0
2	C	2117	EDO	3	0
2	J	2104	EDO	14	0
2	J	2123	EDO	6	0
2	B	2018	EDO	1	0
2	I	2051	EDO	6	0
2	H	2113	EDO	4	0
2	J	2109	EDO	14	0
2	G	2102	EDO	3	0
2	H	2058	EDO	11	0
2	E	2090	EDO	5	0
2	A	2029	EDO	7	0
2	I	2046	EDO	4	0
2	E	2127	EDO	9	0
2	B	2030	EDO	10	0
2	C	2036	EDO	1	0
2	F	2006	EDO	2	0
2	D	2031	EDO	4	0
2	H	2060	EDO	4	0
2	G	2050	EDO	5	0
2	G	2057	EDO	7	0
2	C	2067	EDO	4	0
2	F	2098	EDO	3	0
2	G	2009	EDO	4	0
2	H	2111	EDO	3	0
2	G	2112	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2115	EDO	7	0
2	J	2014	EDO	3	0
2	A	2001	EDO	6	0
2	B	2028	EDO	11	0
2	B	2125	EDO	8	0
2	J	2110	EDO	3	0
2	A	2122	EDO	4	0
2	E	2091	EDO	5	0
2	F	2087	EDO	2	0
2	E	2005	EDO	5	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.