



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:08 AM UTC

PDB ID : 1X0R / pdb_00001x0r
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

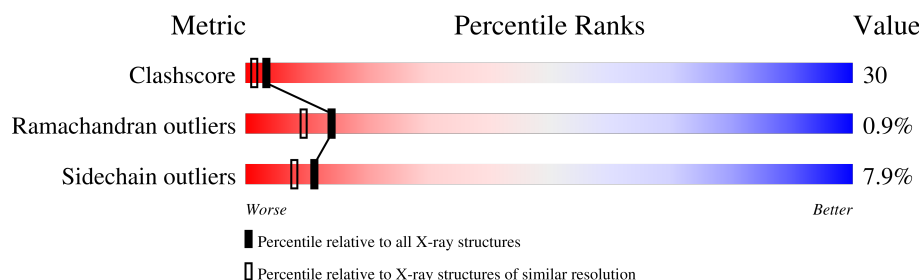
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 ≥ 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	45% 35% 16% ..
1	B	249	36% 40% 20% ..
1	C	249	41% 36% 19% ..
1	D	249	43% 38% 15% ..
1	E	249	36% 40% 19% ..
1	F	249	37% 43% 15% ..
1	G	249	40% 40% 16% ..
1	H	249	41% 43% 12% ..

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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	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	-
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

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
1	A	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	B	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	C	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	D	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	E	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	F	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	G	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	H	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	I	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	J	244	Total 1973	C 1268	N 347	O 352	S 2	Se 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

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

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

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

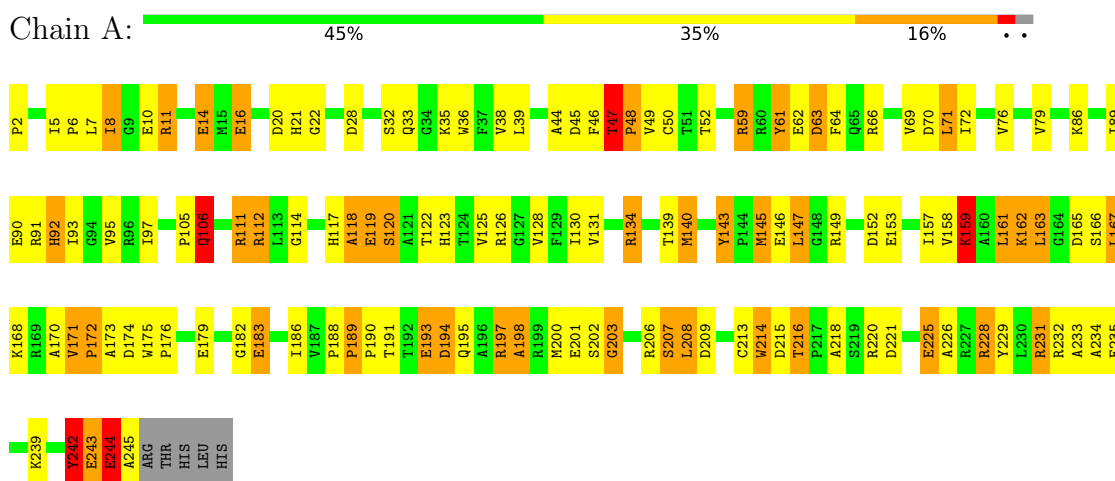
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	140	Total O 140 140	0	0
3	B	120	Total O 120 120	0	0
3	C	136	Total O 136 136	0	0
3	D	132	Total O 132 132	0	0
3	E	133	Total O 133 133	0	0
3	F	115	Total O 115 115	0	0
3	G	98	Total O 98 98	0	0
3	H	94	Total O 94 94	0	0
3	I	106	Total O 106 106	0	0
3	J	115	Total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

3 Residue-property plots

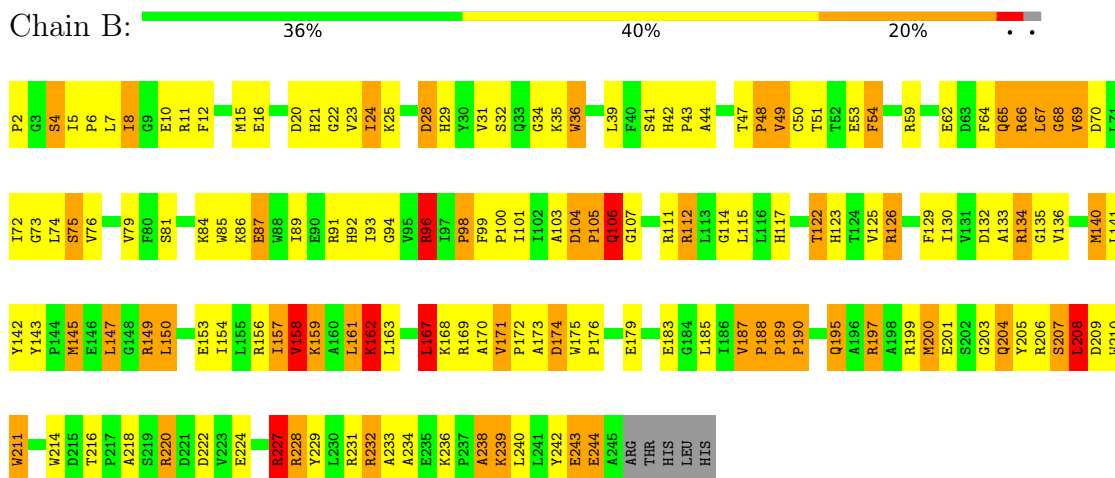
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

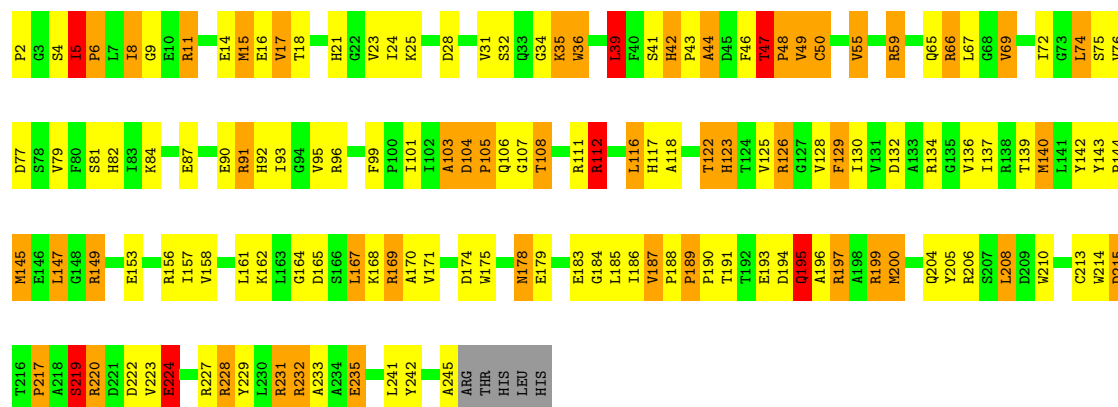


- Molecule 1: Probable peroxiredoxin



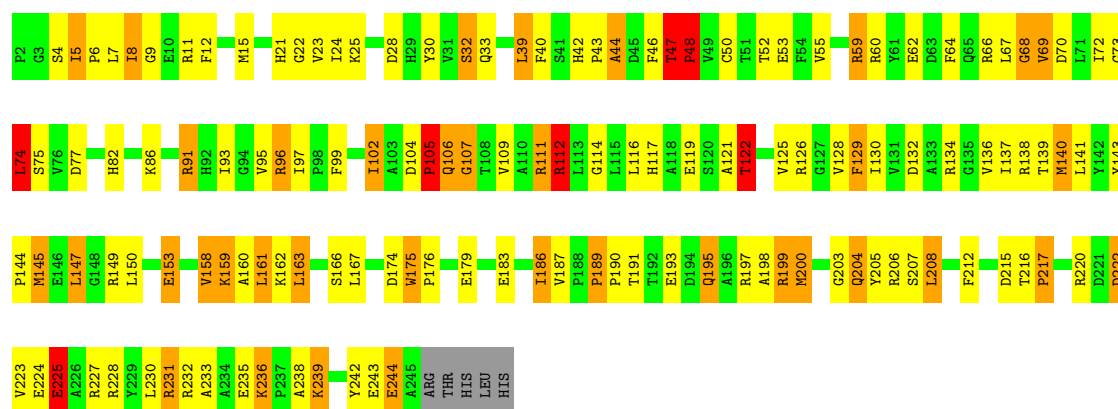
- Molecule 1: Probable peroxiredoxin





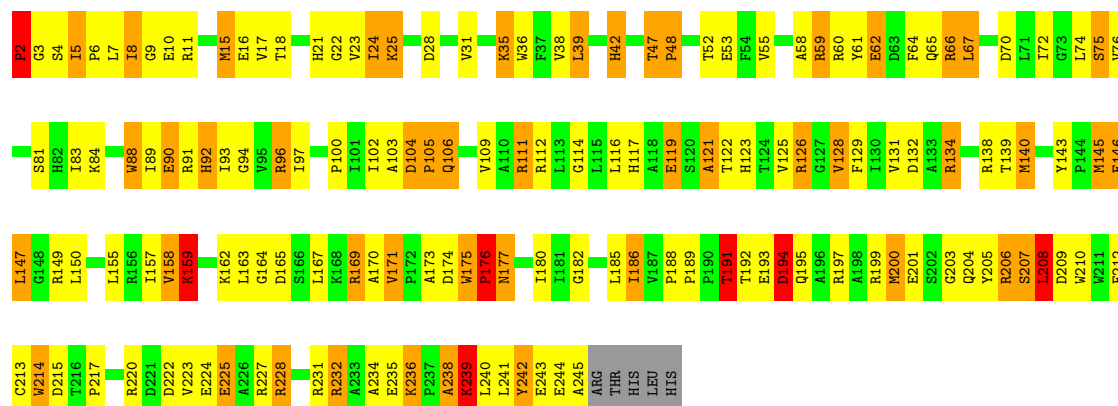
- Molecule 1: Probable peroxiredoxin

Chain D: 43% 38% 15% . .



- Molecule 1: Probable peroxiredoxin

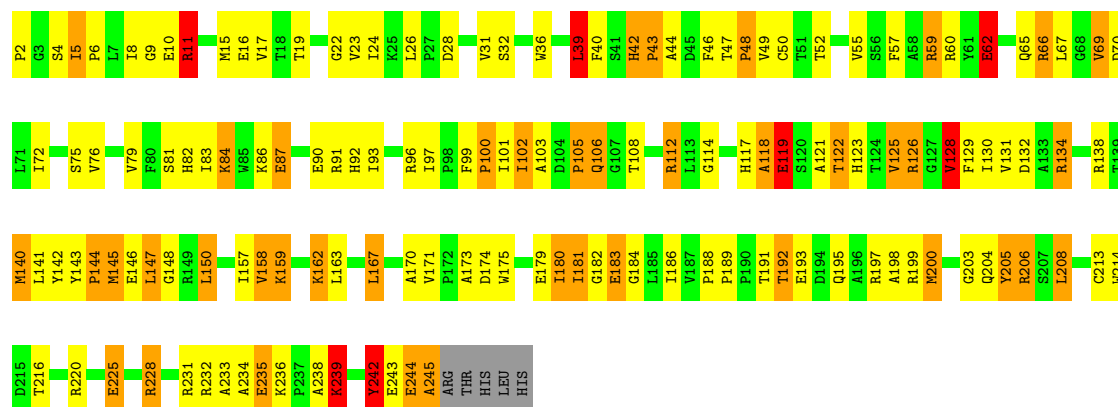
Chain E: 36% 40% 19% . .



- Molecule 1: Probable peroxiredoxin

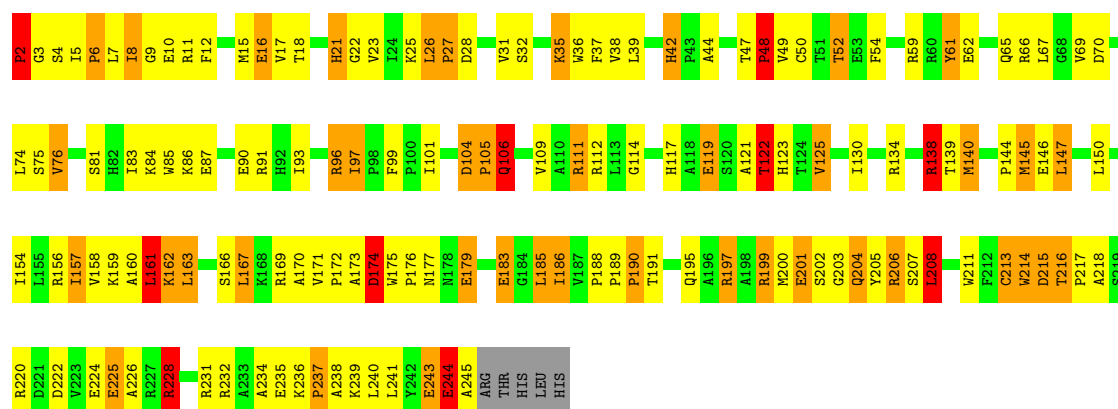
Chain F: 37% 43% 15% . .





• Molecule 1: Probable peroxiredoxin

Chain J: 38% 39% 17% . .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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.	Xtriage
Total number of atoms	21431	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.40	70/2024 (3.5%)	1.99	71/2745 (2.6%)
1	B	2.38	90/2024 (4.4%)	2.06	78/2745 (2.8%)
1	C	2.41	87/2024 (4.3%)	2.07	77/2745 (2.8%)
1	D	2.41	91/2024 (4.5%)	2.04	53/2745 (1.9%)
1	E	2.43	94/2024 (4.6%)	2.29	80/2745 (2.9%)
1	F	2.37	87/2024 (4.3%)	1.96	54/2745 (2.0%)
1	G	2.35	94/2024 (4.6%)	2.03	67/2745 (2.4%)
1	H	2.40	83/2024 (4.1%)	1.95	62/2745 (2.3%)
1	I	2.34	78/2024 (3.9%)	2.02	72/2745 (2.6%)
1	J	2.49	88/2024 (4.3%)	2.35	102/2745 (3.7%)
All	All	2.40	862/20240 (4.3%)	2.08	716/27450 (2.6%)

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 (862) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	104	ASP	CA-CB	17.26	1.72	1.53
1	D	189	PRO	CA-C	16.30	1.60	1.51
1	J	27	PRO	CA-C	15.42	1.74	1.52
1	J	140	MSE	SE-CE	-15.18	1.50	1.95
1	D	68	GLY	N-CA	14.86	1.67	1.45
1	C	140	MSE	SE-CE	-13.96	1.53	1.95
1	G	140	MSE	SE-CE	-13.09	1.56	1.95
1	E	121	ALA	CA-CB	12.63	1.76	1.53
1	E	140	MSE	SE-CE	-12.42	1.58	1.95
1	I	145	MSE	CB-CG	12.37	1.89	1.52
1	C	157	ILE	CA-CB	12.31	1.69	1.54
1	C	69	VAL	CA-CB	12.11	1.70	1.54
1	A	145	MSE	CB-CG	11.98	1.88	1.52
1	F	223	VAL	CA-CB	11.84	1.68	1.54
1	B	162	LYS	CE-NZ	11.77	1.84	1.49
1	A	89	ILE	CA-CB	11.00	1.66	1.54
1	I	140	MSE	SE-CE	-10.94	1.62	1.95
1	E	239	LYS	N-CA	10.91	1.60	1.46
1	A	175	TRP	CA-C	10.74	1.66	1.53
1	G	26	LEU	C-N	10.66	1.58	1.33
1	F	44	ALA	CA-CB	10.55	1.70	1.53
1	H	93	ILE	CA-CB	10.11	1.66	1.54
1	H	145	MSE	CB-CG	10.05	1.82	1.52
1	J	215	ASP	CA-CB	9.92	1.71	1.54
1	B	104	ASP	CB-CG	-9.91	1.27	1.52
1	E	70	ASP	CG-OD1	9.90	1.44	1.25
1	J	176	PRO	CG-CD	-9.90	1.25	1.51
1	E	239	LYS	CA-C	9.87	1.66	1.52
1	A	228	ARG	CZ-NH1	9.83	1.46	1.32
1	A	182	GLY	C-O	9.79	1.37	1.23
1	A	95	VAL	C-O	9.79	1.35	1.24
1	E	145	MSE	CB-CG	9.69	1.81	1.52
1	E	170	ALA	CA-C	9.60	1.65	1.52
1	B	104	ASP	CA-CB	9.47	1.63	1.53
1	F	222	ASP	C-O	-9.40	1.12	1.24
1	C	18	THR	CA-CB	9.37	1.66	1.53
1	D	222	ASP	CG-OD2	9.31	1.43	1.25
1	A	225	GLU	CG-CD	9.27	1.75	1.52
1	J	138	ARG	CD-NE	-9.25	1.33	1.46
1	A	93	ILE	CA-CB	9.07	1.65	1.54
1	F	23	VAL	CA-CB	9.00	1.65	1.54
1	I	119	GLU	N-CA	9.00	1.57	1.46
1	J	215	ASP	CB-CG	-8.99	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	44	ALA	CA-CB	8.91	1.68	1.53
1	H	62	GLU	CD-OE2	8.86	1.42	1.25
1	E	128	VAL	C-O	8.79	1.32	1.24
1	B	50	CYS	N-CA	8.73	1.57	1.46
1	D	21	HIS	CA-C	8.73	1.64	1.52
1	J	121	ALA	CA-CB	8.70	1.69	1.53
1	D	233	ALA	CA-CB	8.70	1.66	1.53
1	F	140	MSE	SE-CE	-8.69	1.69	1.95
1	H	6	PRO	CA-C	8.66	1.62	1.52
1	I	236	LYS	CA-C	8.61	1.62	1.53
1	H	92	HIS	CA-C	-8.60	1.41	1.52
1	G	65	GLN	N-CA	8.59	1.56	1.46
1	C	145	MSE	CB-CG	8.57	1.78	1.52
1	F	6	PRO	CA-C	8.55	1.63	1.52
1	J	190	PRO	CA-C	8.54	1.63	1.52
1	C	24	ILE	CA-C	-8.53	1.43	1.52
1	B	74	LEU	N-CA	-8.51	1.36	1.46
1	G	8	ILE	CA-CB	8.49	1.62	1.54
1	B	157	ILE	CA-CB	8.47	1.64	1.54
1	C	50	CYS	N-CA	8.47	1.56	1.46
1	G	101	ILE	C-O	8.43	1.32	1.24
1	D	145	MSE	CB-CG	8.42	1.77	1.52
1	A	72	ILE	CA-CB	8.38	1.66	1.54
1	E	177	ASN	N-CA	8.33	1.56	1.46
1	I	103	ALA	CA-CB	-8.24	1.42	1.53
1	D	32	SER	CA-C	-8.22	1.41	1.52
1	C	145	MSE	SE-CE	8.21	2.20	1.95
1	J	238	ALA	CA-C	8.17	1.63	1.52
1	G	145	MSE	SE-CE	8.14	2.19	1.95
1	I	173	ALA	CA-CB	8.13	1.66	1.53
1	H	10	GLU	N-CA	8.10	1.55	1.45
1	B	68	GLY	N-CA	8.07	1.57	1.45
1	C	103	ALA	CA-C	-8.05	1.43	1.52
1	E	89	ILE	CA-C	8.05	1.63	1.52
1	E	102	ILE	CA-CB	8.02	1.63	1.54
1	A	172	PRO	C-O	8.01	1.33	1.23
1	F	103	ALA	CA-C	-7.99	1.43	1.52
1	H	224	GLU	C-O	-7.95	1.14	1.24
1	H	58	ALA	CA-CB	7.91	1.65	1.53
1	B	31	VAL	CA-CB	-7.90	1.45	1.54
1	J	208	LEU	CA-C	7.90	1.62	1.52
1	H	97	ILE	N-CA	7.89	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	171	VAL	CA-CB	-7.89	1.44	1.54
1	B	93	ILE	C-O	-7.89	1.16	1.24
1	J	214	TRP	CG-CD1	7.89	1.56	1.36
1	C	47	THR	CB-CG2	-7.88	1.26	1.52
1	F	52	THR	N-CA	7.88	1.56	1.46
1	B	140	MSE	CG-SE	7.87	2.19	1.95
1	A	145	MSE	SE-CE	7.87	2.19	1.95
1	I	159	LYS	CG-CD	-7.86	1.28	1.52
1	I	70	ASP	CG-OD1	7.86	1.40	1.25
1	E	207	SER	CA-C	-7.86	1.42	1.52
1	E	65	GLN	N-CA	7.85	1.55	1.46
1	H	69	VAL	CA-CB	7.85	1.64	1.54
1	I	140	MSE	CG-SE	7.81	2.18	1.95
1	C	134	ARG	NE-CZ	7.79	1.41	1.33
1	C	228	ARG	CD-NE	7.74	1.57	1.46
1	B	76	VAL	N-CA	-7.73	1.36	1.46
1	G	81	SER	N-CA	7.72	1.55	1.46
1	H	189	PRO	CA-C	7.70	1.56	1.51
1	E	8	ILE	C-O	7.69	1.32	1.24
1	A	70	ASP	CG-OD1	7.68	1.40	1.25
1	D	55	VAL	C-O	7.67	1.33	1.24
1	A	158	VAL	CA-CB	7.67	1.64	1.54
1	D	96	ARG	CZ-NH1	7.65	1.43	1.32
1	J	130	ILE	C-O	-7.64	1.15	1.24
1	J	125	VAL	CA-C	7.63	1.62	1.52
1	E	224	GLU	CG-CD	7.61	1.71	1.52
1	A	119	GLU	N-CA	7.59	1.55	1.46
1	J	160	ALA	CA-CB	7.59	1.65	1.53
1	B	154	ILE	C-O	-7.57	1.15	1.24
1	J	28	ASP	N-CA	7.57	1.55	1.46
1	B	239	LYS	N-CA	7.54	1.55	1.46
1	H	144	PRO	CA-C	7.53	1.60	1.53
1	G	26	LEU	C-O	7.51	1.34	1.24
1	B	79	VAL	CA-CB	7.51	1.65	1.54
1	H	128	VAL	N-CA	-7.50	1.37	1.46
1	D	8	ILE	CB-CG1	7.49	1.68	1.53
1	J	195	GLN	N-CA	-7.49	1.36	1.46
1	H	63	ASP	C-O	7.49	1.33	1.24
1	D	243	GLU	CG-CD	7.48	1.70	1.52
1	F	225	GLU	CG-CD	7.47	1.70	1.52
1	H	145	MSE	SE-CE	7.45	2.17	1.95
1	J	224	GLU	CD-OE1	7.45	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	69	VAL	C-O	-7.44	1.16	1.24
1	C	170	ALA	CA-CB	7.43	1.65	1.53
1	A	233	ALA	C-O	7.40	1.32	1.24
1	J	188	PRO	CA-C	7.40	1.59	1.52
1	G	220	ARG	CA-C	7.40	1.62	1.52
1	H	186	ILE	CA-C	-7.38	1.43	1.52
1	B	51	THR	C-O	7.38	1.32	1.24
1	A	170	ALA	CA-C	7.38	1.63	1.53
1	D	238	ALA	CA-C	7.38	1.62	1.52
1	I	192	THR	C-O	7.36	1.32	1.23
1	H	79	VAL	CA-CB	7.35	1.65	1.54
1	E	119	GLU	CD-OE2	7.32	1.39	1.25
1	A	32	SER	CA-C	-7.32	1.42	1.52
1	A	28	ASP	CA-C	-7.30	1.42	1.52
1	D	140	MSE	SE-CE	-7.29	1.73	1.95
1	I	44	ALA	CA-CB	7.27	1.65	1.53
1	G	21	HIS	CA-C	7.27	1.62	1.52
1	J	186	ILE	CA-CB	7.27	1.64	1.54
1	D	72	ILE	CA-CB	7.26	1.65	1.54
1	C	128	VAL	C-O	-7.26	1.16	1.24
1	H	82	HIS	CA-C	-7.25	1.43	1.52
1	I	87	GLU	CB-CG	-7.24	1.30	1.52
1	F	102	ILE	CA-CB	7.23	1.63	1.54
1	C	205	TYR	CA-C	-7.23	1.43	1.52
1	B	189	PRO	C-O	-7.22	1.18	1.25
1	C	8	ILE	C-O	7.22	1.31	1.24
1	G	206	ARG	CA-C	7.20	1.62	1.52
1	A	162	LYS	CD-CE	7.20	1.74	1.52
1	J	69	VAL	CA-CB	7.20	1.63	1.54
1	C	228	ARG	NE-CZ	7.19	1.41	1.33
1	H	175	TRP	CA-C	7.17	1.61	1.53
1	D	28	ASP	C-O	-7.16	1.15	1.24
1	B	243	GLU	CG-CD	7.15	1.70	1.52
1	E	125	VAL	CA-C	7.15	1.61	1.52
1	A	64	PHE	C-O	7.12	1.32	1.24
1	I	197	ARG	CZ-NH2	7.09	1.42	1.33
1	C	87	GLU	C-O	7.08	1.32	1.24
1	J	4	SER	C-O	-7.08	1.15	1.24
1	G	197	ARG	C-O	-7.06	1.16	1.24
1	B	136	VAL	CA-CB	7.05	1.63	1.54
1	H	214	TRP	CE2-CZ2	-7.05	1.25	1.39
1	G	170	ALA	CA-CB	7.03	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	190	PRO	C-O	7.02	1.32	1.23
1	G	122	THR	CA-CB	-7.02	1.44	1.54
1	J	170	ALA	C-O	7.01	1.32	1.23
1	F	90	GLU	CG-CD	7.00	1.69	1.52
1	E	88	TRP	C-O	7.00	1.32	1.24
1	J	16	GLU	CG-CD	6.98	1.69	1.52
1	I	122	THR	CA-C	6.97	1.60	1.52
1	A	183	GLU	CD-OE2	6.97	1.38	1.25
1	F	215	ASP	CA-C	6.96	1.61	1.52
1	G	162	LYS	CE-NZ	6.93	1.70	1.49
1	F	216	THR	N-CA	-6.92	1.39	1.46
1	D	175	TRP	CA-C	6.92	1.60	1.53
1	J	243	GLU	CG-CD	6.91	1.69	1.52
1	F	216	THR	CA-CB	6.91	1.61	1.53
1	I	23	VAL	CA-CB	6.91	1.63	1.54
1	H	7	LEU	CA-C	-6.90	1.44	1.52
1	H	158	VAL	CA-C	-6.90	1.43	1.52
1	F	17	VAL	CA-CB	6.90	1.67	1.55
1	H	101	ILE	CA-CB	6.90	1.63	1.54
1	J	3	GLY	C-O	-6.89	1.16	1.24
1	F	226	ALA	CA-CB	6.88	1.64	1.53
1	F	233	ALA	CA-CB	6.88	1.64	1.53
1	J	8	ILE	C-O	6.88	1.32	1.24
1	D	12	PHE	C-O	-6.88	1.15	1.24
1	G	186	ILE	CA-CB	6.87	1.63	1.54
1	G	160	ALA	CA-CB	6.87	1.64	1.53
1	J	69	VAL	CA-C	-6.86	1.43	1.52
1	C	213	CYS	CA-C	-6.85	1.44	1.52
1	D	137	ILE	CA-CB	-6.85	1.45	1.53
1	J	96	ARG	CA-C	6.85	1.61	1.52
1	F	131	VAL	CA-CB	6.84	1.63	1.54
1	G	217	PRO	C-O	6.81	1.32	1.24
1	B	199	ARG	CB-CG	-6.80	1.32	1.52
1	I	233	ALA	N-CA	-6.78	1.38	1.46
1	I	181	ILE	CA-CB	6.78	1.63	1.54
1	C	184	GLY	C-O	6.78	1.33	1.23
1	D	4	SER	CA-C	6.78	1.60	1.52
1	F	24	ILE	N-CA	-6.78	1.38	1.46
1	D	67	LEU	C-O	6.77	1.32	1.23
1	E	243	GLU	CG-CD	6.77	1.69	1.52
1	G	52	THR	CA-CB	6.76	1.63	1.53
1	B	145	MSE	CB-CG	6.76	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	186	ILE	CA-CB	6.75	1.63	1.54
1	I	233	ALA	CA-CB	6.75	1.63	1.53
1	C	144	PRO	CG-CD	6.75	1.73	1.50
1	D	95	VAL	C-O	6.75	1.31	1.24
1	B	98	PRO	C-O	-6.74	1.16	1.24
1	D	187	VAL	N-CA	6.74	1.53	1.46
1	F	198	ALA	C-O	6.72	1.32	1.24
1	F	90	GLU	CD-OE2	6.72	1.38	1.25
1	F	15	MSE	CG-SE	6.71	2.15	1.95
1	F	3	GLY	C-O	-6.70	1.16	1.24
1	A	242	TYR	CE2-CZ	6.69	1.54	1.38
1	I	228	ARG	N-CA	-6.69	1.38	1.46
1	B	25	LYS	CA-C	6.68	1.60	1.52
1	E	90	GLU	N-CA	-6.68	1.38	1.46
1	F	168	LYS	CE-NZ	6.66	1.69	1.49
1	C	196	ALA	CA-CB	6.66	1.63	1.53
1	J	150	LEU	CA-C	6.66	1.61	1.53
1	D	186	ILE	CA-CB	-6.65	1.46	1.54
1	A	188	PRO	CA-C	6.64	1.58	1.52
1	E	93	ILE	CG1-CD1	-6.64	1.25	1.51
1	B	49	VAL	N-CA	6.64	1.54	1.46
1	D	225	GLU	CG-CD	6.63	1.68	1.52
1	F	70	ASP	CG-OD1	6.63	1.38	1.25
1	I	22	GLY	C-O	6.63	1.29	1.23
1	H	140	MSE	SE-CE	-6.62	1.75	1.95
1	E	58	ALA	CA-CB	6.62	1.63	1.53
1	C	118	ALA	C-O	-6.61	1.15	1.24
1	E	188	PRO	CA-C	6.61	1.58	1.52
1	J	52	THR	CA-CB	6.61	1.63	1.53
1	G	220	ARG	C-O	6.61	1.31	1.24
1	C	175	TRP	CA-C	6.61	1.59	1.53
1	A	111	ARG	CD-NE	6.60	1.55	1.46
1	G	218	ALA	CA-CB	6.60	1.63	1.53
1	J	26	LEU	C-O	6.60	1.31	1.24
1	J	35	LYS	CA-CB	-6.59	1.43	1.53
1	A	38	VAL	CA-CB	-6.59	1.46	1.54
1	B	218	ALA	CA-CB	6.58	1.64	1.53
1	A	198	ALA	C-O	6.58	1.31	1.24
1	B	233	ALA	C-O	6.58	1.31	1.24
1	C	49	VAL	CA-CB	-6.58	1.46	1.54
1	D	53	GLU	N-CA	6.58	1.54	1.46
1	D	44	ALA	CA-CB	6.57	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	83	ILE	CA-CB	6.57	1.62	1.54
1	J	25	LYS	N-CA	-6.56	1.38	1.46
1	G	131	VAL	C-O	6.56	1.30	1.24
1	E	173	ALA	CA-C	6.55	1.60	1.52
1	A	173	ALA	C-O	6.54	1.31	1.23
1	B	73	GLY	C-O	-6.54	1.17	1.23
1	H	168	LYS	CD-CE	6.54	1.72	1.52
1	B	34	GLY	C-O	6.54	1.32	1.23
1	D	207	SER	CB-OG	-6.54	1.29	1.42
1	H	186	ILE	CA-CB	6.53	1.62	1.54
1	F	218	ALA	CA-CB	6.53	1.63	1.53
1	G	236	LYS	CE-NZ	6.53	1.69	1.49
1	H	186	ILE	C-O	-6.52	1.16	1.24
1	D	136	VAL	CB-CG2	6.52	1.74	1.52
1	H	214	TRP	CG-CD2	-6.52	1.32	1.43
1	D	138	ARG	CB-CG	6.51	1.72	1.52
1	F	173	ALA	CA-CB	6.51	1.64	1.53
1	E	238	ALA	CA-CB	6.51	1.63	1.53
1	D	107	GLY	C-O	6.51	1.32	1.24
1	E	145	MSE	SE-CE	6.51	2.15	1.95
1	D	238	ALA	CA-CB	6.50	1.63	1.53
1	H	109	VAL	CA-CB	6.49	1.62	1.54
1	A	234	ALA	CA-C	6.48	1.61	1.52
1	I	193	GLU	N-CA	-6.48	1.38	1.46
1	I	6	PRO	CA-C	6.48	1.60	1.52
1	I	100	PRO	CA-CB	6.47	1.61	1.53
1	E	64	PHE	C-O	6.47	1.31	1.24
1	D	141	LEU	N-CA	6.46	1.54	1.46
1	B	79	VAL	CB-CG2	6.46	1.73	1.52
1	B	239	LYS	CA-C	6.45	1.61	1.52
1	J	157	ILE	N-CA	-6.45	1.39	1.46
1	A	226	ALA	CA-CB	6.44	1.64	1.53
1	C	82	HIS	C-O	6.44	1.31	1.24
1	E	234	ALA	CA-CB	6.44	1.64	1.53
1	A	197	ARG	CD-NE	6.44	1.55	1.46
1	B	66	ARG	NE-CZ	6.43	1.40	1.33
1	E	31	VAL	CA-C	6.42	1.60	1.52
1	E	111	ARG	CA-C	-6.42	1.44	1.52
1	E	236	LYS	CD-CE	6.41	1.71	1.52
1	D	132	ASP	CA-CB	6.40	1.62	1.53
1	H	12	PHE	CA-C	6.40	1.59	1.53
1	I	31	VAL	CA-C	6.39	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	89	ILE	C-O	6.39	1.31	1.24
1	I	102	ILE	CG1-CD1	6.38	1.76	1.51
1	G	119	GLU	CA-C	6.37	1.61	1.52
1	I	122	THR	C-O	6.37	1.33	1.23
1	J	17	VAL	CA-C	-6.37	1.45	1.52
1	E	104	ASP	N-CA	-6.37	1.39	1.46
1	H	39	LEU	C-O	6.36	1.31	1.24
1	H	187	VAL	CA-C	-6.36	1.48	1.53
1	F	104	ASP	CA-CB	6.36	1.61	1.53
1	E	75	SER	C-O	6.35	1.31	1.23
1	D	39	LEU	N-CA	-6.34	1.38	1.46
1	B	153	GLU	CG-CD	6.34	1.68	1.52
1	I	24	ILE	N-CA	-6.33	1.39	1.46
1	D	96	ARG	CZ-NH2	6.33	1.41	1.33
1	F	128	VAL	CA-CB	6.32	1.62	1.54
1	F	175	TRP	CA-C	6.32	1.60	1.52
1	F	79	VAL	CA-CB	6.32	1.63	1.54
1	B	159	LYS	C-O	-6.31	1.16	1.24
1	C	147	LEU	CA-C	6.31	1.59	1.52
1	D	70	ASP	CG-OD1	6.31	1.37	1.25
1	F	170	ALA	CA-C	6.29	1.61	1.53
1	E	61	TYR	C-O	-6.29	1.16	1.24
1	B	162	LYS	CD-CE	6.29	1.71	1.52
1	H	158	VAL	CB-CG1	6.28	1.73	1.52
1	F	239	LYS	C-O	-6.28	1.16	1.23
1	C	44	ALA	CA-CB	6.28	1.64	1.53
1	E	35	LYS	CD-CE	6.28	1.71	1.52
1	B	243	GLU	CA-C	6.27	1.61	1.52
1	J	49	VAL	CB-CG2	6.27	1.73	1.52
1	G	62	GLU	CD-OE1	6.26	1.37	1.25
1	G	86	LYS	CD-CE	-6.26	1.33	1.52
1	D	129	PHE	C-O	-6.25	1.16	1.24
1	A	170	ALA	C-O	6.25	1.31	1.23
1	G	128	VAL	CA-CB	6.25	1.62	1.54
1	I	93	ILE	CA-CB	6.24	1.62	1.54
1	A	47	THR	CB-CG2	-6.24	1.31	1.52
1	B	47	THR	CA-C	6.24	1.58	1.52
1	C	96	ARG	NE-CZ	6.24	1.40	1.33
1	C	178	ASN	C-O	6.24	1.31	1.23
1	F	204	GLN	CB-CG	-6.23	1.33	1.52
1	J	163	LEU	CB-CG	-6.23	1.41	1.53
1	B	6	PRO	CA-C	6.23	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	ALA	CA-CB	6.23	1.64	1.53
1	B	158	VAL	CA-CB	6.22	1.62	1.54
1	D	179	GLU	CG-CD	6.22	1.67	1.52
1	F	4	SER	CA-C	6.22	1.60	1.52
1	C	5	ILE	CA-CB	-6.22	1.44	1.54
1	A	159	LYS	CG-CD	-6.22	1.33	1.52
1	H	65	GLN	N-CA	6.22	1.54	1.46
1	E	189	PRO	CA-C	-6.22	1.48	1.51
1	B	159	LYS	CG-CD	-6.21	1.33	1.52
1	D	99	PHE	C-O	6.21	1.29	1.24
1	E	65	GLN	CD-OE1	6.21	1.35	1.23
1	I	131	VAL	N-CA	6.21	1.53	1.46
1	J	197	ARG	C-O	-6.21	1.16	1.24
1	F	136	VAL	CA-CB	6.20	1.62	1.54
1	D	33	GLN	CA-C	6.20	1.61	1.52
1	J	61	TYR	CA-C	6.18	1.60	1.52
1	D	116	LEU	CA-C	-6.17	1.45	1.53
1	J	244	GLU	CG-CD	6.16	1.67	1.52
1	C	171	VAL	CA-CB	-6.16	1.47	1.54
1	F	111	ARG	CZ-NH1	6.16	1.41	1.32
1	E	104	ASP	CB-CG	-6.16	1.36	1.52
1	F	147	LEU	CA-C	6.16	1.59	1.52
1	G	120	SER	CA-C	-6.15	1.45	1.52
1	J	220	ARG	CG-CD	6.15	1.70	1.52
1	C	65	GLN	N-CA	6.15	1.53	1.46
1	B	53	GLU	N-CA	6.14	1.53	1.46
1	F	95	VAL	CA-CB	6.14	1.63	1.54
1	J	177	ASN	CA-C	-6.14	1.44	1.52
1	I	121	ALA	CA-CB	6.14	1.63	1.53
1	G	223	VAL	CA-CB	6.14	1.61	1.54
1	I	145	MSE	SE-CE	6.14	2.13	1.95
1	I	128	VAL	N-CA	-6.13	1.39	1.46
1	A	170	ALA	CA-CB	6.13	1.63	1.53
1	H	29	HIS	N-CA	-6.13	1.38	1.46
1	E	180	ILE	C-O	6.12	1.30	1.23
1	H	213	CYS	C-O	-6.12	1.16	1.23
1	I	235	GLU	CG-CD	6.11	1.67	1.52
1	I	11	ARG	CD-NE	6.10	1.54	1.46
1	G	197	ARG	CG-CD	6.09	1.70	1.52
1	C	17	VAL	CA-C	-6.09	1.45	1.52
1	E	111	ARG	CZ-NH2	6.09	1.41	1.33
1	E	100	PRO	C-O	6.09	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	193	GLU	CB-CG	-6.08	1.34	1.52
1	C	4	SER	N-CA	-6.08	1.38	1.45
1	B	44	ALA	CA-CB	6.07	1.63	1.53
1	D	183	GLU	CD-OE2	6.07	1.36	1.25
1	H	197	ARG	CD-NE	6.07	1.54	1.46
1	E	38	VAL	CA-CB	6.07	1.61	1.54
1	E	25	LYS	CE-NZ	6.06	1.67	1.49
1	J	18	THR	CA-CB	6.06	1.62	1.53
1	G	192	THR	CA-C	-6.06	1.45	1.52
1	I	239	LYS	CA-C	6.06	1.60	1.52
1	B	209	ASP	CA-C	-6.06	1.45	1.52
1	F	239	LYS	CA-C	6.05	1.59	1.52
1	C	137	ILE	CB-CG1	6.05	1.65	1.53
1	F	193	GLU	CB-CG	-6.05	1.34	1.52
1	A	62	GLU	CA-C	6.04	1.60	1.52
1	G	12	PHE	CA-C	6.04	1.60	1.53
1	C	219	SER	CB-OG	-6.04	1.30	1.42
1	H	170	ALA	CA-CB	6.04	1.63	1.53
1	I	234	ALA	CA-CB	-6.04	1.42	1.53
1	F	112	ARG	CZ-NH2	6.03	1.41	1.33
1	G	31	VAL	CA-C	6.03	1.60	1.52
1	G	130	ILE	C-O	6.03	1.31	1.24
1	F	225	GLU	CB-CG	6.03	1.70	1.52
1	J	27	PRO	N-CA	6.03	1.55	1.47
1	F	140	MSE	CG-SE	6.02	2.13	1.95
1	H	71	LEU	CA-C	-6.02	1.45	1.52
1	D	160	ALA	C-O	-6.00	1.17	1.24
1	J	26	LEU	C-N	6.00	1.47	1.33
1	C	194	ASP	CG-OD2	6.00	1.36	1.25
1	C	224	GLU	CG-CD	6.00	1.67	1.52
1	G	65	GLN	CA-C	6.00	1.60	1.52
1	H	31	VAL	CA-C	6.00	1.60	1.52
1	C	96	ARG	CZ-NH2	6.00	1.41	1.33
1	B	134	ARG	CG-CD	5.99	1.70	1.52
1	B	141	LEU	C-O	-5.99	1.17	1.24
1	C	233	ALA	CA-CB	5.99	1.62	1.53
1	D	30	TYR	CA-C	5.99	1.60	1.52
1	J	157	ILE	CA-CB	5.99	1.61	1.54
1	B	145	MSE	CG-SE	-5.99	1.77	1.95
1	B	162	LYS	CG-CD	5.99	1.70	1.52
1	B	112	ARG	CA-C	-5.98	1.44	1.52
1	I	150	LEU	C-O	5.98	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	223	VAL	CA-CB	5.97	1.62	1.54
1	G	43	PRO	C-O	-5.97	1.17	1.24
1	B	133	ALA	CA-C	-5.97	1.42	1.52
1	J	225	GLU	CA-C	5.97	1.60	1.52
1	C	112	ARG	NE-CZ	5.96	1.39	1.33
1	E	197	ARG	CZ-NH1	5.96	1.41	1.32
1	H	160	ALA	CA-CB	5.96	1.62	1.53
1	C	184	GLY	CA-C	5.96	1.57	1.52
1	B	228	ARG	NE-CZ	5.95	1.39	1.33
1	G	145	MSE	CB-CG	5.95	1.70	1.52
1	A	128	VAL	CA-C	5.94	1.59	1.52
1	A	220	ARG	NE-CZ	5.94	1.39	1.33
1	B	156	ARG	CZ-NH1	5.94	1.41	1.32
1	J	111	ARG	CZ-NH2	5.94	1.41	1.33
1	H	197	ARG	CG-CD	5.93	1.70	1.52
1	D	224	GLU	C-O	-5.93	1.16	1.24
1	D	128	VAL	CA-C	5.93	1.59	1.52
1	D	130	ILE	CA-C	5.92	1.59	1.52
1	G	181	ILE	CA-CB	5.92	1.61	1.54
1	G	121	ALA	CA-CB	5.92	1.63	1.53
1	G	6	PRO	CA-C	5.92	1.60	1.52
1	E	182	GLY	C-O	5.91	1.31	1.23
1	A	216	THR	CA-C	-5.90	1.45	1.52
1	D	93	ILE	CA-CB	5.90	1.61	1.54
1	G	144	PRO	CA-C	5.90	1.58	1.53
1	J	161	LEU	CA-C	5.90	1.60	1.52
1	C	140	MSE	CG-SE	5.89	2.13	1.95
1	D	200	MSE	CG-SE	5.89	2.13	1.95
1	B	129	PHE	N-CA	-5.88	1.39	1.46
1	E	231	ARG	CZ-NH2	5.88	1.41	1.33
1	B	229	TYR	CA-C	-5.88	1.45	1.52
1	A	153	GLU	CB-CG	5.88	1.70	1.52
1	G	76	VAL	CA-C	5.88	1.60	1.52
1	I	106	GLN	N-CA	5.88	1.53	1.46
1	H	111	ARG	CZ-NH2	5.87	1.41	1.33
1	E	67	LEU	C-O	-5.87	1.16	1.24
1	F	98	PRO	CA-C	-5.87	1.46	1.52
1	B	54	PHE	CA-CB	5.87	1.62	1.53
1	C	196	ALA	C-O	5.87	1.30	1.24
1	J	231	ARG	CG-CD	5.87	1.70	1.52
1	A	220	ARG	CZ-NH2	5.86	1.41	1.33
1	G	86	LYS	CA-CB	5.86	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	116	LEU	CA-C	5.86	1.60	1.52
1	J	12	PHE	CA-C	5.86	1.59	1.53
1	I	125	VAL	CA-CB	5.85	1.62	1.54
1	D	153	GLU	CA-C	5.84	1.60	1.52
1	E	200	MSE	CG-SE	5.84	2.12	1.95
1	H	86	LYS	C-O	-5.84	1.17	1.24
1	H	137	ILE	C-O	5.84	1.30	1.24
1	I	170	ALA	CA-C	5.84	1.60	1.52
1	H	194	ASP	CG-OD1	5.84	1.36	1.25
1	E	192	THR	CA-C	-5.83	1.45	1.52
1	A	221	ASP	N-CA	5.82	1.53	1.46
1	H	207	SER	CA-C	-5.82	1.45	1.52
1	F	112	ARG	CG-CD	5.82	1.70	1.52
1	H	159	LYS	CG-CD	-5.82	1.34	1.52
1	B	22	GLY	C-O	5.82	1.28	1.23
1	E	175	TRP	CA-C	-5.82	1.47	1.53
1	H	72	ILE	C-O	5.82	1.29	1.24
1	J	214	TRP	CE2-CZ2	-5.81	1.27	1.39
1	C	242	TYR	CG-CD1	5.81	1.51	1.39
1	F	140	MSE	N-CA	5.81	1.53	1.46
1	D	4	SER	N-CA	-5.80	1.39	1.45
1	J	213	CYS	C-O	5.80	1.31	1.23
1	I	69	VAL	CA-C	-5.80	1.45	1.52
1	B	115	LEU	CG-CD2	5.79	1.71	1.52
1	H	136	VAL	CA-CB	5.79	1.61	1.54
1	B	23	VAL	C-O	-5.78	1.17	1.24
1	F	110	ALA	C-O	5.78	1.30	1.24
1	D	179	GLU	CA-CB	5.78	1.63	1.53
1	B	140	MSE	CA-C	-5.78	1.45	1.52
1	E	220	ARG	CZ-NH1	5.78	1.40	1.32
1	C	228	ARG	N-CA	-5.77	1.39	1.46
1	F	67	LEU	N-CA	5.77	1.53	1.46
1	E	159	LYS	CG-CD	-5.76	1.35	1.52
1	A	225	GLU	CB-CG	5.75	1.69	1.52
1	G	170	ALA	C-N	5.75	1.37	1.32
1	A	214	TRP	CG-CD2	-5.75	1.33	1.43
1	I	70	ASP	N-CA	-5.75	1.38	1.45
1	A	36	TRP	CA-C	5.75	1.61	1.53
1	I	125	VAL	CB-CG2	-5.74	1.33	1.52
1	H	192	THR	CA-C	-5.74	1.45	1.52
1	E	15	MSE	CG-SE	5.74	2.12	1.95
1	A	191	THR	CB-CG2	5.73	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	PHE	C-O	-5.73	1.17	1.24
1	C	136	VAL	CA-C	5.73	1.59	1.52
1	H	104	ASP	N-CA	-5.73	1.40	1.46
1	I	15	MSE	CG-SE	5.73	2.12	1.95
1	D	106	GLN	N-CA	5.73	1.52	1.46
1	D	23	VAL	N-CA	-5.72	1.39	1.46
1	E	169	ARG	CZ-NH2	5.72	1.40	1.33
1	G	49	VAL	CA-CB	-5.71	1.47	1.54
1	E	243	GLU	CD-OE2	5.71	1.36	1.25
1	D	160	ALA	CA-CB	5.71	1.62	1.53
1	I	171	VAL	N-CA	-5.71	1.40	1.46
1	I	225	GLU	CG-CD	5.70	1.66	1.52
1	D	112	ARG	CG-CD	5.70	1.69	1.52
1	J	31	VAL	CA-C	5.70	1.59	1.52
1	E	191	THR	CA-C	5.70	1.60	1.52
1	E	232	ARG	CB-CG	5.70	1.69	1.52
1	C	101	ILE	CA-C	5.70	1.59	1.52
1	D	25	LYS	CA-C	5.69	1.59	1.52
1	J	85	TRP	N-CA	5.69	1.53	1.46
1	C	11	ARG	C-O	5.69	1.30	1.23
1	D	198	ALA	N-CA	-5.69	1.39	1.46
1	E	224	GLU	CD-OE1	5.68	1.36	1.25
1	F	172	PRO	CA-C	-5.68	1.45	1.52
1	H	131	VAL	CA-CB	-5.68	1.47	1.54
1	C	223	VAL	C-O	5.68	1.30	1.24
1	H	24	ILE	CA-CB	-5.67	1.45	1.55
1	G	242	TYR	CZ-OH	5.67	1.50	1.38
1	H	15	MSE	CG-SE	5.66	2.12	1.95
1	C	224	GLU	CD-OE1	5.66	1.36	1.25
1	H	221	ASP	CA-C	5.66	1.60	1.52
1	B	170	ALA	C-N	5.66	1.37	1.32
1	G	227	ARG	N-CA	-5.65	1.39	1.46
1	J	144	PRO	CG-CD	5.65	1.70	1.50
1	B	64	PHE	C-O	5.64	1.30	1.24
1	H	237	PRO	CB-CG	5.64	1.77	1.49
1	H	204	GLN	C-O	-5.64	1.16	1.24
1	C	99	PHE	C-O	5.63	1.31	1.24
1	E	214	TRP	CG-CD1	5.63	1.51	1.36
1	G	97	ILE	C-N	5.63	1.38	1.33
1	B	69	VAL	CB-CG2	5.63	1.71	1.52
1	I	131	VAL	CA-CB	5.63	1.61	1.54
1	G	228	ARG	CG-CD	5.62	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	126	ARG	CZ-NH1	5.62	1.40	1.32
1	D	102	ILE	CA-C	5.61	1.59	1.52
1	I	82	HIS	N-CA	-5.61	1.39	1.46
1	E	157	ILE	CA-CB	5.61	1.60	1.54
1	A	231	ARG	CA-C	5.61	1.60	1.52
1	I	24	ILE	CA-CB	-5.60	1.45	1.55
1	F	131	VAL	C-O	-5.60	1.18	1.24
1	A	119	GLU	CD-OE2	5.60	1.35	1.25
1	C	214	TRP	CG-CD2	-5.60	1.33	1.43
1	B	28	ASP	CA-C	-5.59	1.45	1.52
1	D	111	ARG	CZ-NH2	5.59	1.40	1.33
1	G	190	PRO	C-O	5.59	1.30	1.23
1	G	235	GLU	CG-CD	5.59	1.66	1.52
1	F	154	ILE	CG1-CD1	5.59	1.73	1.51
1	G	17	VAL	N-CA	5.59	1.52	1.46
1	D	47	THR	CB-CG2	-5.59	1.34	1.52
1	I	206	ARG	CZ-NH1	5.59	1.40	1.32
1	I	183	GLU	CD-OE2	5.58	1.35	1.25
1	E	74	LEU	CA-C	-5.58	1.45	1.52
1	E	243	GLU	N-CA	5.58	1.53	1.46
1	A	66	ARG	CZ-NH2	5.58	1.40	1.33
1	F	2	PRO	CA-C	-5.58	1.41	1.52
1	D	122	THR	CA-C	5.57	1.59	1.52
1	F	12	PHE	CA-C	5.57	1.58	1.53
1	C	158	VAL	N-CA	5.57	1.53	1.46
1	J	216	THR	C-O	-5.57	1.17	1.24
1	H	77	ASP	C-O	5.57	1.31	1.23
1	J	66	ARG	NE-CZ	5.57	1.39	1.33
1	C	206	ARG	CA-C	5.57	1.60	1.52
1	C	214	TRP	CG-CD1	5.57	1.50	1.36
1	G	242	TYR	CD2-CE2	5.57	1.55	1.38
1	A	95	VAL	CA-CB	5.56	1.60	1.54
1	F	156	ARG	C-O	5.56	1.30	1.24
1	C	15	MSE	CG-SE	5.56	2.12	1.95
1	I	102	ILE	C-O	5.56	1.31	1.24
1	A	61	TYR	C-N	-5.56	1.26	1.34
1	A	229	TYR	C-O	5.55	1.30	1.24
1	E	116	LEU	C-O	5.55	1.30	1.24
1	C	101	ILE	N-CA	-5.55	1.39	1.46
1	F	25	LYS	CE-NZ	5.55	1.66	1.49
1	B	81	SER	C-O	-5.54	1.17	1.24
1	H	22	GLY	C-O	5.54	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	SER	N-CA	5.54	1.52	1.45
1	J	206	ARG	NE-CZ	5.54	1.39	1.33
1	F	61	TYR	C-O	-5.53	1.17	1.24
1	A	76	VAL	CA-C	5.52	1.58	1.52
1	A	8	ILE	N-CA	-5.52	1.39	1.46
1	C	79	VAL	CB-CG2	5.52	1.70	1.52
1	B	96	ARG	CZ-NH1	5.52	1.40	1.32
1	E	8	ILE	N-CA	-5.51	1.39	1.46
1	H	145	MSE	CG-SE	-5.51	1.78	1.95
1	E	62	GLU	CG-CD	5.51	1.65	1.52
1	F	184	GLY	CA-C	5.51	1.57	1.52
1	J	66	ARG	CZ-NH2	5.51	1.40	1.33
1	E	66	ARG	CG-CD	5.51	1.69	1.52
1	F	158	VAL	CA-CB	5.51	1.61	1.54
1	B	220	ARG	CG-CD	5.50	1.69	1.52
1	F	51	THR	CA-C	-5.50	1.45	1.52
1	F	159	LYS	CG-CD	-5.50	1.35	1.52
1	F	210	TRP	C-O	-5.50	1.17	1.24
1	H	173	ALA	CA-CB	5.49	1.62	1.53
1	G	159	LYS	CG-CD	-5.49	1.35	1.52
1	H	140	MSE	C-O	5.49	1.29	1.23
1	E	238	ALA	CA-C	5.49	1.59	1.52
1	D	159	LYS	C-O	5.49	1.30	1.24
1	E	66	ARG	CZ-NH1	5.49	1.40	1.32
1	H	12	PHE	N-CA	5.49	1.52	1.45
1	J	119	GLU	C-O	5.48	1.30	1.24
1	I	183	GLU	CG-CD	5.48	1.65	1.52
1	C	39	LEU	CB-CG	5.48	1.64	1.53
1	G	96	ARG	CB-CG	-5.48	1.36	1.52
1	J	243	GLU	CA-CB	5.48	1.62	1.53
1	C	104	ASP	CA-C	5.47	1.59	1.52
1	D	223	VAL	C-O	5.46	1.30	1.24
1	B	145	MSE	SE-CE	5.46	2.11	1.95
1	E	76	VAL	CB-CG1	5.45	1.70	1.52
1	D	136	VAL	CA-CB	5.45	1.61	1.54
1	I	43	PRO	CA-C	-5.45	1.44	1.52
1	G	86	LYS	CA-C	-5.45	1.45	1.52
1	H	93	ILE	N-CA	5.45	1.51	1.46
1	G	124	THR	CB-CG2	-5.44	1.34	1.52
1	E	171	VAL	CB-CG2	5.44	1.70	1.52
1	F	149	ARG	CA-CB	5.43	1.62	1.53
1	H	242	TYR	CA-C	5.43	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	21	HIS	C-O	-5.43	1.17	1.24
1	F	225	GLU	CD-OE2	5.43	1.35	1.25
1	G	136	VAL	CA-CB	5.43	1.60	1.54
1	J	37	PHE	CA-C	5.42	1.59	1.52
1	A	220	ARG	CD-NE	5.42	1.53	1.46
1	C	28	ASP	CG-OD1	5.42	1.35	1.25
1	F	57	PHE	N-CA	5.42	1.52	1.46
1	J	206	ARG	CA-C	5.42	1.60	1.53
1	H	185	LEU	N-CA	-5.41	1.39	1.45
1	G	171	VAL	CA-C	-5.41	1.48	1.52
1	C	55	VAL	C-O	5.41	1.30	1.24
1	F	187	VAL	N-CA	5.41	1.53	1.46
1	B	54	PHE	C-O	5.41	1.30	1.24
1	I	159	LYS	C-O	5.41	1.30	1.24
1	I	16	GLU	C-O	-5.41	1.17	1.24
1	D	193	GLU	CB-CG	-5.40	1.36	1.52
1	G	62	GLU	CD-OE2	5.39	1.35	1.25
1	B	232	ARG	CB-CG	5.39	1.68	1.52
1	D	212	PHE	CB-CG	5.39	1.63	1.50
1	G	40	PHE	C-O	5.39	1.30	1.23
1	J	154	ILE	CB-CG1	5.39	1.64	1.53
1	E	158	VAL	CA-C	-5.39	1.45	1.52
1	B	174	ASP	CA-C	5.38	1.61	1.52
1	E	242	TYR	CD1-CE1	5.38	1.54	1.38
1	G	111	ARG	CZ-NH2	5.38	1.40	1.33
1	H	56	SER	CA-C	5.38	1.59	1.52
1	D	239	LYS	CE-NZ	5.38	1.65	1.49
1	G	195	GLN	CA-CB	-5.37	1.44	1.53
1	H	51	THR	CA-CB	5.37	1.61	1.53
1	B	75	SER	CA-C	5.37	1.59	1.52
1	A	140	MSE	SE-CE	-5.37	1.79	1.95
1	G	125	VAL	C-O	5.36	1.30	1.24
1	A	193	GLU	CB-CG	-5.36	1.36	1.52
1	B	4	SER	CB-OG	5.36	1.52	1.42
1	C	210	TRP	CA-C	5.36	1.60	1.52
1	C	223	VAL	N-CA	-5.36	1.40	1.46
1	J	185	LEU	N-CA	5.36	1.52	1.46
1	E	163	LEU	C-O	5.35	1.30	1.24
1	A	76	VAL	CB-CG1	5.35	1.70	1.52
1	D	111	ARG	CZ-NH1	5.35	1.40	1.32
1	I	57	PHE	C-O	-5.35	1.17	1.24
1	F	145	MSE	CB-CG	5.35	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	153	GLU	CG-CD	5.35	1.65	1.52
1	C	108	THR	CB-CG2	-5.35	1.34	1.52
1	J	62	GLU	CD-OE1	5.35	1.35	1.25
1	C	59	ARG	CZ-NH1	5.35	1.40	1.32
1	H	3	GLY	C-O	-5.35	1.17	1.24
1	H	118	ALA	CA-CB	5.34	1.63	1.53
1	J	239	LYS	CE-NZ	5.34	1.65	1.49
1	F	160	ALA	CA-C	5.34	1.59	1.52
1	D	69	VAL	CA-CB	5.34	1.61	1.54
1	F	116	LEU	CG-CD1	5.34	1.70	1.52
1	D	236	LYS	CG-CD	5.33	1.68	1.52
1	E	6	PRO	CA-C	5.33	1.59	1.52
1	G	65	GLN	CD-NE2	5.33	1.44	1.33
1	I	231	ARG	CG-CD	5.32	1.68	1.52
1	B	85	TRP	CA-CB	5.32	1.61	1.53
1	C	32	SER	CA-CB	5.32	1.62	1.53
1	G	226	ALA	CA-C	-5.32	1.46	1.52
1	B	89	ILE	CA-CB	5.31	1.61	1.54
1	G	197	ARG	CZ-NH1	5.31	1.40	1.32
1	E	128	VAL	CA-C	5.31	1.59	1.52
1	E	22	GLY	C-O	5.31	1.28	1.23
1	C	195	GLN	CB-CG	-5.30	1.36	1.52
1	F	200	MSE	SE-CE	5.30	2.11	1.95
1	F	9	GLY	CA-C	5.30	1.58	1.51
1	E	83	ILE	CA-CB	5.30	1.60	1.54
1	G	134	ARG	CZ-NH1	5.30	1.40	1.32
1	C	46	PHE	N-CA	5.29	1.54	1.46
1	C	23	VAL	CA-CB	5.29	1.61	1.54
1	G	238	ALA	N-CA	5.29	1.52	1.46
1	D	223	VAL	N-CA	-5.28	1.40	1.46
1	F	193	GLU	C-O	5.28	1.30	1.24
1	D	24	ILE	C-O	5.28	1.29	1.23
1	H	208	LEU	C-O	-5.28	1.17	1.23
1	J	172	PRO	CG-CD	5.28	1.68	1.50
1	I	76	VAL	C-O	-5.28	1.17	1.24
1	J	83	ILE	CA-CB	-5.28	1.47	1.54
1	A	206	ARG	CA-C	5.27	1.59	1.52
1	E	242	TYR	CG-CD1	5.27	1.50	1.39
1	J	65	GLN	N-CA	5.27	1.52	1.46
1	B	171	VAL	CA-C	-5.27	1.48	1.52
1	H	228	ARG	CG-CD	5.27	1.68	1.52
1	G	129	PHE	CA-C	-5.27	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	54	PHE	CA-C	-5.26	1.46	1.52
1	B	112	ARG	NE-CZ	5.26	1.38	1.33
1	E	165	ASP	CA-C	-5.26	1.46	1.52
1	F	130	ILE	CA-CB	5.26	1.60	1.54
1	F	236	LYS	CA-C	5.26	1.58	1.52
1	C	90	GLU	N-CA	-5.25	1.39	1.46
1	G	192	THR	CA-CB	5.25	1.64	1.54
1	D	141	LEU	C-O	5.24	1.30	1.23
1	E	140	MSE	CG-SE	5.24	2.11	1.95
1	B	41	SER	C-O	5.24	1.30	1.23
1	D	22	GLY	C-O	-5.24	1.18	1.23
1	A	152	ASP	CA-C	5.24	1.59	1.52
1	A	159	LYS	N-CA	5.24	1.52	1.46
1	D	230	LEU	CA-C	5.24	1.59	1.52
1	C	90	GLU	CB-CG	-5.23	1.36	1.52
1	B	8	ILE	CB-CG1	5.23	1.64	1.53
1	D	193	GLU	N-CA	-5.23	1.40	1.46
1	B	51	THR	CA-CB	5.23	1.61	1.53
1	F	154	ILE	C-O	-5.23	1.18	1.24
1	J	224	GLU	CG-CD	5.23	1.65	1.52
1	E	42	HIS	CA-C	5.23	1.58	1.52
1	G	86	LYS	C-O	5.23	1.30	1.24
1	J	224	GLU	N-CA	-5.22	1.40	1.46
1	C	77	ASP	C-O	-5.22	1.16	1.23
1	I	130	ILE	N-CA	-5.22	1.40	1.46
1	J	21	HIS	C-O	-5.22	1.17	1.24
1	A	225	GLU	N-CA	5.21	1.52	1.46
1	E	5	ILE	CA-CB	-5.21	1.49	1.55
1	D	174	ASP	CB-CG	5.21	1.65	1.52
1	E	55	VAL	CB-CG1	5.21	1.69	1.52
1	F	148	GLY	CA-C	-5.21	1.46	1.52
1	C	227	ARG	N-CA	-5.21	1.39	1.46
1	D	216	THR	CA-C	-5.20	1.46	1.52
1	G	91	ARG	C-O	-5.20	1.18	1.24
1	G	136	VAL	N-CA	5.20	1.52	1.46
1	I	23	VAL	CA-C	-5.20	1.46	1.52
1	D	67	LEU	C-N	-5.20	1.25	1.33
1	F	97	ILE	CA-C	5.20	1.58	1.52
1	D	96	ARG	CA-C	5.20	1.59	1.52
1	D	204	GLN	CB-CG	-5.20	1.36	1.52
1	A	131	VAL	CA-C	-5.20	1.46	1.52
1	A	139	THR	CB-CG2	5.20	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	LYS	C-O	5.19	1.30	1.24
1	G	45	ASP	C-O	5.19	1.30	1.23
1	I	197	ARG	CZ-NH1	5.19	1.40	1.32
1	J	36	TRP	N-CA	5.19	1.52	1.45
1	G	189	PRO	CA-C	5.19	1.55	1.52
1	I	243	GLU	CG-CD	5.18	1.65	1.52
1	A	63	ASP	C-O	5.18	1.30	1.24
1	I	60	ARG	CA-CB	5.18	1.62	1.53
1	I	239	LYS	CD-CE	5.18	1.68	1.52
1	F	112	ARG	CD-NE	5.17	1.53	1.46
1	G	15	MSE	CG-SE	5.17	2.10	1.95
1	I	228	ARG	CD-NE	5.17	1.53	1.46
1	A	69	VAL	N-CA	5.17	1.52	1.46
1	H	74	LEU	CA-C	5.16	1.59	1.52
1	C	165	ASP	N-CA	5.16	1.52	1.46
1	E	186	ILE	CA-C	-5.16	1.46	1.52
1	E	208	LEU	CA-C	5.16	1.59	1.52
1	G	72	ILE	C-O	5.16	1.29	1.24
1	I	55	VAL	N-CA	-5.15	1.40	1.46
1	J	199	ARG	CZ-NH2	5.15	1.40	1.33
1	B	200	MSE	CG-SE	5.15	2.10	1.95
1	B	204	GLN	CB-CG	-5.15	1.36	1.52
1	I	91	ARG	C-O	-5.15	1.18	1.24
1	C	31	VAL	CA-CB	-5.15	1.48	1.54
1	G	96	ARG	C-O	-5.14	1.17	1.24
1	I	42	HIS	CA-C	5.14	1.57	1.52
1	G	20	ASP	C-O	-5.14	1.17	1.24
1	B	66	ARG	CZ-NH2	5.13	1.40	1.33
1	C	112	ARG	CG-CD	5.13	1.67	1.52
1	H	23	VAL	C-O	5.13	1.31	1.24
1	A	139	THR	N-CA	5.13	1.51	1.46
1	I	162	LYS	CD-CE	5.13	1.67	1.52
1	A	90	GLU	CB-CG	-5.12	1.37	1.52
1	I	52	THR	CA-CB	5.12	1.61	1.53
1	C	123	HIS	N-CA	5.12	1.52	1.46
1	J	76	VAL	N-CA	5.12	1.52	1.46
1	B	197	ARG	CD-NE	5.12	1.53	1.46
1	F	112	ARG	NE-CZ	5.12	1.38	1.33
1	G	47	THR	N-CA	5.11	1.53	1.45
1	J	199	ARG	CB-CG	-5.11	1.37	1.52
1	E	126	ARG	CA-C	-5.11	1.47	1.53
1	G	42	HIS	C-O	5.10	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	170	ALA	CA-CB	5.10	1.61	1.53
1	F	179	GLU	CD-OE1	5.10	1.35	1.25
1	I	62	GLU	C-O	5.10	1.30	1.24
1	H	106	GLN	CA-C	-5.10	1.46	1.52
1	I	179	GLU	N-CA	5.10	1.52	1.46
1	G	225	GLU	N-CA	-5.10	1.40	1.46
1	C	91	ARG	NE-CZ	5.09	1.38	1.33
1	D	206	ARG	CZ-NH1	5.09	1.39	1.32
1	B	172	PRO	C-O	5.09	1.30	1.23
1	B	106	GLN	C-O	5.09	1.30	1.24
1	D	227	ARG	CG-CD	5.09	1.67	1.52
1	E	158	VAL	CA-CB	5.09	1.60	1.54
1	E	60	ARG	CG-CD	5.09	1.67	1.52
1	B	87	GLU	CA-C	5.09	1.59	1.52
1	J	226	ALA	CA-C	-5.09	1.46	1.52
1	E	4	SER	C-O	-5.08	1.17	1.24
1	D	193	GLU	C-O	5.08	1.30	1.24
1	H	47	THR	CB-OG1	-5.08	1.35	1.43
1	B	67	LEU	C-O	5.08	1.30	1.23
1	D	7	LEU	CA-C	5.08	1.58	1.52
1	B	21	HIS	C-O	-5.08	1.17	1.24
1	I	46	PHE	CA-C	-5.08	1.46	1.53
1	J	174	ASP	CG-OD1	5.07	1.34	1.25
1	H	214	TRP	CE3-CZ3	-5.07	1.23	1.38
1	D	46	PHE	CA-C	-5.07	1.46	1.53
1	G	166	SER	N-CA	-5.07	1.39	1.46
1	C	76	VAL	CA-C	5.07	1.58	1.52
1	C	169	ARG	C-O	-5.07	1.17	1.23
1	G	79	VAL	CA-CB	5.07	1.61	1.54
1	J	202	SER	C-O	5.06	1.30	1.24
1	A	52	THR	CA-CB	5.06	1.61	1.53
1	J	237	PRO	CB-CG	5.06	1.75	1.49
1	G	100	PRO	C-O	5.06	1.29	1.23
1	I	134	ARG	CA-C	-5.06	1.45	1.52
1	F	41	SER	C-O	5.05	1.30	1.23
1	H	173	ALA	C-O	-5.05	1.18	1.23
1	C	205	TYR	CD2-CE2	5.05	1.53	1.38
1	F	57	PHE	C-O	5.04	1.29	1.24
1	J	234	ALA	N-CA	5.04	1.52	1.46
1	D	166	SER	N-CA	-5.04	1.39	1.46
1	B	197	ARG	C-O	-5.04	1.18	1.24
1	G	63	ASP	N-CA	5.04	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	LEU	CA-C	-5.03	1.46	1.52
1	F	159	LYS	CA-CB	5.03	1.61	1.53
1	C	116	LEU	CG-CD1	5.03	1.69	1.52
1	B	69	VAL	CA-CB	5.03	1.61	1.54
1	D	91	ARG	NE-CZ	5.03	1.38	1.33
1	H	218	ALA	CA-CB	5.03	1.61	1.53
1	H	62	GLU	CB-CG	-5.02	1.37	1.52
1	B	134	ARG	CD-NE	5.02	1.53	1.46
1	F	137	ILE	CA-C	5.02	1.58	1.52
1	I	242	TYR	CE1-CZ	5.02	1.50	1.38
1	E	222	ASP	CA-CB	-5.02	1.45	1.53
1	E	96	ARG	CZ-NH1	5.02	1.39	1.32
1	F	228	ARG	N-CA	-5.02	1.39	1.46
1	G	206	ARG	N-CA	5.02	1.52	1.45
1	J	176	PRO	CB-CG	5.02	1.70	1.51
1	D	60	ARG	N-CA	-5.02	1.39	1.46
1	E	194	ASP	N-CA	-5.01	1.39	1.46
1	E	225	GLU	CD-OE1	5.01	1.34	1.25
1	J	35	LYS	C-O	5.01	1.29	1.23
1	A	183	GLU	CG-CD	5.00	1.64	1.52
1	D	139	THR	CA-CB	5.00	1.62	1.53

All (716) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	175	TRP	CA-C-N	29.63	156.87	119.84
1	E	175	TRP	C-N-CA	29.63	156.87	119.84
1	J	138	ARG	NE-CZ-NH2	-19.05	102.06	119.20
1	J	26	LEU	CA-C-N	18.74	143.27	119.84
1	J	26	LEU	C-N-CA	18.74	143.27	119.84
1	G	26	LEU	C-N-CD	-18.14	50.61	125.00
1	J	27	PRO	N-CA-C	-18.14	75.10	112.47
1	E	175	TRP	N-CA-C	17.70	132.31	109.83
1	J	26	LEU	C-N-CD	-16.58	57.03	125.00
1	J	138	ARG	NE-CZ-NH1	15.92	137.42	121.50
1	J	27	PRO	CA-N-CD	-15.20	90.72	112.00
1	E	175	TRP	C-N-CD	-15.02	63.43	125.00
1	E	175	TRP	O-C-N	14.11	137.23	121.43
1	E	176	PRO	N-CA-C	-13.67	84.30	112.47
1	D	67	LEU	CA-C-N	-13.49	94.97	121.41
1	D	67	LEU	C-N-CA	-13.49	94.97	121.41
1	B	104	ASP	CB-CG-OD2	-12.92	88.69	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	LEU	O-C-N	-12.44	108.13	122.68
1	B	67	LEU	CA-C-N	-12.37	97.17	121.41
1	B	67	LEU	C-N-CA	-12.37	97.17	121.41
1	C	32	SER	CA-CB-OG	-12.05	87.00	111.10
1	C	47	THR	CB-CA-C	11.69	125.71	110.16
1	H	6	PRO	N-CA-C	-11.65	94.90	111.22
1	E	175	TRP	CA-C-O	-11.48	107.85	120.25
1	J	26	LEU	O-C-N	11.32	134.95	121.60
1	J	138	ARG	CD-NE-CZ	11.12	139.97	124.40
1	B	67	LEU	O-C-N	-11.05	109.06	122.65
1	B	199	ARG	CG-CD-NE	-10.91	87.99	112.00
1	I	208	LEU	N-CA-C	-10.82	100.35	114.31
1	G	28	ASP	N-CA-C	10.70	123.95	111.11
1	G	27	PRO	CA-N-CD	-10.66	97.07	112.00
1	J	208	LEU	N-CA-C	-10.63	100.80	113.88
1	J	26	LEU	CB-CA-C	-10.58	96.99	109.47
1	J	27	PRO	N-CA-CB	10.45	114.23	103.25
1	G	26	LEU	CA-C-N	10.37	132.81	119.84
1	G	26	LEU	C-N-CA	10.37	132.81	119.84
1	J	215	ASP	CA-CB-CG	-10.21	102.39	112.60
1	C	74	LEU	CD1-CG-CD2	-10.15	88.46	110.80
1	I	6	PRO	N-CA-C	-10.06	96.28	111.57
1	C	5	ILE	N-CA-CB	-10.04	100.90	111.64
1	E	105	PRO	N-CA-C	-10.01	95.48	111.19
1	A	208	LEU	N-CA-C	-9.97	101.21	113.97
1	C	105	PRO	CA-C-N	-9.92	106.78	122.65
1	C	105	PRO	C-N-CA	-9.92	106.78	122.65
1	D	106	GLN	N-CA-C	-9.79	97.72	113.19
1	J	104	ASP	N-CA-CB	9.55	126.08	110.99
1	J	174	ASP	N-CA-C	9.54	131.12	110.80
1	E	104	ASP	CB-CG-OD2	-9.44	96.70	118.40
1	G	124	THR	N-CA-CB	-9.35	96.09	110.29
1	B	238	ALA	N-CA-C	-9.31	95.49	110.20
1	E	208	LEU	N-CA-C	-9.31	102.06	113.97
1	J	202	SER	N-CA-C	-9.17	101.17	111.71
1	J	97	ILE	N-CA-C	-9.16	99.22	107.56
1	E	227	ARG	CG-CD-NE	-9.15	91.88	112.00
1	G	27	PRO	N-CA-CB	9.12	112.82	103.25
1	D	67	LEU	N-CA-C	-9.10	97.40	110.59
1	F	6	PRO	N-CA-C	-9.04	97.85	111.41
1	J	199	ARG	CG-CD-NE	-9.00	92.20	112.00
1	G	26	LEU	CA-C-O	-8.96	112.53	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	206	ARG	N-CA-C	-8.91	98.52	110.55
1	G	93	ILE	N-CA-C	-8.89	104.07	112.96
1	J	175	TRP	C-N-CD	-8.84	101.16	120.60
1	G	208	LEU	N-CA-C	-8.83	102.67	113.97
1	E	238	ALA	O-C-N	-8.83	112.59	123.01
1	G	112	ARG	CG-CD-NE	-8.75	92.75	112.00
1	B	21	HIS	N-CA-C	-8.73	100.52	113.61
1	E	97	ILE	N-CA-C	-8.73	98.00	107.77
1	J	105	PRO	N-CA-C	-8.70	97.57	111.14
1	D	138	ARG	NE-CZ-NH1	-8.67	112.83	121.50
1	E	191	THR	N-CA-CB	-8.65	97.90	110.80
1	F	48	PRO	N-CA-C	8.64	124.97	113.40
1	A	201	GLU	CA-C-N	-8.58	106.71	120.70
1	A	201	GLU	C-N-CA	-8.58	106.71	120.70
1	J	104	ASP	CB-CG-OD2	-8.58	98.67	118.40
1	F	104	ASP	CB-CG-OD2	-8.50	98.85	118.40
1	F	189	PRO	N-CA-C	8.50	118.63	110.47
1	A	228	ARG	NE-CZ-NH2	-8.49	111.56	119.20
1	I	206	ARG	N-CA-C	-8.48	99.33	110.53
1	G	16	GLU	N-CA-C	-8.48	95.85	109.76
1	D	6	PRO	N-CA-C	-8.47	98.69	111.57
1	H	47	THR	N-CA-C	-8.38	94.81	109.48
1	B	179	GLU	CA-CB-CG	-8.36	97.38	114.10
1	A	194	ASP	N-CA-C	8.26	120.28	111.28
1	J	48	PRO	N-CA-C	8.23	124.97	113.53
1	F	39	LEU	CD1-CG-CD2	-8.21	92.75	110.80
1	I	48	PRO	N-CA-C	8.20	125.19	113.47
1	A	145	MSE	CB-CG-SE	-8.19	88.12	112.70
1	H	112	ARG	CG-CD-NE	-8.19	93.98	112.00
1	C	93	ILE	N-CA-C	-8.19	105.51	113.53
1	E	24	ILE	CB-CG1-CD1	-8.15	96.69	113.80
1	I	244	GLU	N-CA-C	-8.15	103.34	113.28
1	J	145	MSE	CG-SE-CE	-8.14	81.02	98.92
1	I	220	ARG	N-CA-C	-8.13	102.39	111.82
1	D	105	PRO	O-C-N	-8.11	111.69	122.64
1	I	189	PRO	N-CA-C	8.11	118.25	110.47
1	G	238	ALA	N-CA-C	-8.05	96.11	109.24
1	C	199	ARG	CA-CB-CG	8.05	130.19	114.10
1	E	28	ASP	N-CA-C	8.05	121.07	111.33
1	G	68	GLY	CA-C-N	-8.04	112.61	123.14
1	G	68	GLY	C-N-CA	-8.04	112.61	123.14
1	E	104	ASP	CA-C-N	8.02	127.78	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	104	ASP	C-N-CA	8.02	127.78	119.76
1	B	49	VAL	N-CA-C	-8.01	103.00	110.53
1	C	17	VAL	CG1-CB-CG2	8.00	128.40	110.80
1	D	121	ALA	N-CA-C	-7.95	103.56	113.18
1	E	176	PRO	CA-N-CD	-7.92	100.91	112.00
1	D	97	ILE	N-CA-C	-7.88	99.81	107.76
1	G	124	THR	OG1-CB-CG2	7.86	125.03	109.30
1	I	2	PRO	N-CA-CB	7.86	111.65	103.00
1	I	118	ALA	N-CA-C	-7.85	97.54	109.79
1	J	138	ARG	CG-CD-NE	-7.84	94.75	112.00
1	F	112	ARG	NE-CZ-NH2	7.83	126.24	119.20
1	B	175	TRP	C-N-CD	-7.82	103.40	120.60
1	C	39	LEU	CD1-CG-CD2	-7.81	93.61	110.80
1	J	26	LEU	N-CA-C	7.81	121.83	109.64
1	A	201	GLU	N-CA-C	-7.77	102.63	113.20
1	C	17	VAL	N-CA-CB	-7.74	96.92	111.62
1	E	6	PRO	N-CA-C	-7.74	99.80	111.41
1	G	170	ALA	N-CA-C	-7.72	98.46	110.42
1	E	238	ALA	N-CA-C	-7.67	98.08	110.20
1	J	81	SER	CA-CB-OG	-7.67	95.76	111.10
1	I	22	GLY	N-CA-C	-7.67	102.65	111.85
1	I	145	MSE	CB-CG-SE	-7.64	89.77	112.70
1	F	161	LEU	CD1-CG-CD2	7.63	127.58	110.80
1	B	103	ALA	CA-C-O	-7.57	112.36	120.46
1	A	145	MSE	CA-CB-CG	-7.54	99.03	114.10
1	A	97	ILE	CA-C-N	-7.49	111.97	121.04
1	A	97	ILE	C-N-CA	-7.49	111.97	121.04
1	A	32	SER	CA-CB-OG	-7.49	96.13	111.10
1	B	208	LEU	N-CA-C	-7.48	104.40	113.97
1	E	104	ASP	N-CA-CB	7.48	122.20	111.21
1	F	140	MSE	CG-SE-CE	-7.48	82.47	98.92
1	A	143	TYR	N-CA-C	-7.46	100.63	110.40
1	E	191	THR	OG1-CB-CG2	7.45	124.20	109.30
1	F	206	ARG	N-CA-C	-7.44	100.71	110.53
1	B	170	ALA	N-CA-C	-7.43	98.90	110.42
1	I	183	GLU	CG-CD-OE2	7.41	135.45	118.40
1	G	24	ILE	CB-CG1-CD1	-7.38	98.30	113.80
1	A	118	ALA	O-C-N	-7.38	112.77	122.59
1	G	36	TRP	N-CA-C	-7.38	99.89	110.59
1	H	206	ARG	N-CA-C	-7.37	100.80	110.53
1	H	227	ARG	NE-CZ-NH1	-7.35	114.15	121.50
1	J	9	GLY	N-CA-C	-7.35	106.34	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	208	LEU	N-CA-C	-7.34	104.58	113.97
1	D	47	THR	CB-CA-C	7.33	120.88	109.15
1	F	231	ARG	NE-CZ-NH2	-7.32	112.61	119.20
1	J	175	TRP	CA-C-N	7.32	144.56	127.00
1	J	175	TRP	C-N-CA	7.32	144.56	127.00
1	B	207	SER	CA-CB-OG	-7.29	96.53	111.10
1	C	206	ARG	N-CA-C	-7.28	100.23	110.50
1	H	145	MSE	CA-CB-CG	-7.27	99.55	114.10
1	D	206	ARG	N-CA-C	-7.25	100.28	110.50
1	B	74	LEU	CD1-CG-CD2	-7.25	94.86	110.80
1	G	157	ILE	N-CA-C	-7.24	103.47	110.42
1	A	47	THR	CB-CA-C	7.24	120.73	109.15
1	J	6	PRO	N-CA-C	-7.22	101.11	111.22
1	E	238	ALA	CA-C-N	-7.21	107.77	121.54
1	E	238	ALA	C-N-CA	-7.21	107.77	121.54
1	C	199	ARG	CB-CG-CD	7.19	127.83	111.30
1	A	47	THR	N-CA-C	-7.19	96.90	109.48
1	C	208	LEU	N-CA-C	-7.18	104.78	113.97
1	E	186	ILE	N-CA-C	7.16	118.88	108.58
1	G	204	GLN	N-CA-C	7.15	121.83	113.18
1	J	42	HIS	CA-C-N	-7.14	111.62	119.19
1	J	42	HIS	C-N-CA	-7.14	111.62	119.19
1	D	208	LEU	N-CA-C	-7.12	105.12	113.88
1	G	26	LEU	CB-CA-C	7.12	119.12	108.86
1	F	231	ARG	CG-CD-NE	-7.11	96.35	112.00
1	J	26	LEU	CA-C-O	-7.10	110.86	119.67
1	C	9	GLY	N-CA-C	-7.09	106.25	114.69
1	E	175	TRP	CB-CA-C	-7.09	98.29	109.42
1	E	245	ALA	CA-C-O	-7.08	108.75	120.80
1	G	26	LEU	O-C-N	7.08	136.22	121.77
1	F	12	PHE	CA-C-N	7.03	128.63	119.84
1	F	12	PHE	C-N-CA	7.03	128.63	119.84
1	J	28	ASP	N-CA-C	7.03	122.90	111.37
1	J	39	LEU	CA-C-N	-7.00	111.60	122.59
1	J	39	LEU	C-N-CA	-7.00	111.60	122.59
1	J	215	ASP	CB-CG-OD1	-7.00	102.31	118.40
1	A	32	SER	CA-C-N	-6.99	111.46	122.65
1	A	32	SER	C-N-CA	-6.99	111.46	122.65
1	B	104	ASP	CB-CG-OD1	6.96	134.42	118.40
1	F	103	ALA	CA-C-N	-6.96	114.59	123.16
1	F	103	ALA	C-N-CA	-6.96	114.59	123.16
1	J	158	VAL	CG1-CB-CG2	-6.95	95.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	138	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	I	231	ARG	CG-CD-NE	-6.91	96.79	112.00
1	D	97	ILE	CA-C-O	6.91	123.23	119.15
1	F	66	ARG	N-CA-C	-6.91	103.75	111.28
1	J	27	PRO	N-CD-CG	6.90	113.56	103.20
1	I	72	ILE	CA-C-N	-6.89	114.43	122.77
1	I	72	ILE	C-N-CA	-6.89	114.43	122.77
1	G	27	PRO	N-CA-C	-6.89	98.28	112.47
1	D	239	LYS	CD-CE-NZ	6.88	133.93	111.90
1	G	206	ARG	N-CA-C	-6.87	100.81	110.50
1	H	204	GLN	N-CA-C	6.87	121.66	113.28
1	B	122	THR	N-CA-C	6.86	121.69	113.12
1	D	122	THR	OG1-CB-CG2	-6.84	95.62	109.30
1	A	195	GLN	N-CA-C	-6.84	103.91	111.36
1	C	187	VAL	CA-C-N	-6.84	113.34	120.38
1	C	187	VAL	C-N-CA	-6.84	113.34	120.38
1	B	105	PRO	N-CA-C	-6.82	100.49	111.14
1	G	26	LEU	N-CA-CB	6.81	118.27	110.03
1	B	140	MSE	CA-CB-CG	-6.81	100.48	114.10
1	B	36	TRP	N-CA-C	-6.80	100.73	110.59
1	I	122	THR	N-CA-C	6.78	122.09	113.55
1	H	150	LEU	N-CA-C	-6.77	96.01	107.99
1	H	186	ILE	N-CA-C	6.77	118.04	108.36
1	H	96	ARG	CA-C-N	-6.76	117.72	122.59
1	H	96	ARG	C-N-CA	-6.76	117.72	122.59
1	I	170	ALA	N-CA-C	-6.75	99.95	110.42
1	A	6	PRO	N-CA-C	-6.74	101.33	111.57
1	F	227	ARG	NE-CZ-NH2	-6.74	113.14	119.20
1	D	59	ARG	CD-NE-CZ	-6.72	114.98	124.40
1	F	105	PRO	N-CA-C	-6.72	100.53	111.21
1	D	48	PRO	N-CA-C	6.71	123.06	113.47
1	F	201	GLU	N-CA-C	6.71	119.60	111.82
1	J	215	ASP	CB-CG-OD2	6.70	133.80	118.40
1	H	11	ARG	N-CA-C	-6.69	99.63	110.20
1	D	236	LYS	CA-C-N	6.67	127.07	119.93
1	D	236	LYS	C-N-CA	6.67	127.07	119.93
1	I	198	ALA	N-CA-C	-6.67	103.94	111.14
1	B	6	PRO	N-CA-C	-6.66	101.90	111.22
1	I	183	GLU	N-CA-C	-6.65	104.48	112.59
1	F	204	GLN	N-CA-C	6.63	121.38	113.16
1	H	171	VAL	N-CA-CB	-6.63	104.52	111.61
1	I	28	ASP	N-CA-C	6.61	118.49	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	SER	N-CA-C	-6.61	104.00	111.07
1	J	145	MSE	CB-CG-SE	-6.60	92.91	112.70
1	E	206	ARG	N-CA-C	-6.58	100.74	110.48
1	G	86	LYS	CB-CG-CD	6.58	126.43	111.30
1	H	220	ARG	N-CA-C	-6.57	104.12	111.28
1	J	59	ARG	NE-CZ-NH1	-6.57	114.93	121.50
1	B	227	ARG	NE-CZ-NH1	-6.56	114.94	121.50
1	D	220	ARG	N-CA-C	-6.56	104.13	111.28
1	F	47	THR	N-CA-C	-6.52	98.07	109.48
1	E	146	GLU	CA-C-N	-6.50	112.77	122.39
1	E	146	GLU	C-N-CA	-6.50	112.77	122.39
1	A	36	TRP	N-CA-C	-6.50	101.17	110.59
1	C	229	TYR	N-CA-C	-6.50	104.20	111.28
1	H	189	PRO	N-CA-C	6.50	116.70	110.47
1	J	122	THR	OG1-CB-CG2	-6.49	96.33	109.30
1	A	28	ASP	N-CA-C	6.48	119.17	111.33
1	E	47	THR	CA-C-N	6.47	125.70	118.97
1	E	47	THR	C-N-CA	6.47	125.70	118.97
1	J	175	TRP	N-CA-C	-6.47	101.15	110.08
1	A	125	VAL	N-CA-CB	-6.47	100.55	111.23
1	G	191	THR	N-CA-C	-6.47	103.82	112.94
1	F	105	PRO	CB-CA-C	6.46	119.50	111.23
1	B	134	ARG	N-CA-C	-6.46	104.97	112.92
1	B	189	PRO	O-C-N	6.44	124.27	121.31
1	I	189	PRO	O-C-N	6.43	124.27	121.31
1	J	174	ASP	CB-CG-OD2	-6.43	103.61	118.40
1	B	190	PRO	N-CA-C	-6.43	101.37	111.34
1	B	135	GLY	CA-C-N	-6.42	114.81	123.10
1	B	135	GLY	C-N-CA	-6.42	114.81	123.10
1	J	173	ALA	N-CA-C	-6.42	101.19	110.24
1	E	243	GLU	N-CA-C	-6.42	104.21	111.14
1	A	171	VAL	N-CA-CB	-6.41	103.31	111.39
1	C	199	ARG	N-CA-C	-6.40	104.22	111.07
1	C	220	ARG	N-CA-C	-6.36	104.39	111.71
1	E	9	GLY	N-CA-C	-6.36	106.65	114.92
1	C	229	TYR	CA-C-O	-6.36	113.81	120.55
1	F	161	LEU	N-CA-C	-6.36	104.28	111.14
1	C	5	ILE	N-CA-C	6.35	114.39	109.19
1	F	145	MSE	CA-CB-CG	-6.34	101.41	114.10
1	G	217	PRO	CA-C-N	-6.34	112.35	121.42
1	G	217	PRO	C-N-CA	-6.34	112.35	121.42
1	J	39	LEU	CD1-CG-CD2	-6.33	96.88	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	ALA	CA-C-O	-6.33	113.96	120.54
1	B	204	GLN	N-CA-C	6.32	119.15	111.82
1	E	104	ASP	CB-CG-OD1	6.31	132.91	118.40
1	C	48	PRO	N-CA-C	6.30	122.29	113.53
1	B	153	GLU	N-CA-C	-6.29	104.52	111.82
1	D	86	LYS	N-CA-C	-6.29	104.51	111.36
1	E	189	PRO	N-CA-C	6.28	116.50	110.47
1	C	6	PRO	N-CA-C	-6.28	101.61	111.34
1	C	164	GLY	N-CA-C	-6.28	105.02	113.24
1	I	200	MSE	CA-C-N	-6.27	110.39	122.06
1	I	200	MSE	C-N-CA	-6.27	110.39	122.06
1	B	145	MSE	CA-CB-CG	-6.26	101.58	114.10
1	E	138	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	H	36	TRP	N-CA-C	-6.24	102.47	110.53
1	I	125	VAL	N-CA-CB	-6.23	100.94	111.23
1	C	59	ARG	NH1-CZ-NH2	6.23	127.40	119.30
1	G	150	LEU	N-CA-C	-6.22	96.99	107.99
1	F	149	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	C	104	ASP	CA-C-N	6.20	126.66	119.47
1	C	104	ASP	C-N-CA	6.20	126.66	119.47
1	B	79	VAL	CA-C-N	-6.19	111.50	120.29
1	B	79	VAL	C-N-CA	-6.19	111.50	120.29
1	I	118	ALA	O-C-N	-6.19	113.63	121.74
1	E	92	HIS	CA-C-N	-6.18	114.49	121.85
1	E	92	HIS	C-N-CA	-6.18	114.49	121.85
1	J	39	LEU	N-CA-C	-6.18	99.16	109.24
1	A	194	ASP	CA-CB-CG	-6.17	106.43	112.60
1	J	49	VAL	N-CA-C	-6.17	104.48	110.72
1	G	6	PRO	N-CA-C	-6.16	99.78	112.47
1	C	112	ARG	CG-CD-NE	6.16	125.56	112.00
1	C	199	ARG	CG-CD-NE	-6.15	98.46	112.00
1	D	47	THR	N-CA-C	-6.15	98.72	109.48
1	J	23	VAL	CA-C-N	-6.14	114.08	122.92
1	J	23	VAL	C-N-CA	-6.14	114.08	122.92
1	F	126	ARG	CA-C-N	-6.14	115.16	122.16
1	F	126	ARG	C-N-CA	-6.14	115.16	122.16
1	F	208	LEU	N-CA-C	-6.14	106.11	113.97
1	A	163	LEU	CB-CA-C	-6.13	101.26	110.88
1	H	33	GLN	N-CA-C	-6.12	105.10	113.30
1	J	44	ALA	N-CA-C	6.12	117.69	108.46
1	F	80	PHE	CA-C-O	-6.11	114.40	120.70
1	I	245	ALA	CA-C-O	-6.11	110.41	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	179	GLU	CA-C-N	-6.10	115.15	122.35
1	H	179	GLU	C-N-CA	-6.10	115.15	122.35
1	B	12	PHE	CA-C-N	6.10	126.45	119.93
1	B	12	PHE	C-N-CA	6.10	126.45	119.93
1	E	239	LYS	N-CA-C	6.08	123.76	110.80
1	I	39	LEU	CD1-CG-CD2	-6.08	97.42	110.80
1	E	94	GLY	CA-C-N	-6.08	115.17	123.14
1	E	94	GLY	C-N-CA	-6.08	115.17	123.14
1	I	32	SER	CB-CA-C	-6.08	100.34	110.68
1	E	204	GLN	CA-CB-CG	6.07	126.24	114.10
1	I	204	GLN	N-CA-C	6.07	120.52	113.18
1	C	47	THR	OG1-CB-CG2	6.07	121.43	109.30
1	H	112	ARG	NE-CZ-NH2	-6.06	113.75	119.20
1	J	204	GLN	N-CA-C	6.06	119.93	112.54
1	J	170	ALA	N-CA-C	-6.06	101.03	110.42
1	E	138	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	D	183	GLU	CG-CD-OE1	-6.05	104.48	118.40
1	F	5	ILE	N-CA-C	6.05	115.71	108.45
1	I	228	ARG	NE-CZ-NH1	6.05	127.55	121.50
1	E	145	MSE	CB-CG-SE	-6.04	94.58	112.70
1	H	74	LEU	CD1-CG-CD2	-6.04	97.51	110.80
1	B	72	ILE	CA-C-N	-6.04	116.29	122.27
1	B	72	ILE	C-N-CA	-6.04	116.29	122.27
1	G	199	ARG	NE-CZ-NH1	-6.04	115.47	121.50
1	G	48	PRO	N-CA-C	6.03	121.91	113.53
1	G	171	VAL	N-CA-CB	-6.03	105.16	111.61
1	E	48	PRO	N-CA-C	6.02	122.08	113.47
1	C	189	PRO	N-CA-C	6.02	118.04	110.70
1	A	48	PRO	N-CA-C	6.02	124.86	112.47
1	A	206	ARG	N-CA-C	-6.01	100.70	110.20
1	C	122	THR	OG1-CB-CG2	-6.00	97.30	109.30
1	E	81	SER	CA-CB-OG	-6.00	99.10	111.10
1	H	22	GLY	N-CA-C	-6.00	105.49	111.85
1	I	9	GLY	N-CA-C	-5.98	107.57	114.69
1	H	12	PHE	CA-C-N	5.98	126.33	119.93
1	H	12	PHE	C-N-CA	5.98	126.33	119.93
1	I	236	LYS	CA-C-N	-5.98	113.81	119.85
1	I	236	LYS	C-N-CA	-5.98	113.81	119.85
1	B	145	MSE	N-CA-C	5.97	118.75	111.82
1	C	122	THR	N-CA-CB	-5.97	102.65	110.59
1	E	21	HIS	N-CA-C	-5.97	105.30	113.30
1	A	170	ALA	N-CA-C	-5.96	101.69	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	ARG	CG-CD-NE	-5.96	98.89	112.00
1	B	48	PRO	N-CA-C	5.96	121.81	113.53
1	H	220	ARG	CB-CA-C	-5.96	100.90	110.79
1	A	125	VAL	CG1-CB-CG2	5.95	123.89	110.80
1	B	159	LYS	CD-CE-NZ	5.94	130.92	111.90
1	H	121	ALA	N-CA-C	-5.94	105.99	113.18
1	B	85	TRP	N-CA-C	-5.93	104.90	111.36
1	A	243	GLU	CA-C-O	5.92	127.00	120.90
1	G	145	MSE	CB-CG-SE	-5.92	94.93	112.70
1	J	10	GLU	CB-CA-C	-5.92	99.46	109.83
1	H	134	ARG	N-CA-C	-5.92	105.24	112.88
1	I	140	MSE	CG-SE-CE	-5.92	85.90	98.92
1	J	38	VAL	N-CA-C	-5.92	99.11	107.75
1	J	138	ARG	N-CA-C	-5.92	106.70	114.04
1	J	121	ALA	N-CA-C	-5.92	105.82	113.16
1	D	97	ILE	CA-C-N	-5.91	113.89	121.04
1	D	97	ILE	C-N-CA	-5.91	113.89	121.04
1	J	16	GLU	N-CA-C	-5.91	99.61	109.24
1	I	121	ALA	N-CA-C	-5.90	105.58	112.89
1	J	190	PRO	N-CA-C	-5.89	101.84	111.21
1	D	64	PHE	N-CA-C	-5.89	104.94	111.36
1	B	24	ILE	CB-CG1-CD1	-5.89	101.44	113.80
1	F	93	ILE	N-CA-C	-5.88	106.54	113.42
1	E	131	VAL	CG1-CB-CG2	-5.88	97.87	110.80
1	H	16	GLU	N-CA-C	-5.87	99.67	109.24
1	I	128	VAL	CG1-CB-CG2	5.87	123.71	110.80
1	J	231	ARG	CG-CD-NE	-5.87	99.10	112.00
1	J	31	VAL	CA-C-O	-5.86	114.96	121.17
1	J	31	VAL	O-C-N	5.85	127.64	121.91
1	J	2	PRO	CA-CB-CG	-5.85	93.39	104.50
1	H	122	THR	N-CA-CB	-5.84	101.93	110.40
1	B	104	ASP	OD1-CG-OD2	5.83	136.89	122.90
1	H	193	GLU	N-CA-CB	-5.83	101.55	110.12
1	C	36	TRP	N-CA-C	-5.83	102.68	110.55
1	D	140	MSE	CG-SE-CE	-5.83	86.10	98.92
1	B	67	LEU	N-CA-C	-5.82	103.02	110.53
1	D	24	ILE	CA-C-N	-5.82	114.69	122.72
1	D	24	ILE	C-N-CA	-5.82	114.69	122.72
1	A	189	PRO	N-CA-C	5.81	116.05	110.47
1	B	87	GLU	N-CA-CB	-5.80	101.58	110.16
1	B	47	THR	CA-C-N	5.80	125.48	119.05
1	B	47	THR	C-N-CA	5.80	125.48	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	GLN	CA-CB-CG	5.79	125.69	114.10
1	J	138	ARG	N-CA-CB	-5.79	102.25	110.81
1	D	74	LEU	CA-C-N	-5.78	112.38	121.87
1	D	74	LEU	C-N-CA	-5.78	112.38	121.87
1	J	145	MSE	CA-CB-CG	-5.78	102.54	114.10
1	D	105	PRO	CA-C-N	-5.77	111.71	121.18
1	D	105	PRO	C-N-CA	-5.77	111.71	121.18
1	C	66	ARG	N-CA-C	-5.76	105.08	111.71
1	B	188	PRO	CB-CA-C	5.76	117.95	110.92
1	J	93	ILE	N-CA-C	-5.76	106.68	113.42
1	B	199	ARG	CB-CA-C	-5.76	101.23	110.79
1	G	159	LYS	CD-CE-NZ	5.76	130.33	111.90
1	H	2	PRO	N-CA-CB	5.76	109.33	103.00
1	I	57	PHE	CA-C-N	5.76	127.99	120.28
1	I	57	PHE	C-N-CA	5.76	127.99	120.28
1	A	72	ILE	CA-C-N	-5.75	116.38	122.30
1	A	72	ILE	C-N-CA	-5.75	116.38	122.30
1	C	140	MSE	CA-CB-CG	-5.74	102.62	114.10
1	H	204	GLN	CB-CG-CD	-5.74	102.84	112.60
1	J	161	LEU	CD1-CG-CD2	5.74	123.42	110.80
1	B	16	GLU	N-CA-C	-5.73	100.36	109.76
1	H	149	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	A	183	GLU	CG-CD-OE2	5.72	131.56	118.40
1	F	81	SER	N-CA-C	-5.72	104.95	111.07
1	H	210	TRP	CA-C-N	-5.72	113.49	122.65
1	H	210	TRP	C-N-CA	-5.72	113.49	122.65
1	E	236	LYS	CA-C-N	-5.71	114.08	119.85
1	E	236	LYS	C-N-CA	-5.71	114.08	119.85
1	E	121	ALA	N-CA-C	-5.71	106.32	113.28
1	J	91	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	H	153	GLU	N-CA-C	-5.70	105.82	112.89
1	C	231	ARG	CA-C-N	-5.70	112.20	120.29
1	C	231	ARG	C-N-CA	-5.70	112.20	120.29
1	F	24	ILE	CB-CG1-CD1	-5.69	101.84	113.80
1	A	145	MSE	CB-CA-C	5.69	121.16	110.63
1	H	36	TRP	CA-C-N	-5.69	113.00	122.21
1	H	36	TRP	C-N-CA	-5.69	113.00	122.21
1	B	183	GLU	CA-C-N	-5.68	113.67	121.06
1	B	183	GLU	C-N-CA	-5.68	113.67	121.06
1	A	146	GLU	CA-C-N	-5.68	114.76	122.77
1	A	146	GLU	C-N-CA	-5.68	114.76	122.77
1	H	32	SER	N-CA-C	-5.68	106.19	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	GLY	N-CA-C	-5.68	106.16	114.90
1	C	149	ARG	N-CA-C	5.68	117.39	110.41
1	G	158	VAL	CB-CA-C	-5.67	104.71	111.97
1	C	232	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	J	174	ASP	OD1-CG-OD2	5.67	136.50	122.90
1	J	101	ILE	CB-CA-C	-5.66	102.07	110.33
1	B	69	VAL	N-CA-C	5.66	116.26	108.12
1	H	227	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	G	195	GLN	CB-CG-CD	-5.63	103.02	112.60
1	J	199	ARG	CB-CA-C	-5.63	102.04	110.88
1	A	168	LYS	CA-CB-CG	-5.63	102.84	114.10
1	C	95	VAL	CA-C-N	-5.63	114.95	122.72
1	C	95	VAL	C-N-CA	-5.63	114.95	122.72
1	B	227	ARG	NH1-CZ-NH2	5.62	126.61	119.30
1	I	228	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	F	65	GLN	O-C-N	5.61	128.07	122.12
1	B	238	ALA	CA-C-N	-5.61	110.83	121.54
1	B	238	ALA	C-N-CA	-5.61	110.83	121.54
1	D	11	ARG	N-CA-C	-5.60	101.99	110.28
1	D	4	SER	N-CA-CB	-5.59	101.90	110.85
1	E	191	THR	CB-CA-C	5.59	119.72	109.99
1	I	118	ALA	CA-C-N	-5.59	110.87	121.54
1	I	118	ALA	C-N-CA	-5.59	110.87	121.54
1	E	39	LEU	CD1-CG-CD2	-5.58	98.51	110.80
1	G	74	LEU	CD1-CG-CD2	-5.58	98.52	110.80
1	J	8	ILE	CA-C-N	-5.58	114.31	122.46
1	J	8	ILE	C-N-CA	-5.58	114.31	122.46
1	J	156	ARG	CA-C-N	-5.58	113.53	120.56
1	J	156	ARG	C-N-CA	-5.58	113.53	120.56
1	I	119	GLU	N-CA-CB	5.58	119.91	110.49
1	B	238	ALA	O-C-N	-5.57	116.43	123.01
1	E	47	THR	N-CA-C	-5.57	99.72	109.48
1	E	231	ARG	N-CA-C	-5.57	105.29	111.36
1	A	47	THR	OG1-CB-CG2	5.56	120.42	109.30
1	I	130	ILE	CA-C-N	-5.56	115.26	122.99
1	I	130	ILE	C-N-CA	-5.56	115.26	122.99
1	B	126	ARG	CG-CD-NE	-5.56	99.77	112.00
1	A	183	GLU	CG-CD-OE1	-5.56	105.62	118.40
1	D	9	GLY	N-CA-C	-5.56	108.47	115.08
1	J	228	ARG	CB-CG-CD	5.56	124.08	111.30
1	J	99	PHE	CA-C-N	5.55	125.46	119.85
1	J	99	PHE	C-N-CA	5.55	125.46	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASP	N-CA-C	-5.55	99.71	108.14
1	C	42	HIS	CA-C-N	5.55	125.21	119.05
1	C	42	HIS	C-N-CA	5.55	125.21	119.05
1	I	145	MSE	CA-CB-CG	-5.54	103.01	114.10
1	G	214	TRP	CA-C-O	-5.54	115.52	121.45
1	J	140	MSE	CA-CB-CG	-5.54	103.02	114.10
1	C	49	VAL	N-CA-C	-5.54	105.13	110.72
1	C	242	TYR	N-CA-C	-5.54	105.34	111.71
1	I	119	GLU	CB-CG-CD	5.53	122.01	112.60
1	J	106	GLN	CA-CB-CG	5.53	125.17	114.10
1	B	94	GLY	CA-C-N	-5.53	115.89	123.14
1	B	94	GLY	C-N-CA	-5.53	115.89	123.14
1	G	204	GLN	CB-CG-CD	-5.53	103.20	112.60
1	C	199	ARG	CB-CA-C	-5.53	102.20	110.88
1	D	47	THR	OG1-CB-CG2	5.53	120.36	109.30
1	G	112	ARG	N-CA-C	5.53	119.28	112.54
1	B	168	LYS	CA-CB-CG	-5.53	103.05	114.10
1	G	231	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	F	84	LYS	N-CA-C	-5.52	105.41	111.82
1	J	214	TRP	CA-C-N	5.52	132.10	122.82
1	J	214	TRP	C-N-CA	5.52	132.10	122.82
1	A	97	ILE	CA-C-O	5.52	122.41	119.15
1	C	103	ALA	CA-C-O	-5.52	114.45	120.36
1	J	179	GLU	CB-CG-CD	-5.52	103.22	112.60
1	J	146	GLU	CA-C-N	-5.51	114.24	122.39
1	J	146	GLU	C-N-CA	-5.51	114.24	122.39
1	E	2	PRO	N-CA-C	5.51	125.87	112.10
1	B	112	ARG	CB-CG-CD	5.51	123.96	111.30
1	G	97	ILE	CA-C-N	-5.51	114.66	120.94
1	G	97	ILE	C-N-CA	-5.51	114.66	120.94
1	A	179	GLU	CA-C-N	-5.50	116.08	122.63
1	A	179	GLU	C-N-CA	-5.50	116.08	122.63
1	D	4	SER	N-CA-C	-5.50	101.20	109.95
1	J	59	ARG	CA-CB-CG	-5.50	103.10	114.10
1	A	59	ARG	CB-CG-CD	-5.50	98.65	111.30
1	F	21	HIS	N-CA-C	-5.50	105.36	113.61
1	A	22	GLY	CA-C-N	5.50	128.45	120.98
1	A	22	GLY	C-N-CA	5.50	128.45	120.98
1	A	179	GLU	CA-CB-CG	-5.49	103.11	114.10
1	D	74	LEU	CD1-CG-CD2	-5.49	98.71	110.80
1	I	97	ILE	N-CA-C	-5.49	102.22	107.76
1	F	146	GLU	CA-C-N	-5.48	114.28	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	146	GLU	C-N-CA	-5.48	114.28	122.39
1	I	26	LEU	N-CA-C	-5.48	102.56	110.40
1	C	130	ILE	N-CA-C	-5.48	99.86	107.80
1	F	207	SER	N-CA-CB	-5.48	101.81	111.39
1	H	103	ALA	N-CA-C	-5.48	99.48	108.41
1	F	2	PRO	CA-N-CD	-5.47	104.33	112.00
1	C	227	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	A	79	VAL	CA-C-N	-5.47	112.52	120.29
1	A	79	VAL	C-N-CA	-5.47	112.52	120.29
1	G	24	ILE	CA-C-N	-5.47	115.17	122.72
1	G	24	ILE	C-N-CA	-5.47	115.17	122.72
1	C	2	PRO	N-CA-CB	5.46	109.01	103.00
1	D	73	GLY	N-CA-C	-5.46	105.09	112.57
1	I	65	GLN	CB-CA-C	5.46	119.85	110.79
1	C	11	ARG	NE-CZ-NH2	-5.45	114.29	119.20
1	G	17	VAL	N-CA-CB	-5.44	102.53	111.45
1	B	211	TRP	N-CA-C	-5.44	106.42	113.16
1	H	48	PRO	N-CA-C	5.44	121.09	113.53
1	E	23	VAL	CA-C-N	-5.42	114.11	122.68
1	E	23	VAL	C-N-CA	-5.42	114.11	122.68
1	F	227	ARG	N-CA-C	-5.42	105.53	111.82
1	E	111	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	E	145	MSE	CG-SE-CE	5.42	110.84	98.92
1	F	163	LEU	CB-CA-C	-5.42	102.34	110.90
1	A	120	SER	N-CA-C	5.42	118.23	108.48
1	B	75	SER	CA-C-O	-5.41	115.67	121.45
1	A	158	VAL	CB-CA-C	5.40	119.67	112.22
1	C	210	TRP	CA-C-N	-5.40	114.01	122.65
1	C	210	TRP	C-N-CA	-5.40	114.01	122.65
1	E	93	ILE	N-CA-C	-5.39	107.11	113.42
1	G	195	GLN	CA-CB-CG	5.39	124.88	114.10
1	E	134	ARG	CG-CD-NE	-5.38	100.15	112.00
1	B	176	PRO	CA-N-CD	5.37	119.02	111.50
1	G	42	HIS	CA-C-N	-5.37	113.00	118.85
1	G	42	HIS	C-N-CA	-5.37	113.00	118.85
1	C	228	ARG	CD-NE-CZ	5.36	131.91	124.40
1	G	242	TYR	CA-C-N	5.36	127.74	120.44
1	G	242	TYR	C-N-CA	5.36	127.74	120.44
1	H	203	GLY	CA-C-O	5.36	126.11	119.25
1	G	47	THR	N-CA-C	-5.35	100.11	109.48
1	I	180	ILE	CB-CA-C	-5.35	105.48	111.80
1	G	97	ILE	N-CA-C	-5.35	102.35	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	LYS	CD-CE-NZ	-5.35	94.78	111.90
1	F	158	VAL	CG1-CB-CG2	-5.34	99.05	110.80
1	I	79	VAL	N-CA-C	-5.34	104.56	112.04
1	D	199	ARG	CA-CB-CG	-5.34	103.42	114.10
1	J	134	ARG	CG-CD-NE	-5.34	100.26	112.00
1	A	97	ILE	N-CA-C	-5.34	102.37	107.76
1	C	143	TYR	N-CA-C	-5.34	102.93	110.29
1	B	122	THR	N-CA-CB	-5.33	102.27	110.42
1	A	16	GLU	N-CA-C	-5.32	100.50	109.07
1	A	118	ALA	CA-C-N	-5.32	111.38	121.54
1	A	118	ALA	C-N-CA	-5.32	111.38	121.54
1	C	35	LYS	N-CA-C	5.32	118.48	109.76
1	H	31	VAL	CB-CA-C	-5.32	104.96	112.14
1	A	140	MSE	CG-SE-CE	5.32	110.62	98.92
1	E	193	GLU	CA-C-N	-5.32	111.64	120.68
1	E	193	GLU	C-N-CA	-5.32	111.64	120.68
1	F	216	THR	OG1-CB-CG2	-5.30	98.70	109.30
1	B	167	LEU	N-CA-CB	-5.30	102.14	110.46
1	G	189	PRO	O-C-N	5.30	123.64	121.15
1	J	201	GLU	CA-C-N	5.30	127.91	120.28
1	J	201	GLU	C-N-CA	5.30	127.91	120.28
1	B	28	ASP	N-CA-C	5.29	117.73	111.33
1	H	5	ILE	CA-C-N	5.29	125.29	120.21
1	H	5	ILE	C-N-CA	5.29	125.29	120.21
1	H	155	LEU	N-CA-C	-5.29	105.43	111.14
1	E	155	LEU	CA-C-N	-5.29	113.20	120.28
1	E	155	LEU	C-N-CA	-5.29	113.20	120.28
1	G	79	VAL	CB-CA-C	-5.29	103.70	112.26
1	B	227	ARG	CG-CD-NE	-5.28	100.39	112.00
1	I	134	ARG	CA-CB-CG	-5.27	103.55	114.10
1	A	182	GLY	CA-C-N	-5.27	114.24	122.73
1	A	182	GLY	C-N-CA	-5.27	114.24	122.73
1	I	81	SER	CB-CA-C	-5.26	102.61	110.88
1	F	91	ARG	N-CA-C	5.26	118.16	111.69
1	H	180	ILE	CB-CA-C	-5.26	105.50	111.55
1	I	193	GLU	CB-CA-C	-5.26	101.91	110.85
1	C	134	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	D	70	ASP	CA-CB-CG	-5.26	107.34	112.60
1	H	158	VAL	CB-CA-C	-5.24	104.98	112.22
1	J	215	ASP	N-CA-CB	-5.24	103.09	111.43
1	C	84	LYS	CB-CA-C	-5.24	102.09	110.79
1	C	206	ARG	CG-CD-NE	-5.24	100.47	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	9	GLY	N-CA-C	-5.24	108.84	115.08
1	H	98	PRO	N-CA-C	5.24	122.23	114.80
1	E	186	ILE	N-CA-CB	-5.23	105.02	110.72
1	B	36	TRP	CB-CA-C	-5.23	100.62	110.51
1	A	215	ASP	CA-C-N	-5.23	116.83	123.15
1	A	215	ASP	C-N-CA	-5.23	116.83	123.15
1	E	35	LYS	N-CA-C	5.22	118.73	109.96
1	G	27	PRO	N-CD-CG	5.22	111.03	103.20
1	C	147	LEU	CB-CA-C	-5.22	101.79	110.14
1	A	39	LEU	CD1-CG-CD2	-5.21	99.33	110.80
1	C	220	ARG	CG-CD-NE	-5.21	100.53	112.00
1	D	23	VAL	CA-C-N	-5.21	115.29	122.69
1	D	23	VAL	C-N-CA	-5.21	115.29	122.69
1	D	153	GLU	N-CA-C	-5.21	105.77	111.82
1	G	27	PRO	CB-CA-C	5.21	120.16	111.56
1	H	75	SER	N-CA-C	-5.21	101.00	108.60
1	B	66	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	B	149	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	I	93	ILE	N-CA-C	-5.20	107.33	113.42
1	B	84	LYS	CB-CA-C	-5.20	100.69	110.67
1	H	168	LYS	CA-CB-CG	-5.19	103.72	114.10
1	E	59	ARG	CB-CG-CD	-5.19	99.36	111.30
1	C	215	ASP	N-CA-C	-5.19	101.50	108.19
1	A	134	ARG	N-CA-C	-5.18	106.54	112.92
1	I	148	GLY	N-CA-C	-5.18	105.11	112.37
1	I	183	GLU	CG-CD-OE1	-5.18	106.48	118.40
1	C	16	GLU	CB-CG-CD	-5.18	103.79	112.60
1	A	59	ARG	NH1-CZ-NH2	5.17	126.02	119.30
1	I	175	TRP	C-N-CD	-5.17	109.23	120.60
1	J	11	ARG	N-CA-C	-5.17	102.63	110.28
1	J	54	PHE	CA-CB-CG	-5.16	108.64	113.80
1	G	235	GLU	CA-CB-CG	5.16	124.41	114.10
1	J	218	ALA	N-CA-C	-5.15	102.85	110.48
1	F	65	GLN	CB-CG-CD	-5.15	103.84	112.60
1	H	60	ARG	N-CA-C	-5.15	106.59	112.92
1	I	159	LYS	CB-CA-C	-5.14	102.58	110.81
1	G	140	MSE	CA-CB-CG	-5.14	103.82	114.10
1	C	164	GLY	CA-C-O	-5.14	114.85	120.40
1	B	51	THR	CA-C-N	-5.14	112.88	120.28
1	B	51	THR	C-N-CA	-5.14	112.88	120.28
1	J	47	THR	N-CA-C	-5.13	100.50	109.48
1	I	138	ARG	NE-CZ-NH1	-5.13	116.37	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	87	GLU	N-CA-C	-5.13	105.60	111.14
1	B	197	ARG	N-CA-C	-5.12	105.59	111.07
1	D	231	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	D	138	ARG	NH1-CZ-NH2	5.12	125.96	119.30
1	J	104	ASP	CB-CG-OD1	5.12	130.17	118.40
1	A	163	LEU	CB-CG-CD1	-5.11	95.36	110.70
1	F	103	ALA	CA-C-O	-5.11	115.03	120.40
1	F	206	ARG	CG-CD-NE	-5.11	100.75	112.00
1	D	161	LEU	N-CA-C	-5.11	105.62	111.14
1	H	79	VAL	CA-C-N	-5.11	113.04	120.29
1	H	79	VAL	C-N-CA	-5.11	113.04	120.29
1	J	231	ARG	CD-NE-CZ	5.11	131.55	124.40
1	G	22	GLY	CA-C-O	-5.10	118.64	122.37
1	A	22	GLY	CA-C-O	-5.10	118.64	122.37
1	C	5	ILE	CG1-CB-CG2	5.10	126.00	110.70
1	C	23	VAL	CA-C-N	-5.10	116.09	123.03
1	C	23	VAL	C-N-CA	-5.10	116.09	123.03
1	F	145	MSE	CB-CG-SE	-5.10	97.41	112.70
1	E	35	LYS	CA-CB-CG	-5.10	103.91	114.10
1	E	47	THR	CA-C-O	5.09	126.39	120.23
1	E	75	SER	N-CA-C	-5.09	101.37	108.96
1	I	126	ARG	CA-C-N	-5.09	116.19	122.15
1	I	126	ARG	C-N-CA	-5.09	116.19	122.15
1	B	187	VAL	CA-C-O	5.09	123.65	119.47
1	D	158	VAL	N-CA-C	5.09	115.31	110.42
1	I	42	HIS	N-CA-C	-5.09	100.21	108.82
1	J	22	GLY	N-CA-C	-5.09	105.74	111.85
1	A	92	HIS	CA-C-N	-5.09	115.80	121.85
1	A	92	HIS	C-N-CA	-5.09	115.80	121.85
1	D	145	MSE	CB-CG-SE	-5.08	97.45	112.70
1	F	11	ARG	CA-CB-CG	-5.08	103.93	114.10
1	H	126	ARG	CG-CD-NE	-5.08	100.81	112.00
1	H	47	THR	CA-C-N	5.08	124.69	119.05
1	H	47	THR	C-N-CA	5.08	124.69	119.05
1	J	245	ALA	CA-C-O	-5.07	112.18	120.80
1	G	112	ARG	CA-CB-CG	-5.07	103.96	114.10
1	I	84	LYS	CD-CE-NZ	-5.07	95.68	111.90
1	A	106	GLN	N-CA-CB	5.07	119.06	110.49
1	E	111	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	B	206	ARG	N-CA-C	-5.07	103.46	110.35
1	E	228	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	I	47	THR	CB-CA-C	5.07	117.26	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	156	ARG	CA-C-N	-5.06	113.52	120.46
1	C	156	ARG	C-N-CA	-5.06	113.52	120.46
1	E	143	TYR	N-CA-C	-5.06	103.77	110.40
1	H	189	PRO	N-CA-CB	-5.06	100.36	103.19
1	A	165	ASP	CA-C-N	-5.06	112.29	121.14
1	A	165	ASP	C-N-CA	-5.06	112.29	121.14
1	C	77	ASP	CA-C-O	-5.06	116.22	121.99
1	H	71	LEU	CA-C-N	-5.06	115.42	122.75
1	H	71	LEU	C-N-CA	-5.06	115.42	122.75
1	F	32	SER	CA-CB-OG	-5.05	100.99	111.10
1	C	200	MSE	CG-SE-CE	5.05	110.04	98.92
1	G	170	ALA	CA-C-N	-5.05	117.88	123.43
1	G	170	ALA	C-N-CA	-5.05	117.88	123.43
1	F	112	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	B	15	MSE	CA-CB-CG	-5.05	104.01	114.10
1	F	143	TYR	N-CA-C	-5.05	103.79	110.40
1	I	5	ILE	CA-C-N	5.05	125.26	120.31
1	I	5	ILE	C-N-CA	5.05	125.26	120.31
1	I	122	THR	OG1-CB-CG2	-5.05	99.21	109.30
1	E	164	GLY	CA-C-O	5.04	125.94	120.75
1	C	235	GLU	N-CA-C	5.03	117.75	109.76
1	I	105	PRO	CB-CA-C	5.01	117.65	111.23
1	J	122	THR	N-CA-CB	-5.01	103.39	110.81
1	F	66	ARG	NE-CZ-NH1	5.01	126.51	121.50
1	I	244	GLU	CA-CB-CG	-5.01	104.08	114.10
1	J	199	ARG	CB-CG-CD	5.00	122.81	111.30
1	D	231	ARG	NE-CZ-NH2	5.00	123.70	119.20

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

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Mol	Chain	Res	Type	Group
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

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	110	0
1	B	1973	0	1959	125	0
1	C	1973	0	1959	116	0
1	D	1973	0	1959	106	0
1	E	1973	0	1959	141	0
1	F	1973	0	1959	131	0
1	G	1973	0	1959	100	0
1	H	1973	0	1959	101	0
1	I	1973	0	1959	139	0
1	J	1973	0	1959	122	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	35	0
2	E	68	0	101	56	0
2	F	48	0	72	43	0
2	G	36	0	54	37	0
2	H	36	0	54	38	1
2	I	44	0	66	55	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1220	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 30.

All (1220) 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:A:225:GLU:CD	1:A:225:GLU:CG	1.75	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
1:E:121:ALA:CB	1:E:121:ALA:CA	1.76	1.56
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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:236:LYS:HZ1	2:F:2043:EDO:H22	1.34	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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:239:LYS:HE2	1:B:244:GLU:CD	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:70:ASP:CG	2:H:2113:EDO:H12	2.13	0.74
1:B:49:VAL:N	2:B:2028:EDO:C1	2.50	0.73
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:16:GLU:C	2:J:2123:EDO:H21	2.16	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: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
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:E:121:ALA:CB	1:E:121:ALA:C	2.66	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:59:ARG:HH12	1:J:179:GLU:CD	2.02	0.67
1:J:244:GLU:O	1:J:244:GLU:CD	2.37	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
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
2:J:2014:EDO:C1	2:J:2014:EDO:HO1	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:2029:EDO:C2	2:A:2029:EDO:HO2	2.07	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: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
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
2:J:2049:EDO:C2	2:J:2049:EDO:HO2	2.08	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: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
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
2:J:2068:EDO:C2	2:J:2068:EDO:HO2	2.08	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:I:36:TRP:CD1	1:I:162:LYS:HZ1	2.16	0.64
2:J:2008:EDO:C2	2:J:2008:EDO:HO2	2.07	0.64
1:B:43:PRO:HG3	1:B:145:MSE:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:179:GLU:CD	1:D:59:ARG:NH1	2.57	0.63
2:C:2067:EDO:C2	2:C:2067:EDO:HO2	2.09	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: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
2:G:2050:EDO:C2	2:G:2050:EDO:HO2	2.09	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
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: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:G:183:GLU:H	2:G:2057:EDO:HO2	1.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2058:EDO:C2	2:H:2058: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
1:I:50:CYS:HG	2:I:2121:EDO:HO1	1.46	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: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:E:132:ASP:CG	2:E:2039:EDO:H12	2.25	0.61
1:B:203:GLY:C	2:B:2030:EDO:H21	2.25	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
1:A:243:GLU:CD	3:A:2163:HOH:O	2.42	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
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
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: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
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:132:ASP:CG	2:I:2045:EDO:H21	2.26	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
1:G:39:LEU:C	1:G:39:LEU:HD23	2.26	0.60
2:G:2009:EDO:C1	2:G:2009:EDO:HO1	2.10	0.60
1:H:145:MSE:CB	1:H:145:MSE:CE	2.79	0.60
1:D:235:GLU:HA	2:D:2119:EDO:H12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2120:EDO:C1	2:E:2120:EDO:HO1	2.07	0.60
1:I:182:GLY:HA3	2:I:2103:EDO:H21	1.84	0.60
2:I:2103:EDO:HO2	1:J:236:LYS:HZ1	1.50	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:C:232:ARG:O	2:C:2004:EDO:O2	2.16	0.59
2:C:2128:EDO:C2	2:C:2128:EDO:HO2	2.08	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:I:59:ARG:NH1	1:J:179:GLU:CD	2.60	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:F:2043:EDO:C2	2:F:2043:EDO:HO2	2.08	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
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
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:C:2024:EDO:C2	2:C:2024:EDO:HO2	2.09	0.59
1:H:18:THR:HB	2:H:2044:EDO:O2	2.03	0.59
2:A:2012:EDO:C1	2:A:2012:EDO:HO1	2.07	0.58
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2126:EDO:C2	2:C:2126:EDO:HO2	2.08	0.58
1:D:68:GLY:H	1:D:162:LYS:HE3	1.67	0.58
1:A:216:THR:C	2:A:2063:EDO:H11	2.28	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:E:2032:EDO:C2	2:E:2032:EDO:HO2	2.10	0.57
2:J:2049:EDO:O2	2:J:2049:EDO:C1	2.47	0.57
1:A:200:MSE:C	1:A:202:SER:H	2.11	0.57
1:F:105:PRO:HG2	1:G:122:THR:HB	1.87	0.57
2:F:2006:EDO:C1	2:F:2006:EDO:HO1	2.11	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
1:D:106:GLN:O	1:D:111:ARG:CZ	2.53	0.57
2:G:2056:EDO:C2	2:G:2056:EDO:HO2	2.09	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
2:C:2085:EDO:C2	2:C:2085:EDO:HO2	2.10	0.57
1:E:5:ILE:HG22	1:E:114:GLY:HA3	1.87	0.57
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:C:5:ILE:HG12	1:C:142:TYR:OH	2.05	0.56
1:J:97:ILE:CG1	2:J:2109:EDO:H11	2.32	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
2:A:2063:EDO:C1	2:A:2063:EDO:HO1	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:GLU:OE1	2:C:2080:EDO:H21	2.04	0.56
1:E:169:ARG:HH12	2:E:2089:EDO:C2	2.17	0.56
2:J:2105:EDO:C2	2:J:2105:EDO:HO2	2.07	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
1:I:192:THR:HG1	2:I:2115:EDO:H11	1.70	0.56
1:J:86:LYS:O	2:J:2109:EDO:O1	2.16	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:J:90:GLU:OE2	1:J:96:ARG:HG3	2.06	0.55
1:C:44:ALA:O	1:C:47:THR:HB	2.06	0.55
2:C:2085:EDO:C1	2:C:2085:EDO:HO1	2.11	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:B:132:ASP:CG	2:B:2025:EDO:H21	2.32	0.55
1:G:183:GLU:N	2:G:2057:EDO:HO2	2.03	0.55
1:F:104:ASP:OD2	1:F:104:ASP:N	2.40	0.55
2:J:2104:EDO:C2	2:J:2104:EDO:HO2	2.10	0.55
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:74:LEU:HD13	1:G:74:LEU:C	2.32	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: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: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: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:J:222:ASP:OD2	2:J:2110:EDO:C1	2.56	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
2:G:2102:EDO:C2	2:G:2102:EDO:HO2	2.09	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:49:VAL:H	2:I:2121:EDO:HO2	1.52	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
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
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:36:TRP:CD1	1:C:162:LYS:HZ2	2.28	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
2:B:2023:EDO:C2	2:B:2023:EDO:HO2	2.11	0.51
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
1:A:200:MSE:C	1:A:202:SER:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:GLY:N	2:D:2035:EDO:H21	2.26	0.51
1:E:238:ALA:O	1:E:239:LYS:HB3	2.10	0.51
1:C:224:GLU:CD	1:C:231:ARG:HH22	2.19	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
2:C:2004:EDO:C1	2:C:2004:EDO:HO1	2.10	0.51
1:D:74:LEU:HD13	1:D:74:LEU:C	2.36	0.51
1:I:238:ALA:C	1:I:239:LYS:HD2	2.36	0.51
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
2:D:2074:EDO:C1	2:D:2074:EDO:HO1	2.13	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
1:E:194:ASP:OD1	1:E:194:ASP:C	2.54	0.50
1:H:74:LEU:C	1:H:74:LEU:HD13	2.36	0.50
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: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
1:B:243:GLU:C	1:B:244:GLU:OE1	2.55	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:E:235:GLU:O	2:E:2005:EDO:O2	2.17	0.50
1:H:140:MSE:CE	1:H:142:TYR:OH	2.60	0.50
2:I:2115:EDO:C2	2:I:2115:EDO:HO2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:PRO:N	1:H:10:GLU:OE2	2.44	0.50
1:H:215:ASP:C	1:H:217:PRO:HD3	2.37	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
1:I:203:GLY:C	2:I:2051:EDO:H21	2.37	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:A:243:GLU:C	1:A:245:ALA:N	2.65	0.49
1:B:244:GLU:N	1:B:244:GLU:CD	2.71	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:D:163:LEU:HD21	1:D:222:ASP:CG	2.38	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
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
2:D:2118:EDO:C2	2:D:2118:EDO:HO2	2.10	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
2:C:2004:EDO:C2	2:C:2004:EDO:HO2	2.16	0.48
1:F:25:LYS:NZ	3:F:556:HOH:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:I:36:TRP:NE1	1:I:162:LYS:HZ3	2.06	0.48
1:I:39:LEU:HD12	1:I:39:LEU:C	2.38	0.48
2:E:2005:EDO:C2	3:E:513:HOH:O	2.62	0.48
1:F:232:ARG:O	2:F:2006:EDO:O1	2.31	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:C:103:ALA:C	1:C:105:PRO:HD3	2.37	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
2:A:2022:EDO:C2	1:B:236:LYS:HZ1	2.25	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2010:EDO:C2	2:H:2010:EDO:HO2	2.13	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
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:132:ASP:OD1	1:G:132:ASP:C	2.58	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:H:132:ASP:C	1:H:132:ASP:OD1	2.58	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
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:E:139:THR:C	1:E:140:MSE:HG3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2089:EDO:C2	2:E:2089:EDO:HO2	2.12	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: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: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:G:236:LYS:NZ	1:G:236:LYS:CD	2.68	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: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:E:88:TRP:HA	2:E:2076:EDO:C1	2.46	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:C:179:GLU:CD	1:D:59:ARG:HH12	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:211:TRP:CD1	1:J:211:TRP:H	2.33	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: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:J:240:LEU:H	1:J:243:GLU:CD	2.22	0.45
1:B:220:ARG:CD	1:B:224:GLU:OE2	2.65	0.45
1:B:232:ARG:O	2:B:2002:EDO:O1	2.28	0.45
1:B:244:GLU:CD	1:B:244:GLU:H	2.25	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:J:104:ASP:CG	1:J:104:ASP:O	2.61	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:36:TRP:NE1	1:I:162:LYS:HZ2	2.13	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
1:I:36:TRP:CD1	1:I:162:LYS:HZ3	2.36	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:139:THR:C	1:C:140:MSE:HG3	2.43	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:A:239:LYS:HZ1	1:A:244:GLU:HA	1.83	0.43
1:B:24:ILE:HD13	1:B:24:ILE:HG21	1.75	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
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
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:I:117:HIS:C	1:I:118:ALA:O	2.58	0.43
1:B:187:VAL:O	1:B:188:PRO:C	2.60	0.43
1:D:203:GLY:C	2:D:2035:EDO:C2	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:132:ASP:C	1:E:132:ASP:OD1	2.62	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:20:ASP:OD2	1:B:86:LYS:NZ	2.50	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASP:CG	1:A:86:LYS:HZ2	2.20	0.42
1:A:61:TYR:HD1	1:A:71:LEU:HD12	1.85	0.42
2:A:2124:EDO:C1	2:A:2124:EDO:HO1	2.13	0.42
1:C:139:THR:OG1	1:D:144:PRO:HD3	2.19	0.42
1:E:2:PRO:HB2	1:F:10:GLU:CD	2.41	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: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:G:164:GLY:C	2:G:2112:EDO:H22	2.44	0.42
1:C:187:VAL:O	1:C:188:PRO:C	2.62	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:H:39:LEU:C	1:H:39:LEU:HD12	2.45	0.42
1:J:208:LEU:C	2:J:2105:EDO:H12	2.45	0.42
1:A:189:PRO:HA	1:A:190:PRO:HD3	1.78	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:G:211:TRP:CD1	1:G:211:TRP:H	2.37	0.42
1:J:97:ILE:N	2:J:2109:EDO:C1	2.55	0.42
1:F:81:SER:O	1:F:82:HIS:C	2.62	0.41
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PRO:HG2	1:C:122:THR:OG1	2.21	0.41
1:E:104:ASP:CG	1:E:104:ASP:O	2.61	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:H:74:LEU:C	1:H:74:LEU:CD1	2.93	0.41
1:I:19:THR:HA	1:I:102:ILE:HA	2.02	0.41
1:A:243:GLU:C	1:A:245:ALA:H	2.27	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:D:203:GLY:C	2:D:2035:EDO:H21	2.45	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:HE1	1:E:112:ARG:HG2	2.02	0.41
1:E:15:MSE:SE	1:E:109:VAL:HG13	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:GLU:HG2	2:G:2057:EDO:C2	2.50	0.41
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:I:49:VAL:N	2:I:2121:EDO:HO2	2.15	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:28:ASP:O	1:B:29:HIS:C	2.62	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: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:E:212:PHE:C	1:E:212:PHE:HD2	2.29	0.40
1:G:240:LEU:HD23	1:G:240:LEU:HA	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	10	6
1	B	242/249 (97%)	234 (97%)	6 (2%)	2 (1%)	16	11
1	C	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	30	27
1	D	242/249 (97%)	231 (96%)	9 (4%)	2 (1%)	16	11
1	E	242/249 (97%)	233 (96%)	6 (2%)	3 (1%)	10	6
1	F	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	30	27
1	G	242/249 (97%)	232 (96%)	7 (3%)	3 (1%)	10	6
1	H	242/249 (97%)	233 (96%)	7 (3%)	2 (1%)	16	11
1	I	242/249 (97%)	234 (97%)	7 (3%)	1 (0%)	30	27
1	J	242/249 (97%)	236 (98%)	3 (1%)	3 (1%)	10	6
All	All	2420/2490 (97%)	2332 (96%)	67 (3%)	21 (1%)	14	9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	176	PRO

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

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%)	192 (91%)	18 (9%)	10	6
1	B	210/211 (100%)	190 (90%)	20 (10%)	8	5
1	C	210/211 (100%)	189 (90%)	21 (10%)	7	4
1	D	210/211 (100%)	194 (92%)	16 (8%)	12	9
1	E	210/211 (100%)	199 (95%)	11 (5%)	21	18
1	F	210/211 (100%)	196 (93%)	14 (7%)	15	11
1	G	210/211 (100%)	194 (92%)	16 (8%)	12	9
1	H	210/211 (100%)	195 (93%)	15 (7%)	13	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	210/211 (100%)	191 (91%)	19 (9%)	9	6
1	J	210/211 (100%)	194 (92%)	16 (8%)	12	9
All	All	2100/2110 (100%)	1934 (92%)	166 (8%)	11	8

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	11	ARG
1	A	14	GLU
1	A	16	GLU
1	A	47	THR
1	A	112	ARG
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	207	SER
1	A	208	LEU
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	96	ARG
1	B	106	GLN
1	B	112	ARG
1	B	147	LEU
1	B	150	LEU
1	B	158	VAL
1	B	159	LYS
1	B	161	LEU
1	B	162	LYS
1	B	167	LEU
1	B	195	GLN

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Mol	Chain	Res	Type
1	B	208	LEU
1	B	227	ARG
1	B	228	ARG
1	B	244	GLU
1	C	5	ILE
1	C	11	ARG
1	C	17	VAL
1	C	39	LEU
1	C	47	THR
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	168	LYS
1	C	195	GLN
1	C	197	ARG
1	C	199	ARG
1	C	204	GLN
1	C	208	LEU
1	C	217	PRO
1	C	219	SER
1	C	220	ARG
1	C	224	GLU
1	D	5	ILE
1	D	47	THR
1	D	48	PRO
1	D	74	LEU
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	217	PRO
1	D	225	GLU
1	D	236	LYS
1	D	244	GLU
1	E	2	PRO

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Mol	Chain	Res	Type
1	E	11	ARG
1	E	16	GLU
1	E	35	LYS
1	E	147	LEU
1	E	159	LYS
1	E	167	LEU
1	E	191	THR
1	E	194	ASP
1	E	201	GLU
1	E	208	LEU
1	F	2	PRO
1	F	24	ILE
1	F	77	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	204	GLN
1	F	208	LEU
1	F	217	PRO
1	F	239	LYS
1	F	244	GLU
1	G	15	MSE
1	G	17	VAL
1	G	96	ARG
1	G	106	GLN
1	G	111	ARG
1	G	112	ARG
1	G	124	THR
1	G	144	PRO
1	G	147	LEU
1	G	150	LEU
1	G	159	LYS
1	G	161	LEU
1	G	167	LEU
1	G	179	GLU
1	G	208	LEU
1	G	242	TYR
1	H	39	LEU
1	H	59	ARG

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Mol	Chain	Res	Type
1	H	74	LEU
1	H	93	ILE
1	H	144	PRO
1	H	147	LEU
1	H	159	LYS
1	H	161	LEU
1	H	167	LEU
1	H	179	GLU
1	H	201	GLU
1	H	204	GLN
1	H	208	LEU
1	H	228	ARG
1	H	239	LYS
1	I	4	SER
1	I	11	ARG
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	159	LYS
1	I	167	LEU
1	I	208	LEU
1	I	235	GLU
1	I	239	LYS
1	I	244	GLU
1	J	2	PRO
1	J	48	PRO
1	J	74	LEU
1	J	106	GLN
1	J	122	THR
1	J	145	MSE
1	J	147	LEU
1	J	161	LEU
1	J	162	LYS
1	J	166	SER

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Mol	Chain	Res	Type
1	J	167	LEU
1	J	183	GLU
1	J	204	GLN
1	J	208	LEU
1	J	228	ARG
1	J	244	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	106	GLN
1	A	117	HIS
1	A	123	HIS
1	B	65	GLN
1	B	106	GLN
1	B	117	HIS
1	B	123	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	106	GLN
1	E	117	HIS
1	E	195	GLN
1	E	204	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	123	HIS
1	H	195	GLN
1	I	117	HIS
1	I	123	HIS
1	I	195	GLN

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Mol	Chain	Res	Type
1	J	92	HIS
1	J	117	HIS
1	J	123	HIS
1	J	195	GLN
1	J	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	2109	-	3,3,3	1.31	1 (33%)	2,2,2	1.14	0
2	EDO	I	2115	-	3,3,3	3.68	2 (66%)	2,2,2	0.93	0
2	EDO	G	2009	-	3,3,3	3.75	2 (66%)	2,2,2	1.17	0
2	EDO	I	2046	-	3,3,3	2.26	1 (33%)	2,2,2	1.02	0
2	EDO	J	2123	-	3,3,3	3.44	2 (66%)	2,2,2	1.90	1 (50%)
2	EDO	G	2101	-	3,3,3	2.29	2 (66%)	2,2,2	1.83	1 (50%)
2	EDO	C	2082	-	3,3,3	3.29	1 (33%)	2,2,2	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	2012	-	3,3,3	4.06	2 (66%)	2,2,2	0.32	0
2	EDO	F	2038	-	3,3,3	2.49	2 (66%)	2,2,2	0.69	0
2	EDO	I	2107	-	3,3,3	1.51	1 (33%)	2,2,2	0.58	0
2	EDO	H	2111	-	3,3,3	2.50	3 (100%)	2,2,2	1.01	0
2	EDO	H	2060	-	3,3,3	1.02	0	2,2,2	0.21	0
2	EDO	C	2026	-	3,3,3	1.07	0	2,2,2	0.77	0
2	EDO	G	2112	-	3,3,3	2.68	2 (66%)	2,2,2	0.46	0
2	EDO	E	2076	-	3,3,3	2.55	2 (66%)	2,2,2	0.93	0
2	EDO	B	2013	-	3,3,3	2.47	2 (66%)	2,2,2	0.73	0
2	EDO	A	2029	-	3,3,3	3.27	2 (66%)	2,2,2	0.71	0
2	EDO	F	2006	-	3,3,3	3.55	2 (66%)	2,2,2	0.88	0
2	EDO	A	2065	-	3,3,3	2.63	2 (66%)	2,2,2	0.68	0
2	EDO	E	2092	-	3,3,3	1.84	2 (66%)	2,2,2	1.23	0
2	EDO	G	2050	-	3,3,3	2.99	2 (66%)	2,2,2	0.29	0
2	EDO	A	2122	-	3,3,3	3.16	1 (33%)	2,2,2	1.26	0
2	EDO	C	2085	-	3,3,3	4.06	2 (66%)	2,2,2	1.35	0
2	EDO	J	2008	-	3,3,3	5.00	2 (66%)	2,2,2	1.19	0
2	EDO	A	2011	-	3,3,3	2.72	2 (66%)	2,2,2	1.29	0
2	EDO	G	2093	-	3,3,3	3.06	2 (66%)	2,2,2	1.14	0
2	EDO	C	2004	-	3,3,3	4.51	2 (66%)	2,2,2	0.49	0
2	EDO	F	2096	-	3,3,3	2.42	2 (66%)	2,2,2	0.96	0
2	EDO	A	2017	-	3,3,3	2.06	2 (66%)	2,2,2	0.95	0
2	EDO	J	2110	-	3,3,3	2.52	2 (66%)	2,2,2	1.06	0
2	EDO	B	2018	-	3,3,3	2.12	2 (66%)	2,2,2	0.81	0
2	EDO	E	2088	-	3,3,3	2.87	2 (66%)	2,2,2	1.17	0
2	EDO	E	2120	-	3,3,3	3.00	2 (66%)	2,2,2	0.72	0
2	EDO	G	2047	-	3,3,3	2.84	2 (66%)	2,2,2	0.74	0
2	EDO	F	2098	-	3,3,3	4.18	2 (66%)	2,2,2	0.77	0
2	EDO	J	2104	-	3,3,3	3.81	2 (66%)	2,2,2	2.00	1 (50%)
2	EDO	D	2003	-	3,3,3	2.80	2 (66%)	2,2,2	0.88	0
2	EDO	D	2073	-	3,3,3	2.10	2 (66%)	2,2,2	0.64	0
2	EDO	J	2014	-	3,3,3	3.45	2 (66%)	2,2,2	0.70	0
2	EDO	I	2045	-	3,3,3	2.97	2 (66%)	2,2,2	0.46	0
2	EDO	I	2052	-	3,3,3	2.63	2 (66%)	2,2,2	1.00	0
2	EDO	B	2062	-	3,3,3	1.86	1 (33%)	2,2,2	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	J	2055	-	3,3,3	2.13	1 (33%)	2,2,2	0.83	0
2	EDO	B	2025	-	3,3,3	2.95	2 (66%)	2,2,2	0.67	0
2	EDO	B	2028	-	3,3,3	2.33	2 (66%)	2,2,2	1.14	0
2	EDO	I	2099	-	3,3,3	2.53	2 (66%)	2,2,2	1.80	1 (50%)
2	EDO	I	2103	-	3,3,3	2.85	2 (66%)	2,2,2	1.83	1 (50%)
2	EDO	B	2015	-	3,3,3	2.38	2 (66%)	2,2,2	0.68	0
2	EDO	G	2056	-	3,3,3	3.16	2 (66%)	2,2,2	0.88	0
2	EDO	H	2113	-	3,3,3	2.51	1 (33%)	2,2,2	0.81	0
2	EDO	E	2089	-	3,3,3	3.50	2 (66%)	2,2,2	0.23	0
2	EDO	C	2075	-	3,3,3	2.19	2 (66%)	2,2,2	1.20	0
2	EDO	I	2007	-	3,3,3	3.82	2 (66%)	2,2,2	1.40	0
2	EDO	B	2020	-	3,3,3	2.99	2 (66%)	2,2,2	0.74	0
2	EDO	J	2068	-	3,3,3	2.92	2 (66%)	2,2,2	0.05	0
2	EDO	J	2049	-	3,3,3	2.98	2 (66%)	2,2,2	0.86	0
2	EDO	E	2039	-	3,3,3	2.11	2 (66%)	2,2,2	0.33	0
2	EDO	F	2043	-	3,3,3	3.08	2 (66%)	2,2,2	1.33	0
2	EDO	B	2030	-	3,3,3	1.00	0	2,2,2	0.34	0
2	EDO	B	2021	-	3,3,3	4.05	2 (66%)	2,2,2	0.13	0
2	EDO	F	2037	-	3,3,3	2.52	2 (66%)	2,2,2	1.04	0
2	EDO	J	2061	-	3,3,3	2.25	1 (33%)	2,2,2	0.96	0
2	EDO	D	2118	-	3,3,3	3.21	2 (66%)	2,2,2	0.27	0
2	EDO	H	2058	-	3,3,3	3.36	2 (66%)	2,2,2	1.47	1 (50%)
2	EDO	F	2097	-	3,3,3	3.00	2 (66%)	2,2,2	0.13	0
2	EDO	D	2071	-	3,3,3	2.92	2 (66%)	2,2,2	0.52	0
2	EDO	F	2095	-	3,3,3	3.09	2 (66%)	2,2,2	0.98	0
2	EDO	E	2077	-	3,3,3	2.75	2 (66%)	2,2,2	0.91	0
2	EDO	C	2083	-	3,3,3	2.80	2 (66%)	2,2,2	1.22	0
2	EDO	A	2124	-	3,3,3	4.45	2 (66%)	2,2,2	0.76	0
2	EDO	H	2059	-	3,3,3	4.04	3 (100%)	2,2,2	0.51	0
2	EDO	B	2002	-	3,3,3	4.64	2 (66%)	2,2,2	1.19	0
2	EDO	E	2079	-	3,3,3	2.72	2 (66%)	2,2,2	1.14	0
2	EDO	H	2054	-	3,3,3	2.28	2 (66%)	2,2,2	0.92	0
2	EDO	E	2090	-	3,3,3	2.71	2 (66%)	2,2,2	0.60	0
2	EDO	C	2067	-	3,3,3	2.84	1 (33%)	2,2,2	0.42	0
2	EDO	I	2100	-	3,3,3	1.81	1 (33%)	2,2,2	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	J	2053	-	3,3,3	3.39	2 (66%)	2,2,2	0.32	0
2	EDO	B	2125	-	3,3,3	2.75	3 (100%)	2,2,2	0.96	0
2	EDO	E	2005	-	3,3,3	4.50	2 (66%)	2,2,2	0.49	0
2	EDO	I	2121	-	3,3,3	1.27	0	2,2,2	0.77	0
2	EDO	C	2126	-	3,3,3	3.27	2 (66%)	2,2,2	0.57	0
2	EDO	C	2084	-	3,3,3	3.19	2 (66%)	2,2,2	1.22	0
2	EDO	H	2010	-	3,3,3	4.00	2 (66%)	2,2,2	0.42	0
2	EDO	D	2035	-	3,3,3	1.28	0	2,2,2	0.30	0
2	EDO	J	2069	-	3,3,3	2.87	2 (66%)	2,2,2	0.47	0
2	EDO	C	2036	-	3,3,3	2.72	2 (66%)	2,2,2	1.08	0
2	EDO	D	2074	-	3,3,3	3.77	2 (66%)	2,2,2	1.37	0
2	EDO	G	2057	-	3,3,3	1.47	1 (33%)	2,2,2	0.86	0
2	EDO	A	2016	-	3,3,3	2.18	2 (66%)	2,2,2	0.57	0
2	EDO	A	2001	-	3,3,3	2.52	2 (66%)	2,2,2	0.22	0
2	EDO	J	2048	-	3,3,3	3.09	2 (66%)	2,2,2	0.90	0
2	EDO	J	2106	-	3,3,3	2.41	1 (33%)	2,2,2	0.96	0
2	EDO	B	2027	-	3,3,3	1.72	2 (66%)	2,2,2	1.11	0
2	EDO	J	2108	-	3,3,3	1.61	1 (33%)	2,2,2	0.81	0
2	EDO	G	2102	-	3,3,3	3.11	2 (66%)	2,2,2	0.76	0
2	EDO	B	2023	-	3,3,3	3.24	2 (66%)	2,2,2	0.97	0
2	EDO	C	2128	-	3,3,3	3.40	2 (66%)	2,2,2	0.95	0
2	EDO	H	2114	-	3,3,3	3.18	2 (66%)	2,2,2	0.91	0
2	EDO	D	2031	-	3,3,3	3.00	2 (66%)	2,2,2	0.57	0
2	EDO	A	2066	-	3,3,3	3.00	2 (66%)	2,2,2	0.48	0
2	EDO	C	2081	-	3,3,3	2.81	3 (100%)	2,2,2	0.89	0
2	EDO	A	2063	-	3,3,3	3.43	2 (66%)	2,2,2	1.00	0
2	EDO	A	2019	-	3,3,3	2.74	2 (66%)	2,2,2	0.75	0
2	EDO	C	2064	-	3,3,3	2.74	2 (66%)	2,2,2	0.58	0
2	EDO	F	2086	-	3,3,3	2.51	2 (66%)	2,2,2	1.42	0
2	EDO	E	2040	-	3,3,3	2.65	2 (66%)	2,2,2	0.82	0
2	EDO	C	2024	-	3,3,3	3.44	2 (66%)	2,2,2	0.81	0
2	EDO	H	2044	-	3,3,3	2.22	2 (66%)	2,2,2	0.28	0
2	EDO	B	2070	-	3,3,3	2.82	2 (66%)	2,2,2	0.89	0
2	EDO	C	2080	-	3,3,3	2.76	2 (66%)	2,2,2	0.44	0
2	EDO	J	2105	-	3,3,3	3.06	2 (66%)	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	2033	-	3,3,3	2.34	2 (66%)	2,2,2	0.99	0
2	EDO	F	2034	-	3,3,3	2.21	1 (33%)	2,2,2	0.27	0
2	EDO	D	2072	-	3,3,3	2.69	2 (66%)	2,2,2	0.60	0
2	EDO	A	2022	-	3,3,3	2.04	1 (33%)	2,2,2	1.01	0
2	EDO	E	2127	-	3,3,3	2.61	2 (66%)	2,2,2	1.43	0
2	EDO	E	2091	-	3,3,3	3.32	2 (66%)	2,2,2	1.24	0
2	EDO	F	2094	-	3,3,3	3.03	2 (66%)	2,2,2	1.38	0
2	EDO	E	2032	-	3,3,3	3.07	1 (33%)	2,2,2	0.82	0
2	EDO	F	2087	-	3,3,3	1.68	1 (33%)	2,2,2	0.78	0
2	EDO	A	2116	-	3,3,3	3.07	2 (66%)	2,2,2	0.46	0
2	EDO	E	2042	-	3,3,3	2.19	2 (66%)	2,2,2	0.83	0
2	EDO	C	2117	-	3,3,3	2.42	2 (66%)	2,2,2	0.48	0
2	EDO	I	2051	-	3,3,3	2.01	1 (33%)	2,2,2	1.09	0
2	EDO	D	2119	-	3,3,3	2.61	2 (66%)	2,2,2	0.94	0
2	EDO	E	2078	-	3,3,3	2.45	1 (33%)	2,2,2	1.31	0
2	EDO	E	2041	-	3,3,3	1.71	1 (33%)	2,2,2	1.02	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	2109	-	-	0/1/1/1	-
2	EDO	I	2115	-	-	0/1/1/1	-
2	EDO	G	2009	-	-	1/1/1/1	-
2	EDO	I	2046	-	-	0/1/1/1	-
2	EDO	J	2123	-	-	1/1/1/1	-
2	EDO	G	2101	-	-	1/1/1/1	-
2	EDO	C	2082	-	-	0/1/1/1	-
2	EDO	A	2012	-	-	1/1/1/1	-
2	EDO	F	2038	-	-	0/1/1/1	-
2	EDO	I	2107	-	-	0/1/1/1	-
2	EDO	H	2111	-	-	0/1/1/1	-
2	EDO	H	2060	-	-	1/1/1/1	-
2	EDO	C	2026	-	-	1/1/1/1	-
2	EDO	G	2112	-	-	0/1/1/1	-
2	EDO	E	2076	-	-	1/1/1/1	-
2	EDO	B	2013	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	2029	-	-	1/1/1/1	-
2	EDO	F	2006	-	-	1/1/1/1	-
2	EDO	A	2065	-	-	1/1/1/1	-
2	EDO	E	2092	-	-	1/1/1/1	-
2	EDO	G	2050	-	-	0/1/1/1	-
2	EDO	A	2122	-	-	1/1/1/1	-
2	EDO	C	2085	-	-	1/1/1/1	-
2	EDO	J	2008	-	-	1/1/1/1	-
2	EDO	A	2011	-	-	0/1/1/1	-
2	EDO	G	2093	-	-	1/1/1/1	-
2	EDO	C	2004	-	-	1/1/1/1	-
2	EDO	F	2096	-	-	1/1/1/1	-
2	EDO	A	2017	-	-	1/1/1/1	-
2	EDO	J	2110	-	-	0/1/1/1	-
2	EDO	B	2018	-	-	1/1/1/1	-
2	EDO	E	2088	-	-	1/1/1/1	-
2	EDO	E	2120	-	-	1/1/1/1	-
2	EDO	G	2047	-	-	0/1/1/1	-
2	EDO	F	2098	-	-	1/1/1/1	-
2	EDO	J	2104	-	-	1/1/1/1	-
2	EDO	D	2003	-	-	1/1/1/1	-
2	EDO	D	2073	-	-	1/1/1/1	-
2	EDO	J	2014	-	-	0/1/1/1	-
2	EDO	I	2045	-	-	1/1/1/1	-
2	EDO	I	2052	-	-	1/1/1/1	-
2	EDO	B	2062	-	-	0/1/1/1	-
2	EDO	J	2055	-	-	1/1/1/1	-
2	EDO	B	2025	-	-	1/1/1/1	-
2	EDO	B	2028	-	-	1/1/1/1	-
2	EDO	I	2099	-	-	1/1/1/1	-
2	EDO	I	2103	-	-	1/1/1/1	-
2	EDO	B	2015	-	-	0/1/1/1	-
2	EDO	G	2056	-	-	1/1/1/1	-
2	EDO	H	2113	-	-	0/1/1/1	-
2	EDO	E	2089	-	-	1/1/1/1	-
2	EDO	C	2075	-	-	1/1/1/1	-
2	EDO	I	2007	-	-	1/1/1/1	-
2	EDO	B	2020	-	-	0/1/1/1	-
2	EDO	J	2068	-	-	1/1/1/1	-
2	EDO	J	2049	-	-	0/1/1/1	-
2	EDO	E	2039	-	-	1/1/1/1	-
2	EDO	F	2043	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	2030	-	-	0/1/1/1	-
2	EDO	B	2021	-	-	1/1/1/1	-
2	EDO	F	2037	-	-	1/1/1/1	-
2	EDO	J	2061	-	-	1/1/1/1	-
2	EDO	D	2118	-	-	1/1/1/1	-
2	EDO	H	2058	-	-	1/1/1/1	-
2	EDO	F	2097	-	-	1/1/1/1	-
2	EDO	D	2071	-	-	1/1/1/1	-
2	EDO	F	2095	-	-	0/1/1/1	-
2	EDO	E	2077	-	-	1/1/1/1	-
2	EDO	C	2083	-	-	1/1/1/1	-
2	EDO	A	2124	-	-	1/1/1/1	-
2	EDO	H	2059	-	-	1/1/1/1	-
2	EDO	B	2002	-	-	1/1/1/1	-
2	EDO	E	2079	-	-	1/1/1/1	-
2	EDO	H	2054	-	-	0/1/1/1	-
2	EDO	E	2090	-	-	1/1/1/1	-
2	EDO	C	2067	-	-	1/1/1/1	-
2	EDO	I	2100	-	-	1/1/1/1	-
2	EDO	J	2053	-	-	1/1/1/1	-
2	EDO	B	2125	-	-	1/1/1/1	-
2	EDO	E	2005	-	-	1/1/1/1	-
2	EDO	I	2121	-	-	1/1/1/1	-
2	EDO	C	2126	-	-	1/1/1/1	-
2	EDO	C	2084	-	-	0/1/1/1	-
2	EDO	H	2010	-	-	1/1/1/1	-
2	EDO	D	2035	-	-	1/1/1/1	-
2	EDO	J	2069	-	-	1/1/1/1	-
2	EDO	C	2036	-	-	1/1/1/1	-
2	EDO	D	2074	-	-	1/1/1/1	-
2	EDO	G	2057	-	-	1/1/1/1	-
2	EDO	A	2016	-	-	1/1/1/1	-
2	EDO	A	2001	-	-	1/1/1/1	-
2	EDO	J	2048	-	-	1/1/1/1	-
2	EDO	J	2106	-	-	1/1/1/1	-
2	EDO	B	2027	-	-	0/1/1/1	-
2	EDO	J	2108	-	-	1/1/1/1	-
2	EDO	G	2102	-	-	0/1/1/1	-
2	EDO	B	2023	-	-	0/1/1/1	-
2	EDO	C	2128	-	-	1/1/1/1	-
2	EDO	H	2114	-	-	0/1/1/1	-
2	EDO	D	2031	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	2066	-	-	0/1/1/1	-
2	EDO	C	2081	-	-	0/1/1/1	-
2	EDO	A	2063	-	-	1/1/1/1	-
2	EDO	A	2019	-	-	0/1/1/1	-
2	EDO	C	2064	-	-	1/1/1/1	-
2	EDO	F	2086	-	-	1/1/1/1	-
2	EDO	E	2040	-	-	0/1/1/1	-
2	EDO	C	2024	-	-	1/1/1/1	-
2	EDO	H	2044	-	-	0/1/1/1	-
2	EDO	B	2070	-	-	1/1/1/1	-
2	EDO	C	2080	-	-	1/1/1/1	-
2	EDO	J	2105	-	-	0/1/1/1	-
2	EDO	D	2033	-	-	1/1/1/1	-
2	EDO	F	2034	-	-	1/1/1/1	-
2	EDO	D	2072	-	-	1/1/1/1	-
2	EDO	A	2022	-	-	1/1/1/1	-
2	EDO	E	2127	-	-	0/1/1/1	-
2	EDO	E	2091	-	-	1/1/1/1	-
2	EDO	F	2094	-	-	1/1/1/1	-
2	EDO	E	2032	-	-	1/1/1/1	-
2	EDO	F	2087	-	-	1/1/1/1	-
2	EDO	A	2116	-	-	1/1/1/1	-
2	EDO	E	2042	-	-	1/1/1/1	-
2	EDO	C	2117	-	-	0/1/1/1	-
2	EDO	I	2051	-	-	1/1/1/1	-
2	EDO	D	2119	-	-	1/1/1/1	-
2	EDO	E	2078	-	-	0/1/1/1	-
2	EDO	E	2041	-	-	1/1/1/1	-

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2008	EDO	O1-C1	7.43	1.80	1.42
2	E	2005	EDO	O2-C2	6.54	1.75	1.42
2	C	2004	EDO	O2-C2	6.06	1.73	1.42
2	F	2098	EDO	O2-C2	5.88	1.72	1.42
2	B	2002	EDO	O1-C1	5.82	1.71	1.42
2	H	2059	EDO	O2-C2	5.82	1.71	1.42
2	A	2012	EDO	O2-C2	5.56	1.70	1.42
2	D	2074	EDO	O1-C1	5.55	1.70	1.42
2	H	2010	EDO	O2-C2	5.55	1.70	1.42
2	A	2124	EDO	O1-C1	5.44	1.69	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2124	EDO	O2-C2	5.43	1.69	1.42
2	A	2122	EDO	O2-C2	5.40	1.69	1.42
2	B	2002	EDO	O2-C2	5.34	1.69	1.42
2	B	2021	EDO	O2-C2	5.24	1.68	1.42
2	C	2082	EDO	O2-C2	5.21	1.68	1.42
2	E	2089	EDO	O2-C2	5.19	1.68	1.42
2	I	2007	EDO	O1-C1	5.18	1.68	1.42
2	F	2006	EDO	O1-C1	5.16	1.68	1.42
2	C	2085	EDO	O1-C1	5.10	1.68	1.42
2	B	2023	EDO	O2-C2	5.04	1.67	1.42
2	G	2009	EDO	O1-C1	4.97	1.67	1.42
2	C	2004	EDO	O1-C1	4.90	1.67	1.42
2	I	2115	EDO	O2-C2	4.89	1.67	1.42
2	D	2118	EDO	O2-C2	4.86	1.66	1.42
2	J	2104	EDO	O2-C2	4.83	1.66	1.42
2	E	2032	EDO	O2-C2	4.83	1.66	1.42
2	C	2085	EDO	O2-C2	4.80	1.66	1.42
2	G	2050	EDO	O2-C2	4.68	1.66	1.42
2	G	2056	EDO	O2-C2	4.64	1.65	1.42
2	G	2102	EDO	O2-C2	4.62	1.65	1.42
2	C	2024	EDO	O2-C2	4.60	1.65	1.42
2	C	2067	EDO	O2-C2	4.55	1.65	1.42
2	F	2043	EDO	O2-C2	4.53	1.65	1.42
2	C	2128	EDO	O2-C2	4.51	1.65	1.42
2	C	2126	EDO	O2-C2	4.49	1.65	1.42
2	B	2021	EDO	O1-C1	4.49	1.65	1.42
2	D	2031	EDO	O2-C2	4.42	1.64	1.42
2	J	2068	EDO	O2-C2	4.40	1.64	1.42
2	G	2093	EDO	O2-C2	4.40	1.64	1.42
2	J	2049	EDO	O2-C2	4.37	1.64	1.42
2	H	2058	EDO	O2-C2	4.35	1.64	1.42
2	J	2014	EDO	O1-C1	4.33	1.64	1.42
2	E	2120	EDO	O1-C1	4.33	1.64	1.42
2	J	2123	EDO	O1-C1	4.32	1.64	1.42
2	B	2020	EDO	O1-C1	4.31	1.64	1.42
2	A	2063	EDO	O1-C1	4.31	1.64	1.42
2	E	2088	EDO	O1-C1	4.30	1.64	1.42
2	J	2105	EDO	O2-C2	4.25	1.63	1.42
2	A	2012	EDO	O1-C1	4.23	1.63	1.42
2	J	2008	EDO	O2-C2	4.23	1.63	1.42
2	J	2053	EDO	O2-C2	4.22	1.63	1.42
2	J	2104	EDO	O1-C1	4.21	1.63	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2029	EDO	O2-C2	4.20	1.63	1.42
2	H	2114	EDO	O1-C1	4.18	1.63	1.42
2	E	2091	EDO	O2-C2	4.15	1.63	1.42
2	D	2071	EDO	O2-C2	4.15	1.63	1.42
2	J	2048	EDO	O2-C2	4.14	1.63	1.42
2	H	2010	EDO	O1-C1	4.09	1.62	1.42
2	A	2063	EDO	O2-C2	4.08	1.62	1.42
2	D	2072	EDO	O2-C2	4.07	1.62	1.42
2	D	2003	EDO	O2-C2	4.05	1.62	1.42
2	J	2014	EDO	O2-C2	4.04	1.62	1.42
2	C	2084	EDO	O2-C2	4.03	1.62	1.42
2	I	2045	EDO	O1-C1	4.02	1.62	1.42
2	E	2091	EDO	O1-C1	3.98	1.62	1.42
2	I	2007	EDO	O2-C2	3.97	1.62	1.42
2	I	2103	EDO	O1-C1	3.97	1.62	1.42
2	A	2065	EDO	O1-C1	3.96	1.62	1.42
2	G	2009	EDO	O2-C2	3.95	1.62	1.42
2	E	2078	EDO	O1-C1	3.94	1.62	1.42
2	F	2098	EDO	O1-C1	3.92	1.62	1.42
2	J	2053	EDO	O1-C1	3.91	1.62	1.42
2	E	2005	EDO	O1-C1	3.91	1.62	1.42
2	A	2116	EDO	O2-C2	3.90	1.62	1.42
2	C	2036	EDO	O1-C1	3.89	1.61	1.42
2	H	2058	EDO	O1-C1	3.87	1.61	1.42
2	A	2011	EDO	O2-C2	3.86	1.61	1.42
2	B	2025	EDO	O1-C1	3.84	1.61	1.42
2	C	2084	EDO	O1-C1	3.79	1.61	1.42
2	J	2061	EDO	O1-C1	3.77	1.61	1.42
2	I	2115	EDO	O1-C1	3.77	1.61	1.42
2	A	2029	EDO	O1-C1	3.76	1.61	1.42
2	J	2123	EDO	O2-C2	3.76	1.61	1.42
2	F	2095	EDO	O1-C1	3.75	1.61	1.42
2	A	2066	EDO	O2-C2	3.75	1.61	1.42
2	F	2034	EDO	O2-C2	3.74	1.61	1.42
2	F	2095	EDO	O2-C2	3.74	1.61	1.42
2	H	2113	EDO	O1-C1	3.73	1.61	1.42
2	F	2094	EDO	O1-C1	3.72	1.61	1.42
2	J	2106	EDO	O1-C1	3.70	1.61	1.42
2	F	2097	EDO	O1-C1	3.70	1.61	1.42
2	C	2081	EDO	O2-C2	3.69	1.60	1.42
2	F	2086	EDO	O1-C1	3.66	1.60	1.42
2	C	2064	EDO	O1-C1	3.66	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2094	EDO	O2-C2	3.66	1.60	1.42
2	F	2097	EDO	O2-C2	3.64	1.60	1.42
2	G	2047	EDO	O2-C2	3.63	1.60	1.42
2	E	2079	EDO	O2-C2	3.62	1.60	1.42
2	C	2024	EDO	O1-C1	3.61	1.60	1.42
2	A	2019	EDO	O1-C1	3.60	1.60	1.42
2	B	2070	EDO	O1-C1	3.57	1.60	1.42
2	C	2083	EDO	O2-C2	3.55	1.60	1.42
2	J	2069	EDO	O2-C2	3.55	1.60	1.42
2	E	2127	EDO	O2-C2	3.55	1.60	1.42
2	C	2080	EDO	O2-C2	3.55	1.60	1.42
2	F	2037	EDO	O2-C2	3.54	1.60	1.42
2	F	2096	EDO	O2-C2	3.50	1.59	1.42
2	J	2110	EDO	O2-C2	3.50	1.59	1.42
2	J	2055	EDO	O2-C2	3.47	1.59	1.42
2	A	2116	EDO	O1-C1	3.44	1.59	1.42
2	I	2052	EDO	O1-C1	3.40	1.59	1.42
2	C	2128	EDO	O1-C1	3.40	1.59	1.42
2	A	2066	EDO	O1-C1	3.40	1.59	1.42
2	J	2069	EDO	O1-C1	3.39	1.59	1.42
2	E	2090	EDO	O2-C2	3.38	1.59	1.42
2	E	2077	EDO	O1-C1	3.38	1.59	1.42
2	B	2028	EDO	O2-C2	3.36	1.59	1.42
2	D	2033	EDO	O2-C2	3.35	1.59	1.42
2	E	2077	EDO	O2-C2	3.35	1.59	1.42
2	I	2046	EDO	O2-C2	3.35	1.59	1.42
2	H	2114	EDO	O2-C2	3.31	1.59	1.42
2	D	2119	EDO	O2-C2	3.30	1.58	1.42
2	G	2112	EDO	O1-C1	3.30	1.58	1.42
2	G	2047	EDO	O1-C1	3.29	1.58	1.42
2	C	2083	EDO	O1-C1	3.27	1.58	1.42
2	J	2048	EDO	O1-C1	3.27	1.58	1.42
2	E	2040	EDO	O1-C1	3.26	1.58	1.42
2	B	2025	EDO	O2-C2	3.25	1.58	1.42
2	E	2076	EDO	O2-C2	3.23	1.58	1.42
2	E	2090	EDO	O1-C1	3.22	1.58	1.42
2	F	2038	EDO	O1-C1	3.21	1.58	1.42
2	H	2044	EDO	O1-C1	3.21	1.58	1.42
2	B	2015	EDO	O1-C1	3.20	1.58	1.42
2	H	2059	EDO	O1-C1	3.18	1.58	1.42
2	J	2105	EDO	O1-C1	3.16	1.58	1.42
2	I	2099	EDO	O2-C2	3.13	1.58	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2111	EDO	O2-C2	3.11	1.58	1.42
2	G	2112	EDO	O2-C2	3.09	1.57	1.42
2	D	2119	EDO	O1-C1	3.09	1.57	1.42
2	A	2022	EDO	O1-C1	3.08	1.57	1.42
2	A	2001	EDO	O1-C1	3.07	1.57	1.42
2	B	2070	EDO	O2-C2	3.07	1.57	1.42
2	C	2075	EDO	O1-C1	3.06	1.57	1.42
2	C	2080	EDO	O1-C1	3.06	1.57	1.42
2	B	2125	EDO	O1-C1	3.06	1.57	1.42
2	E	2040	EDO	O2-C2	3.04	1.57	1.42
2	A	2019	EDO	O2-C2	3.04	1.57	1.42
2	B	2013	EDO	O2-C2	3.04	1.57	1.42
2	I	2052	EDO	O2-C2	3.03	1.57	1.42
2	D	2074	EDO	O2-C2	3.03	1.57	1.42
2	C	2064	EDO	O2-C2	3.02	1.57	1.42
2	C	2117	EDO	O2-C2	3.00	1.57	1.42
2	B	2062	EDO	O1-C1	3.00	1.57	1.42
2	I	2099	EDO	O1-C1	2.99	1.57	1.42
2	G	2101	EDO	O2-C2	2.96	1.57	1.42
2	E	2089	EDO	O1-C1	2.96	1.57	1.42
2	B	2125	EDO	O2-C2	2.96	1.57	1.42
2	H	2054	EDO	O2-C2	2.96	1.57	1.42
2	B	2013	EDO	O1-C1	2.95	1.57	1.42
2	G	2093	EDO	O1-C1	2.93	1.57	1.42
2	E	2079	EDO	O1-C1	2.92	1.57	1.42
2	I	2100	EDO	O2-C2	2.91	1.56	1.42
2	E	2041	EDO	O1-C1	2.90	1.56	1.42
2	F	2087	EDO	O1-C1	2.89	1.56	1.42
2	I	2045	EDO	O2-C2	2.87	1.56	1.42
2	C	2126	EDO	O1-C1	2.86	1.56	1.42
2	F	2006	EDO	O2-C2	2.83	1.56	1.42
2	I	2051	EDO	O2-C2	2.82	1.56	1.42
2	F	2043	EDO	O1-C1	2.82	1.56	1.42
2	C	2117	EDO	O1-C1	2.81	1.56	1.42
2	A	2001	EDO	O2-C2	2.81	1.56	1.42
2	E	2120	EDO	O2-C2	2.80	1.56	1.42
2	B	2020	EDO	O2-C2	2.77	1.56	1.42
2	I	2103	EDO	O2-C2	2.76	1.56	1.42
2	G	2102	EDO	O1-C1	2.73	1.56	1.42
2	F	2038	EDO	O2-C2	2.73	1.56	1.42
2	J	2049	EDO	O1-C1	2.71	1.55	1.42
2	A	2016	EDO	O1-C1	2.71	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2042	EDO	O2-C2	2.68	1.55	1.42
2	D	2118	EDO	O1-C1	2.68	1.55	1.42
2	C	2036	EDO	O2-C2	2.63	1.55	1.42
2	A	2011	EDO	O1-C1	2.62	1.55	1.42
2	H	2054	EDO	O1-C1	2.60	1.55	1.42
2	J	2110	EDO	O1-C1	2.60	1.55	1.42
2	D	2071	EDO	O1-C1	2.57	1.55	1.42
2	E	2039	EDO	O2-C2	2.57	1.55	1.42
2	E	2042	EDO	O1-C1	2.56	1.55	1.42
2	A	2017	EDO	O2-C2	2.56	1.55	1.42
2	J	2108	EDO	O2-C2	2.55	1.55	1.42
2	G	2101	EDO	O1-C1	2.55	1.55	1.42
2	E	2076	EDO	O1-C1	2.55	1.55	1.42
2	A	2016	EDO	O2-C2	2.55	1.55	1.42
2	D	2073	EDO	O1-C1	2.53	1.55	1.42
2	G	2056	EDO	O1-C1	2.53	1.55	1.42
2	D	2003	EDO	O1-C1	2.53	1.55	1.42
2	D	2073	EDO	O2-C2	2.52	1.54	1.42
2	B	2015	EDO	O2-C2	2.50	1.54	1.42
2	F	2037	EDO	O1-C1	2.50	1.54	1.42
2	B	2018	EDO	O2-C2	2.50	1.54	1.42
2	E	2088	EDO	O2-C2	2.50	1.54	1.42
2	D	2031	EDO	O1-C1	2.49	1.54	1.42
2	E	2127	EDO	O1-C1	2.47	1.54	1.42
2	J	2068	EDO	O1-C1	2.47	1.54	1.42
2	A	2017	EDO	O1-C1	2.47	1.54	1.42
2	C	2081	EDO	O1-C1	2.46	1.54	1.42
2	E	2092	EDO	O1-C1	2.45	1.54	1.42
2	E	2039	EDO	O1-C1	2.43	1.54	1.42
2	F	2086	EDO	O2-C2	2.33	1.54	1.42
2	G	2057	EDO	O1-C1	2.32	1.53	1.42
2	B	2018	EDO	O1-C1	2.29	1.53	1.42
2	D	2072	EDO	O1-C1	2.25	1.53	1.42
2	B	2028	EDO	O1-C1	2.23	1.53	1.42
2	H	2111	EDO	O1-C1	2.23	1.53	1.42
2	D	2033	EDO	O1-C1	2.21	1.53	1.42
2	H	2059	EDO	C2-C1	2.21	1.65	1.48
2	F	2096	EDO	O1-C1	2.20	1.53	1.42
2	C	2075	EDO	O2-C2	2.18	1.53	1.42
2	J	2109	EDO	O2-C2	2.18	1.53	1.42
2	B	2027	EDO	O1-C1	2.18	1.53	1.42
2	I	2107	EDO	O1-C1	2.14	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2023	EDO	O1-C1	2.13	1.53	1.42
2	B	2125	EDO	C2-C1	2.12	1.64	1.48
2	A	2065	EDO	O2-C2	2.12	1.52	1.42
2	E	2092	EDO	O2-C2	2.04	1.52	1.42
2	G	2050	EDO	O1-C1	2.04	1.52	1.42
2	H	2044	EDO	O2-C2	2.03	1.52	1.42
2	H	2111	EDO	C2-C1	2.02	1.64	1.48
2	C	2081	EDO	C2-C1	2.02	1.64	1.48
2	B	2027	EDO	O2-C2	2.01	1.52	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2101	EDO	O2-C2-C1	-2.56	92.91	112.39
2	J	2123	EDO	O2-C2-C1	-2.52	93.21	112.39
2	I	2099	EDO	O2-C2-C1	-2.47	93.54	112.39
2	J	2104	EDO	O2-C2-C1	-2.14	96.06	112.39
2	H	2058	EDO	O2-C2-C1	-2.08	96.52	112.39
2	I	2103	EDO	O1-C1-C2	-2.02	96.97	112.39

There are no chirality outliers.

All (92) 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

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Mol	Chain	Res	Type	Atoms
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
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	2070	EDO	O1-C1-C2-O2
2	B	2013	EDO	O1-C1-C2-O2
2	E	2090	EDO	O1-C1-C2-O2
2	J	2055	EDO	O1-C1-C2-O2
2	C	2085	EDO	O1-C1-C2-O2
2	E	2089	EDO	O1-C1-C2-O2
2	F	2034	EDO	O1-C1-C2-O2
2	F	2037	EDO	O1-C1-C2-O2
2	F	2098	EDO	O1-C1-C2-O2
2	G	2009	EDO	O1-C1-C2-O2
2	I	2045	EDO	O1-C1-C2-O2
2	I	2100	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	2064	EDO	O1-C1-C2-O2
2	C	2075	EDO	O1-C1-C2-O2
2	C	2083	EDO	O1-C1-C2-O2
2	D	2071	EDO	O1-C1-C2-O2
2	D	2072	EDO	O1-C1-C2-O2
2	E	2032	EDO	O1-C1-C2-O2
2	F	2096	EDO	O1-C1-C2-O2
2	I	2051	EDO	O1-C1-C2-O2
2	A	2016	EDO	O1-C1-C2-O2
2	A	2116	EDO	O1-C1-C2-O2
2	C	2036	EDO	O1-C1-C2-O2
2	D	2033	EDO	O1-C1-C2-O2
2	D	2074	EDO	O1-C1-C2-O2
2	E	2079	EDO	O1-C1-C2-O2
2	F	2006	EDO	O1-C1-C2-O2
2	H	2058	EDO	O1-C1-C2-O2
2	I	2052	EDO	O1-C1-C2-O2
2	I	2099	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	J	2069	EDO	O1-C1-C2-O2
2	J	2104	EDO	O1-C1-C2-O2
2	J	2108	EDO	O1-C1-C2-O2
2	J	2123	EDO	O1-C1-C2-O2
2	A	2017	EDO	O1-C1-C2-O2
2	B	2125	EDO	O1-C1-C2-O2
2	C	2067	EDO	O1-C1-C2-O2
2	C	2126	EDO	O1-C1-C2-O2
2	C	2128	EDO	O1-C1-C2-O2
2	D	2003	EDO	O1-C1-C2-O2
2	D	2119	EDO	O1-C1-C2-O2
2	E	2088	EDO	O1-C1-C2-O2
2	E	2092	EDO	O1-C1-C2-O2
2	F	2086	EDO	O1-C1-C2-O2
2	F	2094	EDO	O1-C1-C2-O2
2	F	2097	EDO	O1-C1-C2-O2
2	G	2057	EDO	O1-C1-C2-O2
2	H	2010	EDO	O1-C1-C2-O2
2	J	2048	EDO	O1-C1-C2-O2
2	J	2061	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	B	2028	EDO	O1-C1-C2-O2
2	C	2026	EDO	O1-C1-C2-O2
2	C	2080	EDO	O1-C1-C2-O2
2	D	2118	EDO	O1-C1-C2-O2
2	E	2120	EDO	O1-C1-C2-O2
2	G	2056	EDO	O1-C1-C2-O2
2	B	2021	EDO	O1-C1-C2-O2
2	D	2073	EDO	O1-C1-C2-O2
2	J	2106	EDO	O1-C1-C2-O2

There are no ring outliers.

107 monomers are involved in 504 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2109	EDO	14	0
2	I	2115	EDO	7	0
2	G	2009	EDO	4	0
2	I	2046	EDO	4	0
2	J	2123	EDO	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2082	EDO	2	0
2	A	2012	EDO	11	0
2	F	2038	EDO	4	0
2	I	2107	EDO	11	0
2	H	2111	EDO	3	0
2	H	2060	EDO	4	0
2	G	2112	EDO	3	0
2	E	2076	EDO	7	0
2	A	2029	EDO	7	0
2	F	2006	EDO	3	0
2	A	2065	EDO	5	0
2	E	2092	EDO	1	0
2	G	2050	EDO	5	0
2	A	2122	EDO	4	0
2	C	2085	EDO	10	0
2	J	2008	EDO	6	0
2	A	2011	EDO	1	0
2	G	2093	EDO	6	0
2	C	2004	EDO	11	0
2	A	2017	EDO	2	0
2	J	2110	EDO	3	0
2	B	2018	EDO	1	0
2	E	2088	EDO	2	0
2	E	2120	EDO	6	0
2	G	2047	EDO	2	0
2	F	2098	EDO	2	0
2	J	2104	EDO	14	0
2	D	2003	EDO	4	0
2	J	2014	EDO	3	0
2	I	2045	EDO	2	0
2	J	2055	EDO	2	0
2	B	2025	EDO	2	0
2	B	2028	EDO	10	0
2	I	2099	EDO	3	0
2	I	2103	EDO	4	0
2	G	2056	EDO	7	0
2	H	2113	EDO	4	0
2	E	2089	EDO	4	0
2	C	2075	EDO	7	0
2	I	2007	EDO	5	0
2	B	2020	EDO	2	0
2	J	2068	EDO	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2049	EDO	10	0
2	E	2039	EDO	2	0
2	F	2043	EDO	13	0
2	B	2030	EDO	10	0
2	B	2021	EDO	4	0
2	J	2061	EDO	2	0
2	D	2118	EDO	7	0
2	H	2058	EDO	11	0
2	F	2097	EDO	5	0
2	F	2095	EDO	2	0
2	E	2077	EDO	1	0
2	A	2124	EDO	7	0
2	H	2059	EDO	2	0
2	B	2002	EDO	6	0
2	E	2079	EDO	2	0
2	H	2054	EDO	1	0
2	E	2090	EDO	5	0
2	C	2067	EDO	4	0
2	I	2100	EDO	2	0
2	J	2053	EDO	3	0
2	B	2125	EDO	8	0
2	E	2005	EDO	5	0
2	I	2121	EDO	11	0
2	C	2126	EDO	6	0
2	C	2084	EDO	1	0
2	H	2010	EDO	9	0
2	D	2035	EDO	13	0
2	C	2036	EDO	1	0
2	D	2074	EDO	2	0
2	G	2057	EDO	7	0
2	A	2001	EDO	6	0
2	J	2106	EDO	2	0
2	J	2108	EDO	3	0
2	G	2102	EDO	3	0
2	B	2023	EDO	3	0
2	C	2128	EDO	8	0
2	H	2114	EDO	0	1
2	D	2031	EDO	4	0
2	A	2066	EDO	1	0
2	A	2063	EDO	7	0
2	C	2064	EDO	2	0
2	F	2086	EDO	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2040	EDO	1	0
2	C	2024	EDO	12	0
2	H	2044	EDO	4	0
2	C	2080	EDO	2	0
2	J	2105	EDO	5	0
2	F	2034	EDO	5	0
2	D	2072	EDO	3	0
2	A	2022	EDO	3	0
2	E	2127	EDO	9	0
2	E	2091	EDO	5	0
2	E	2032	EDO	3	0
2	F	2087	EDO	2	0
2	A	2116	EDO	1	0
2	E	2042	EDO	2	0
2	C	2117	EDO	3	0
2	I	2051	EDO	6	0
2	D	2119	EDO	2	0
2	E	2078	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.