



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 04:17 AM UTC

PDB ID : 3FA3 / pdb\_00003fa3  
Title : Crystal structure of 2,3-dimethylmalate lyase, a PEP mutase/isocitrate lyase superfamily member, trigonal crystal form  
Authors : Narayanan, B.C.; Herzberg, O.  
Deposited on : 2008-11-14  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

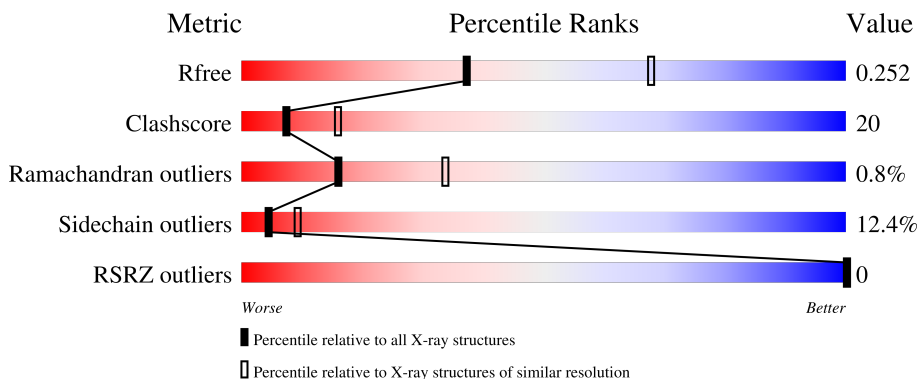
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	
1	B	302	
1	C	302	
1	D	302	
1	E	302	

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Mol	Chain	Length	Quality of chain		
1	F	302	61%	31%	8%
1	G	302	63%	31%	5%
1	H	302	59%	36%	• •
1	I	302	58%	35%	6% •
1	J	302	57%	33%	7% •
1	K	302	58%	35%	6% •
1	L	302	51%	40%	8% •
1	M	302	55%	39%	6% •
1	N	302	54%	36%	6% • •
1	O	302	56%	38%	5% •
1	P	302	50%	42%	7% •

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
4	GOL	G	601	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36360 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.

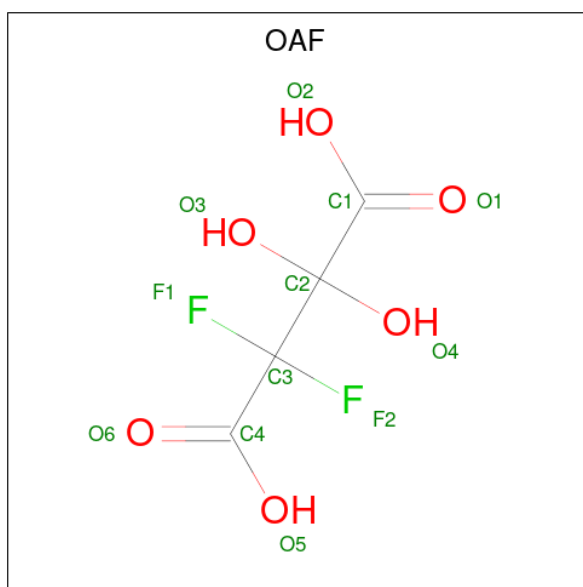
- Molecule 1 is a protein called 2,3-dimethylmalate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2222	1379	397	430	16	0	0	0
1	B	302	2230	1384	399	431	16	0	0	0
1	C	301	2228	1384	398	430	16	0	0	0
1	D	301	2226	1384	398	428	16	0	0	0
1	E	301	2228	1384	398	430	16	0	0	0
1	F	301	2224	1381	397	430	16	0	0	0
1	G	301	2228	1384	398	430	16	0	0	0
1	H	301	2228	1384	398	430	16	0	0	0
1	I	300	2216	1376	397	427	16	0	0	0
1	J	292	2162	1344	383	420	15	0	0	0
1	K	300	2218	1376	397	429	16	0	0	0
1	L	300	2215	1375	396	428	16	0	0	0
1	M	300	2220	1378	397	429	16	0	0	0
1	N	292	2161	1342	383	421	15	0	0	0
1	O	301	2211	1374	397	424	16	0	0	0
1	P	301	2225	1381	398	430	16	0	0	0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

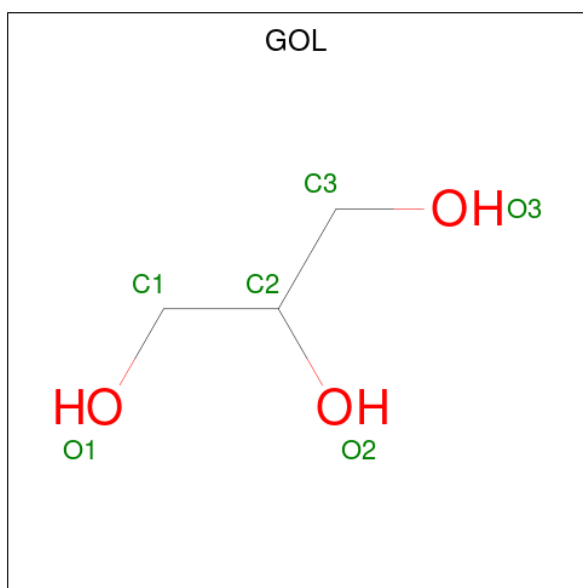
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	E	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0
2	G	1	Total 1	Mn 1	0	0
2	H	1	Total 1	Mn 1	0	0
2	I	1	Total 1	Mn 1	0	0
2	J	1	Total 1	Mn 1	0	0
2	K	1	Total 1	Mn 1	0	0
2	L	1	Total 1	Mn 1	0	0
2	M	1	Total 1	Mn 1	0	0
2	N	1	Total 1	Mn 1	0	0
2	O	1	Total 1	Mn 1	0	0
2	P	1	Total 1	Mn 1	0	0

- Molecule 3 is 2,2-difluoro-3,3-dihydroxybutanedioic acid (CCD ID: OAF) (formula: C<sub>4</sub>H<sub>4</sub>F<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	F			O
3	A	1	12	4	2	6	0	0
3	B	1	12	4	2	6	0	0
3	C	1	12	4	2	6	0	0
3	D	1	12	4	2	6	0	0
3	E	1	12	4	2	6	0	0
3	F	1	12	4	2	6	0	0
3	G	1	12	4	2	6	0	0
3	H	1	12	4	2	6	0	0
3	I	1	12	4	2	6	0	0
3	K	1	12	4	2	6	0	0
3	L	1	12	4	2	6	0	0
3	M	1	12	4	2	6	0	0
3	O	1	12	4	2	6	0	0
3	P	1	12	4	2	6	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	0	0
5	B	59	Total O 59 59	0	0
5	C	52	Total O 52 52	0	0
5	D	57	Total O 57 57	0	0
5	E	65	Total O 65 65	0	0
5	F	55	Total O 55 55	0	0

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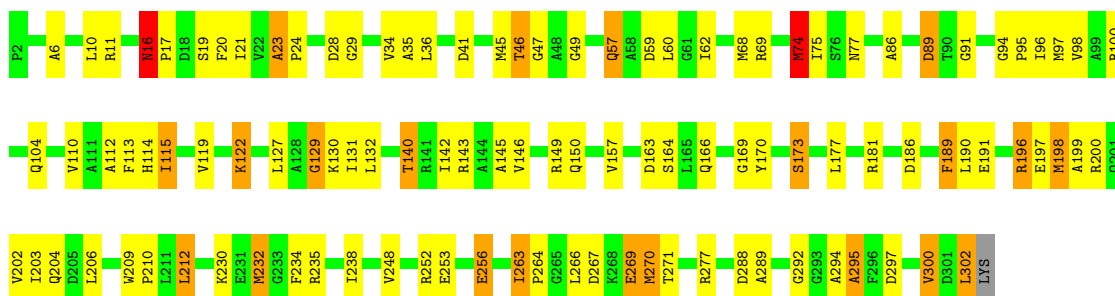
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	G	66	Total O 66 66	0	0
5	H	68	Total O 68 68	0	0
5	I	29	Total O 29 29	0	0
5	J	29	Total O 29 29	0	0
5	K	27	Total O 27 27	0	0
5	L	24	Total O 24 24	0	0
5	M	38	Total O 38 38	0	0
5	N	28	Total O 28 28	0	0
5	O	24	Total O 24 24	0	0
5	P	24	Total O 24 24	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

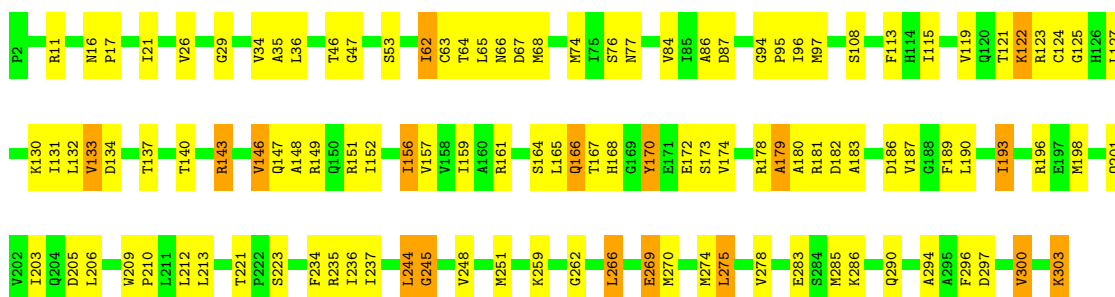
- Molecule 1: 2,3-dimethylmalate lyase

Chain A: 



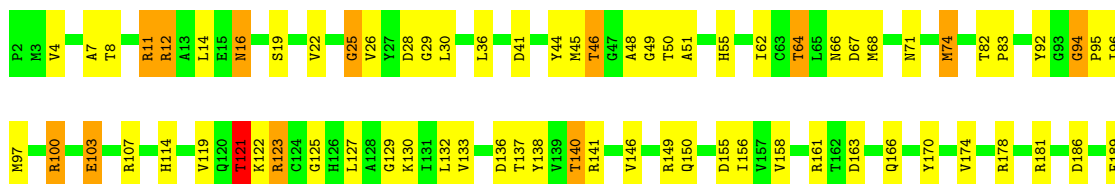
- Molecule 1: 2,3-dimethylmalate lyase

Chain B: 



- Molecule 1: 2,3-dimethylmalate lyase

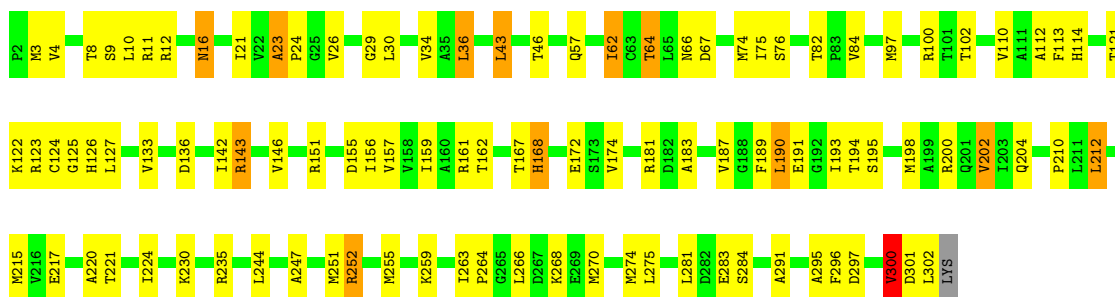
Chain C: 





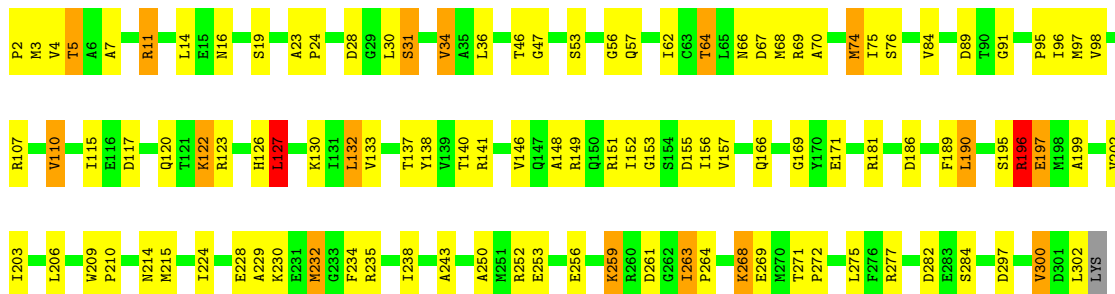
- Molecule 1: 2,3-dimethylmalate lyase

Chain D: 66% 30%



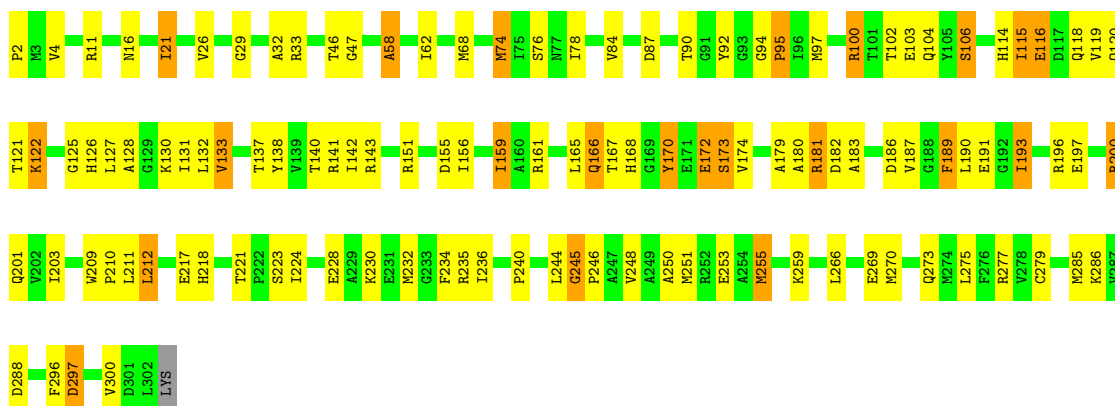
- Molecule 1: 2,3-dimethylmalate lyase

Chain E: 64% 30% 5%



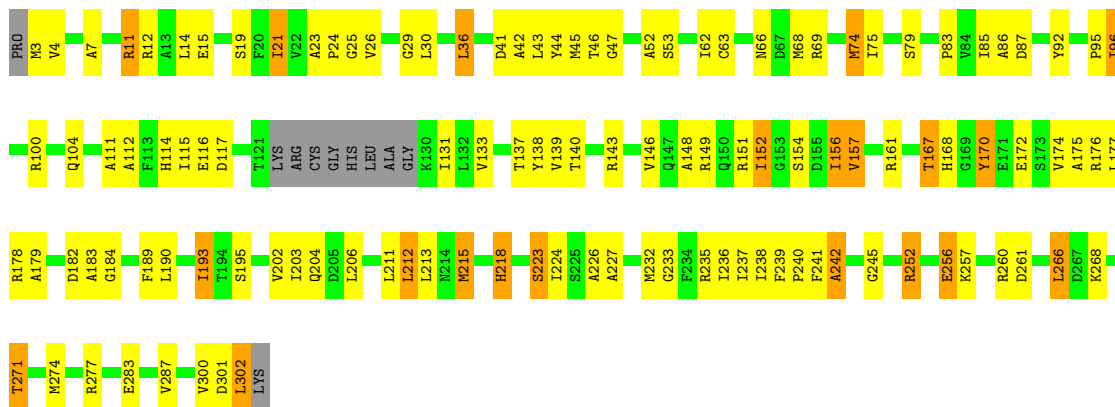
- Molecule 1: 2,3-dimethylmalate lyase

Chain F: 61% 31% 8%



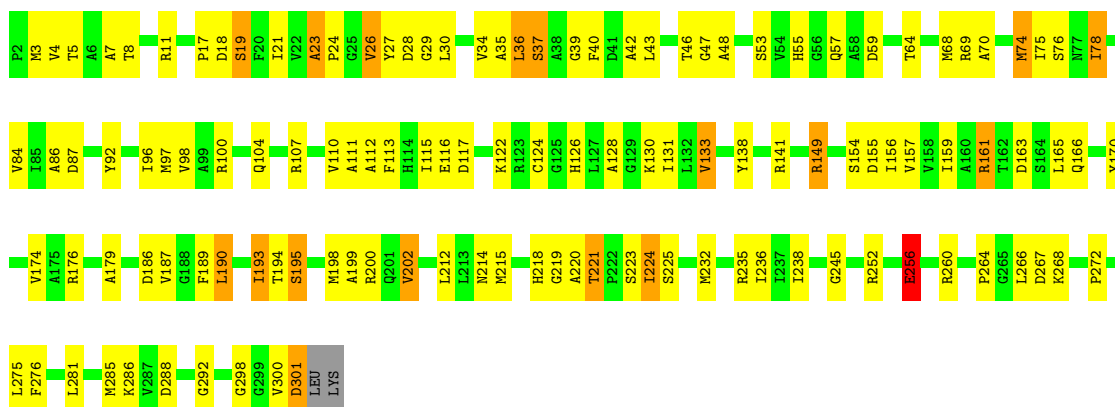
- Molecule 1: 2,3-dimethylmalate lyase





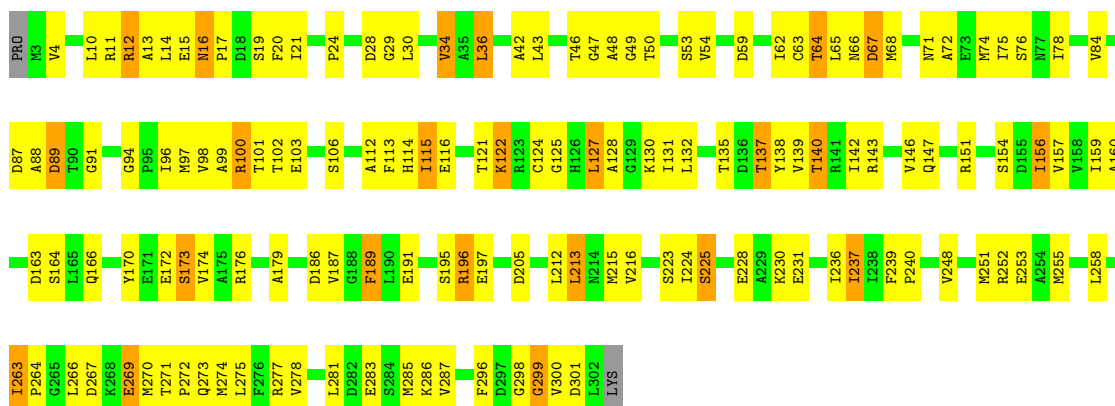
- Molecule 1: 2,3-dimethylmalate lyase

Chain K: 58% 35% 6%



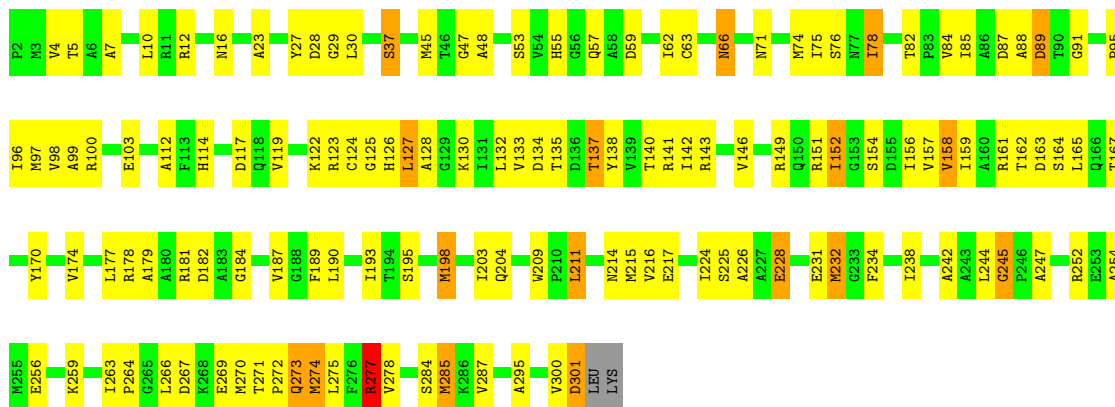
- Molecule 1: 2,3-dimethylmalate lyase

Chain L: 51% 40% 8%



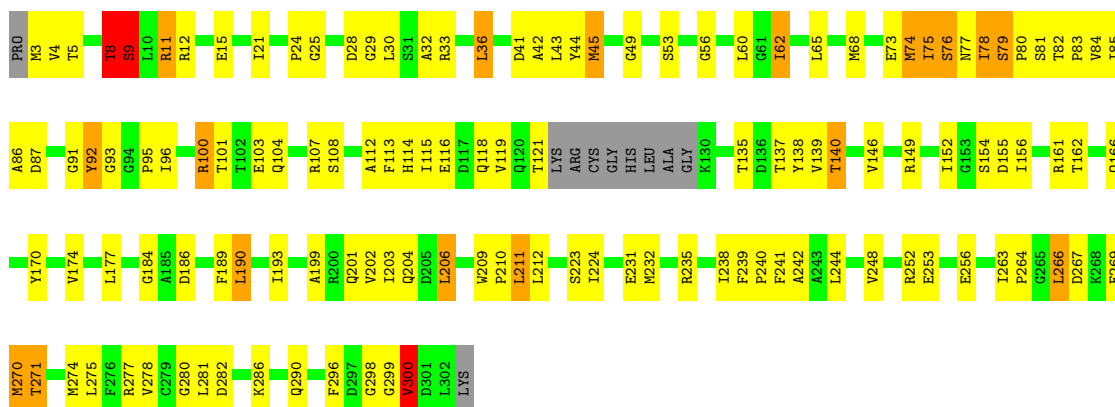
- Molecule 1: 2,3-dimethylmalate lyase

Chain M: 55% 39% 6%



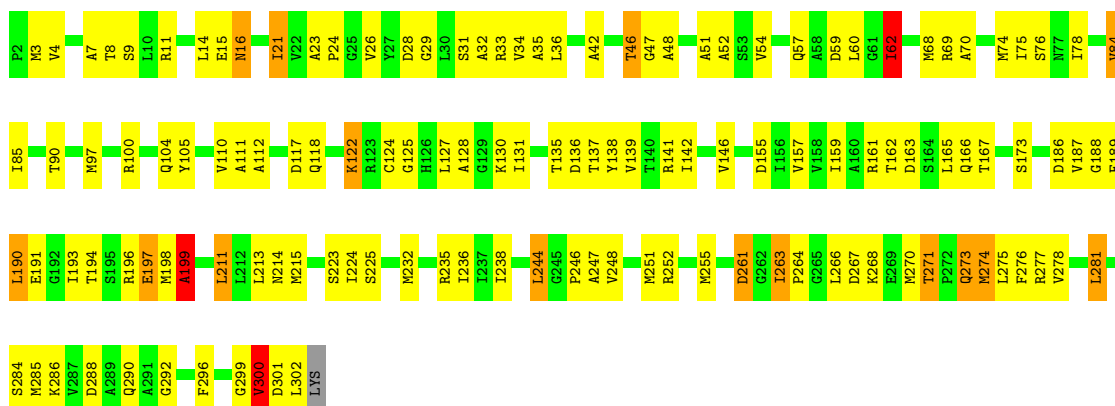
- Molecule 1: 2,3-dimethylmalate lyase

Chain N: 54% 36% 6% ..



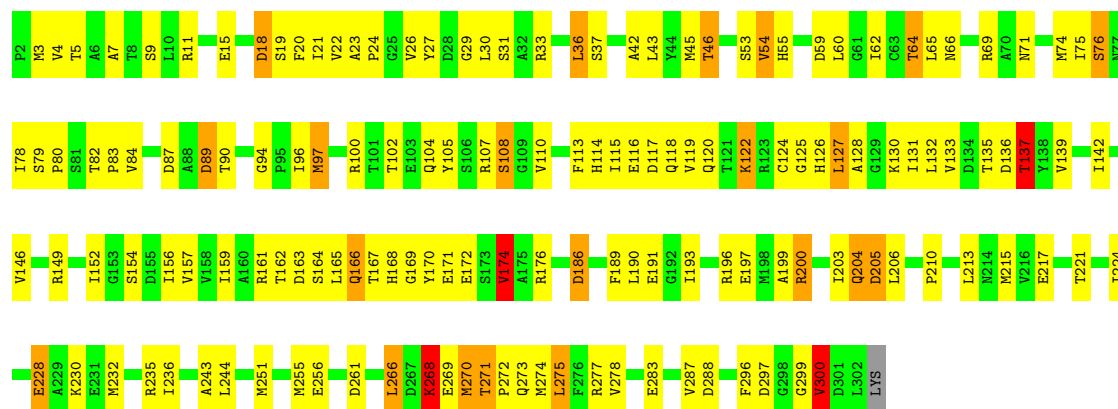
- Molecule 1: 2,3-dimethylmalate lyase

Chain O: 56% 38% 5% .



- Molecule 1: 2,3-dimethylmalate lyase

Chain P: 50% 42% 7% .



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.57Å 160.57Å 161.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.60) 94.3 (50.00-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.255 0.190 , 0.252	Depositor DCC
$R_{free}$ test set	6752 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 22.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.447 for -h,-k,l 0.084 for h,-h-k,-l 0.083 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	36360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5454e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OAF, GOL, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.38	7/2255 (0.3%)	1.42	13/3053 (0.4%)
1	B	1.32	3/2263 (0.1%)	1.32	5/3063 (0.2%)
1	C	1.41	7/2261 (0.3%)	1.38	17/3060 (0.6%)
1	D	1.38	6/2259 (0.3%)	1.40	11/3057 (0.4%)
1	E	1.39	5/2261 (0.2%)	1.37	12/3060 (0.4%)
1	F	1.26	6/2257 (0.3%)	1.37	14/3056 (0.5%)
1	G	1.38	9/2261 (0.4%)	1.36	13/3060 (0.4%)
1	H	1.40	6/2261 (0.3%)	1.39	19/3060 (0.6%)
1	I	1.25	3/2249 (0.1%)	1.34	10/3044 (0.3%)
1	J	1.18	2/2192 (0.1%)	1.34	7/2967 (0.2%)
1	K	1.18	2/2251 (0.1%)	1.34	17/3046 (0.6%)
1	L	1.14	0/2247	1.26	10/3041 (0.3%)
1	M	1.17	4/2253 (0.2%)	1.36	16/3049 (0.5%)
1	N	1.21	2/2191 (0.1%)	1.31	5/2966 (0.2%)
1	O	1.21	5/2244 (0.2%)	1.31	15/3039 (0.5%)
1	P	1.17	4/2258 (0.2%)	1.29	14/3056 (0.5%)
All	All	1.28	71/35963 (0.2%)	1.35	198/48677 (0.4%)

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	300	VAL	CA-CB	-9.99	1.44	1.54
1	D	283	GLU	CG-CD	-9.45	1.28	1.52
1	E	196	ARG	C-N	-7.74	1.23	1.33
1	E	4	VAL	CA-CB	7.74	1.66	1.54
1	C	158	VAL	CA-CB	7.69	1.62	1.53
1	I	156	ILE	CA-CB	6.96	1.61	1.54
1	F	142	ILE	CA-CB	6.91	1.62	1.54
1	A	35	ALA	CA-CB	-6.77	1.42	1.53
1	D	296	PHE	C-N	6.68	1.43	1.33
1	P	300	VAL	CA-CB	-6.67	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	294	ALA	CA-CB	-6.60	1.43	1.53
1	J	4	VAL	CA-CB	6.57	1.62	1.55
1	B	62	ILE	CA-CB	6.51	1.62	1.54
1	C	4	VAL	CA-CB	6.36	1.65	1.54
1	F	128	ALA	CA-CB	-6.28	1.42	1.53
1	P	18	ASP	C-N	6.27	1.41	1.33
1	G	72	ALA	CA-CB	-6.22	1.43	1.53
1	F	159	ILE	CA-CB	6.17	1.61	1.54
1	K	193	ILE	CA-CB	6.17	1.61	1.54
1	G	127	LEU	CA-C	-6.11	1.45	1.52
1	O	159	ILE	CA-CB	6.07	1.62	1.54
1	G	202	VAL	CA-CB	6.03	1.61	1.54
1	E	148	ALA	CA-CB	-6.02	1.44	1.53
1	C	25	GLY	C-O	-5.97	1.19	1.24
1	B	152	ILE	CA-CB	5.96	1.61	1.54
1	H	12	ARG	CA-C	5.83	1.60	1.52
1	C	71	ASN	N-CA	-5.79	1.39	1.46
1	N	75	ILE	CA-CB	5.72	1.60	1.54
1	G	4	VAL	CA-CB	5.71	1.65	1.55
1	J	157	VAL	CA-CB	5.68	1.60	1.53
1	K	23	ALA	CA-CB	-5.62	1.46	1.53
1	D	295	ALA	CA-CB	-5.61	1.44	1.53
1	D	259	LYS	CA-C	5.54	1.59	1.52
1	F	240	PRO	CA-C	5.53	1.60	1.52
1	A	129	GLY	C-O	-5.53	1.17	1.24
1	G	30	LEU	C-O	-5.49	1.17	1.24
1	P	23	ALA	CA-C	5.38	1.59	1.52
1	G	28	ASP	C-O	-5.37	1.17	1.24
1	O	4	VAL	CA-CB	5.36	1.60	1.53
1	C	296	PHE	CA-C	-5.34	1.46	1.53
1	A	89	ASP	CA-C	5.32	1.59	1.52
1	I	294	ALA	CA-CB	-5.31	1.44	1.52
1	A	21	ILE	C-O	5.30	1.30	1.24
1	P	261	ASP	C-O	-5.28	1.19	1.23
1	M	254	ALA	CA-CB	-5.27	1.44	1.53
1	C	50	THR	CA-C	5.26	1.59	1.52
1	G	237	ILE	CA-CB	5.26	1.61	1.54
1	H	123	ARG	C-O	-5.24	1.17	1.23
1	O	193	ILE	CA-CB	5.23	1.61	1.54
1	H	44	TYR	N-CA	-5.22	1.40	1.46
1	I	102	THR	CA-CB	-5.22	1.45	1.53
1	A	131	ILE	CA-CB	-5.20	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	32	ALA	CA-CB	-5.18	1.45	1.53
1	D	23	ALA	CA-CB	-5.17	1.46	1.53
1	M	55	HIS	CA-C	-5.16	1.45	1.52
1	H	215	MET	CA-C	-5.13	1.47	1.53
1	F	180	ALA	CA-C	5.12	1.59	1.52
1	E	197	GLU	CA-C	5.11	1.59	1.52
1	M	174	VAL	CA-CB	5.10	1.60	1.54
1	G	121	THR	CA-C	-5.09	1.47	1.53
1	D	26	VAL	CA-C	5.08	1.58	1.52
1	O	128	ALA	CA-CB	-5.08	1.45	1.53
1	A	295	ALA	CA-CB	-5.07	1.45	1.53
1	H	237	ILE	CA-C	5.06	1.58	1.52
1	B	245	GLY	N-CA	5.06	1.51	1.44
1	G	156	ILE	CA-CB	5.05	1.61	1.54
1	O	271	THR	CA-CB	5.04	1.61	1.53
1	E	195	SER	C-N	-5.04	1.26	1.33
1	M	135	THR	CA-CB	5.03	1.61	1.53
1	F	200	ARG	CG-CD	5.03	1.67	1.52
1	A	6	ALA	CA-CB	-5.02	1.44	1.53

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	300	VAL	N-CA-C	-9.37	104.01	113.10
1	A	263	ILE	CA-C-N	9.31	128.92	119.24
1	A	263	ILE	C-N-CA	9.31	128.92	119.24
1	I	271	THR	CA-C-N	8.59	129.12	119.32
1	I	271	THR	C-N-CA	8.59	129.12	119.32
1	C	291	ALA	N-CA-C	8.38	123.62	113.23
1	M	89	ASP	CB-CA-C	-7.95	107.40	116.63
1	E	169	GLY	N-CA-C	7.85	121.98	112.48
1	C	25	GLY	N-CA-C	7.71	123.00	110.97
1	J	167	THR	CB-CA-C	-7.56	98.19	110.74
1	O	54	VAL	CB-CA-C	-7.37	102.19	112.14
1	H	202	VAL	CB-CA-C	-7.37	100.15	112.16
1	N	62	ILE	N-CA-C	-7.37	105.95	113.10
1	J	170	TYR	N-CA-C	7.34	119.92	111.11
1	L	16	ASN	CA-C-N	7.05	126.67	119.19
1	L	16	ASN	C-N-CA	7.05	126.67	119.19
1	P	271	THR	CA-C-N	-6.95	111.40	119.32
1	P	271	THR	C-N-CA	-6.95	111.40	119.32
1	P	94	GLY	CA-C-N	6.94	128.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	94	GLY	C-N-CA	6.94	128.51	119.84
1	D	296	PHE	O-C-N	6.93	130.58	122.19
1	H	143	ARG	N-CA-C	-6.92	103.74	111.28
1	K	55	HIS	N-CA-C	6.90	122.80	113.97
1	H	114	HIS	N-CA-C	6.84	119.62	108.26
1	F	245	GLY	CA-C-N	6.83	127.11	119.32
1	F	245	GLY	C-N-CA	6.83	127.11	119.32
1	H	298	GLY	N-CA-C	-6.82	106.28	113.58
1	O	199	ALA	CA-C-N	6.76	129.23	120.44
1	O	199	ALA	C-N-CA	6.76	129.23	120.44
1	L	114	HIS	N-CA-C	6.75	119.41	108.34
1	F	230	LYS	N-CA-C	-6.74	103.02	111.11
1	E	53	SER	N-CA-C	6.72	118.39	111.14
1	F	138	TYR	N-CA-C	6.71	118.39	111.14
1	D	168	HIS	N-CA-C	6.70	121.16	112.92
1	M	16	ASN	CA-C-N	6.63	128.13	119.84
1	M	16	ASN	C-N-CA	6.63	128.13	119.84
1	K	98	VAL	N-CA-C	-6.61	103.88	110.62
1	L	287	VAL	N-CA-C	6.58	117.34	110.62
1	D	230	LYS	N-CA-C	-6.57	103.22	111.11
1	M	216	VAL	CB-CA-C	-6.57	102.77	110.91
1	O	62	ILE	N-CA-C	-6.54	106.42	112.96
1	E	230	LYS	N-CA-C	-6.52	104.09	111.07
1	L	15	GLU	N-CA-C	-6.49	105.00	113.12
1	I	230	LYS	N-CA-C	-6.47	104.23	111.28
1	D	16	ASN	CA-C-N	-6.41	113.00	120.12
1	D	16	ASN	C-N-CA	-6.41	113.00	120.12
1	C	114	HIS	N-CA-C	6.40	119.58	108.76
1	L	94	GLY	CA-C-N	6.37	127.81	119.84
1	L	94	GLY	C-N-CA	6.37	127.81	119.84
1	J	252	ARG	N-CA-C	-6.32	104.31	111.07
1	K	256	GLU	CA-C-N	6.28	128.70	120.28
1	K	256	GLU	C-N-CA	6.28	128.70	120.28
1	K	224	ILE	N-CA-C	6.23	116.84	107.75
1	K	221	THR	CA-C-N	-6.19	113.90	120.03
1	K	221	THR	C-N-CA	-6.19	113.90	120.03
1	K	4	VAL	N-CA-C	6.12	118.26	109.51
1	O	51	ALA	N-CA-C	-6.11	103.78	111.11
1	C	121	THR	N-CA-C	-6.10	102.97	110.65
1	K	199	ALA	N-CA-C	-6.06	104.59	111.14
1	H	168	HIS	N-CA-C	6.06	120.81	113.17
1	C	239	PHE	CA-C-N	6.05	127.41	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	PHE	C-N-CA	6.05	127.41	119.84
1	D	202	VAL	CB-CA-C	-6.05	104.13	112.24
1	B	146	VAL	N-CA-C	6.05	116.23	110.42
1	P	33	ARG	CA-C-N	6.02	128.15	120.56
1	P	33	ARG	C-N-CA	6.02	128.15	120.56
1	K	292	GLY	N-CA-C	-6.00	106.75	114.85
1	C	82	THR	CA-C-N	-6.00	113.76	119.76
1	C	82	THR	C-N-CA	-6.00	113.76	119.76
1	P	169	GLY	N-CA-C	6.00	117.65	111.95
1	H	230	LYS	N-CA-C	-5.97	104.68	111.07
1	M	277	ARG	N-CA-CB	5.96	118.61	109.91
1	M	245	GLY	CA-C-N	5.96	125.83	119.28
1	M	245	GLY	C-N-CA	5.96	125.83	119.28
1	I	16	ASN	CA-C-N	5.93	127.26	119.84
1	I	16	ASN	C-N-CA	5.93	127.26	119.84
1	D	136	ASP	N-CA-C	5.93	117.42	111.07
1	K	87	ASP	N-CA-C	-5.92	102.15	110.50
1	A	16	ASN	CB-CA-C	5.92	116.96	110.15
1	G	6	ALA	N-CA-C	-5.92	106.02	113.18
1	I	105	TYR	N-CA-C	-5.91	104.92	111.36
1	G	98	VAL	N-CA-C	-5.90	104.16	110.36
1	F	114	HIS	N-CA-C	5.89	118.99	109.40
1	M	247	ALA	N-CA-C	-5.86	104.81	111.14
1	O	84	VAL	N-CA-C	5.86	116.32	108.11
1	G	127	LEU	N-CA-C	-5.82	99.17	109.06
1	C	238	ILE	CA-C-N	5.80	128.88	122.74
1	C	238	ILE	C-N-CA	5.80	128.88	122.74
1	A	169	GLY	N-CA-C	5.79	119.97	112.68
1	F	170	TYR	N-CA-C	5.77	117.25	111.07
1	J	74	MET	N-CA-C	-5.74	105.11	111.36
1	F	180	ALA	N-CA-C	5.71	117.51	111.28
1	P	186	ASP	N-CA-C	5.68	118.68	111.69
1	E	127	LEU	N-CA-C	5.67	118.81	110.59
1	H	94	GLY	CA-C-N	5.65	125.11	119.24
1	H	94	GLY	C-N-CA	5.65	125.11	119.24
1	P	152	ILE	N-CA-C	5.64	120.16	113.22
1	I	103	GLU	N-CA-C	-5.63	104.83	110.97
1	E	110	VAL	N-CA-C	5.62	116.96	109.37
1	M	256	GLU	N-CA-CB	5.61	118.30	109.94
1	K	18	ASP	N-CA-C	5.60	119.29	112.23
1	H	136	ASP	N-CA-C	5.60	117.83	111.11
1	H	245	GLY	CA-C-N	5.59	125.44	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	245	GLY	C-N-CA	5.59	125.44	119.28
1	O	211	LEU	N-CA-C	5.59	118.81	110.14
1	C	11	ARG	N-CA-C	-5.58	105.28	111.36
1	F	115	ILE	N-CA-C	5.58	115.98	108.17
1	N	93	GLY	N-CA-C	-5.57	102.66	110.63
1	A	110	VAL	N-CA-C	5.57	116.60	109.30
1	O	263	ILE	CA-C-N	-5.57	112.78	118.85
1	O	263	ILE	C-N-CA	-5.57	112.78	118.85
1	P	221	THR	CA-C-N	-5.57	114.03	119.76
1	P	221	THR	C-N-CA	-5.57	114.03	119.76
1	H	21	ILE	N-CA-C	5.53	116.06	107.99
1	E	126	HIS	N-CA-C	5.52	119.72	113.15
1	J	223	SER	N-CA-C	5.52	117.22	108.67
1	E	152	ILE	N-CA-C	5.51	117.47	112.29
1	M	119	VAL	N-CA-C	-5.47	101.88	110.09
1	D	259	LYS	N-CA-C	5.46	117.69	111.02
1	I	62	ILE	CB-CA-C	-5.46	103.41	112.26
1	K	245	GLY	CA-C-N	5.44	124.90	119.24
1	K	245	GLY	C-N-CA	5.44	124.90	119.24
1	C	103	GLU	N-CA-C	-5.44	105.00	111.69
1	E	133	VAL	N-CA-C	-5.40	100.57	108.99
1	E	261	ASP	N-CA-C	5.39	117.24	111.36
1	O	21	ILE	N-CA-C	5.39	116.14	107.73
1	J	195	SER	N-CA-C	5.38	116.71	108.52
1	F	121	THR	CB-CA-C	-5.38	103.74	111.91
1	F	255	MET	N-CA-C	5.37	117.13	111.28
1	B	262	GLY	N-CA-C	-5.37	107.38	115.32
1	A	114	HIS	N-CA-C	5.36	117.70	109.07
1	K	128	ALA	N-CA-C	5.36	118.21	110.28
1	C	48	ALA	CA-C-N	5.36	125.92	119.98
1	C	48	ALA	C-N-CA	5.36	125.92	119.98
1	G	121	THR	CB-CA-C	-5.35	104.33	111.88
1	E	137	THR	N-CA-C	-5.34	105.54	111.36
1	M	152	ILE	N-CA-C	5.33	117.30	112.29
1	K	163	ASP	N-CA-C	-5.33	106.56	113.16
1	C	132	LEU	N-CA-C	5.32	118.38	110.14
1	L	195	SER	N-CA-C	5.32	116.88	108.96
1	H	16	ASN	CA-C-N	5.31	126.48	119.84
1	H	16	ASN	C-N-CA	5.31	126.48	119.84
1	O	162	THR	N-CA-C	5.30	118.09	109.24
1	N	60	LEU	N-CA-C	5.29	118.86	111.56
1	D	82	THR	N-CA-C	-5.29	102.98	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	197	GLU	N-CA-C	5.28	117.04	111.28
1	A	163	ASP	N-CA-C	-5.28	106.07	112.88
1	M	285	MET	N-CA-C	5.28	117.78	111.71
1	G	202	VAL	CB-CA-C	-5.27	105.13	111.88
1	H	301	ASP	N-CA-C	5.27	118.75	109.80
1	C	94	GLY	CA-C-N	5.26	124.44	118.97
1	C	94	GLY	C-N-CA	5.26	124.44	118.97
1	J	21	ILE	N-CA-C	5.25	116.27	108.23
1	O	163	ASP	N-CA-C	-5.25	106.47	112.92
1	O	292	GLY	N-CA-C	-5.24	108.09	115.32
1	L	163	ASP	N-CA-C	-5.24	106.20	112.59
1	M	103	GLU	N-CA-C	-5.23	105.66	111.36
1	M	170	TYR	N-CA-C	5.22	116.66	111.07
1	G	219	GLY	N-CA-C	-5.21	100.84	113.18
1	N	21	ILE	N-CA-C	5.21	115.35	107.80
1	H	8	THR	N-CA-C	-5.21	105.50	111.07
1	H	113	PHE	N-CA-C	5.20	116.71	108.96
1	A	198	MET	N-CA-C	-5.20	105.50	111.07
1	F	181	ARG	N-CA-C	-5.19	105.62	111.28
1	B	170	TYR	N-CA-C	5.17	116.61	111.07
1	A	119	VAL	N-CA-C	-5.17	98.58	109.34
1	A	74	MET	N-CA-C	-5.17	105.73	111.36
1	H	74	MET	N-CA-C	-5.16	105.73	112.23
1	H	78	ILE	CB-CA-C	5.15	118.30	111.70
1	D	195	SER	N-CA-C	5.14	116.34	108.52
1	B	63	CYS	N-CA-C	5.14	117.80	110.24
1	P	174	VAL	N-CA-C	-5.14	105.53	110.72
1	I	274	MET	N-CA-C	-5.13	105.87	111.82
1	B	156	ILE	N-CA-C	5.12	116.01	109.30
1	M	232	MET	N-CA-C	-5.12	106.29	112.54
1	M	37	SER	N-CA-C	-5.12	106.99	113.18
1	I	209	TRP	N-CA-C	-5.11	98.51	109.81
1	F	102	THR	N-CA-C	-5.11	105.62	111.14
1	F	116	GLU	N-CA-C	5.09	117.85	110.17
1	K	57	GLN	N-CA-C	5.08	116.03	108.86
1	O	85	ILE	CB-CA-C	-5.08	104.02	110.98
1	E	215	MET	N-CA-C	5.07	117.45	109.39
1	G	94	GLY	CA-C-N	5.07	124.51	119.24
1	G	94	GLY	C-N-CA	5.07	124.51	119.24
1	D	174	VAL	CB-CA-C	-5.06	105.24	112.22
1	P	137	THR	N-CA-C	-5.05	105.66	111.07
1	E	256	GLU	N-CA-C	-5.05	105.48	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	195	SER	N-CA-C	5.05	116.52	108.79
1	A	23	ALA	CA-C-N	5.04	124.81	119.76
1	A	23	ALA	C-N-CA	5.04	124.81	119.76
1	G	275	LEU	CD1-CG-CD2	-5.04	99.72	110.80
1	L	137	THR	N-CA-C	-5.03	105.69	111.07
1	A	96	ILE	N-CA-C	-5.03	105.60	110.42
1	P	114	HIS	N-CA-C	5.02	117.25	108.76
1	O	278	VAL	N-CA-CB	5.02	116.08	110.51
1	G	245	GLY	CA-C-N	5.01	124.62	119.05
1	G	245	GLY	C-N-CA	5.01	124.62	119.05
1	F	58	ALA	N-CA-C	5.01	116.57	110.41

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2222	0	2206	91	0
1	B	2230	0	2217	98	0
1	C	2228	0	2224	103	0
1	D	2226	0	2224	79	0
1	E	2228	0	2224	82	0
1	F	2224	0	2213	96	0
1	G	2228	0	2224	85	0
1	H	2228	0	2224	79	0
1	I	2216	0	2209	105	0
1	J	2162	0	2150	95	0
1	K	2218	0	2206	89	0
1	L	2215	0	2203	127	0
1	M	2220	0	2213	115	0
1	N	2161	0	2146	116	0
1	O	2211	0	2196	115	0
1	P	2225	0	2215	147	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	12	0	1	0	0
3	B	12	0	1	0	0
3	C	12	0	1	0	0
3	D	12	0	1	2	0
3	E	12	0	1	0	0
3	F	12	0	1	1	0
3	G	12	0	1	0	0
3	H	12	0	1	1	0
3	I	12	0	1	2	0
3	K	12	0	1	1	0
3	L	12	0	1	1	0
3	M	12	0	1	1	0
3	O	12	0	1	1	0
3	P	12	0	1	1	0
4	A	12	0	16	6	0
4	E	6	0	8	0	0
4	G	6	0	8	2	0
4	M	6	0	8	1	0
5	A	59	0	0	4	0
5	B	59	0	0	3	0
5	C	52	0	0	7	0
5	D	57	0	0	4	0
5	E	65	0	0	7	0
5	F	55	0	0	3	0
5	G	66	0	0	5	0
5	H	68	0	0	2	0
5	I	29	0	0	1	0
5	J	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	27	0	0	0	0
5	L	24	0	0	1	0
5	M	38	0	0	6	0
5	N	28	0	0	4	0
5	O	24	0	0	3	0
5	P	24	0	0	4	0
All	All	36360	0	35348	1446	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1446) 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:N:210:PRO:C	1:N:211:LEU:HD12	1.49	1.33
1:N:210:PRO:O	1:N:211:LEU:HD12	1.23	1.27
1:C:8:THR:HG22	1:C:155:ASP:OD2	1.38	1.19
1:L:10:LEU:O	1:L:14:LEU:HD12	1.41	1.18
1:N:210:PRO:C	1:N:211:LEU:CD1	2.17	1.16
1:B:303:LYS:H	1:B:303:LYS:HD2	1.05	1.11
1:L:12:ARG:HG3	1:L:12:ARG:HH11	0.95	1.10
1:L:12:ARG:HH11	1:L:12:ARG:CG	1.65	1.10
1:K:5:THR:HG23	1:K:8:THR:HG23	1.35	1.09
1:G:53:SER:OG	4:G:601:GOL:H32	1.47	1.09
1:D:270:MET:HE2	5:D:698:HOH:O	1.51	1.08
1:O:271:THR:O	1:O:275:LEU:HD12	1.50	1.08
1:F:212:LEU:HD23	1:F:236:ILE:HB	1.36	1.08
1:L:124:CYS:HB3	1:L:127:LEU:HD13	1.21	1.08
1:P:213:LEU:HD11	1:P:215:MET:HE2	1.35	1.05
1:M:127:LEU:HD13	1:N:300:VAL:CG1	1.87	1.05
1:J:3:MET:CE	1:L:106:SER:HB3	1.87	1.04
1:M:193:ILE:HG23	1:M:198:MET:HG2	1.36	1.04
1:M:127:LEU:HD13	1:N:300:VAL:HG11	1.37	1.03
1:L:11:ARG:HH22	1:L:186:ASP:CG	1.66	1.03
4:A:605:GOL:H12	5:A:814:HOH:O	1.59	1.02
1:M:127:LEU:N	1:M:127:LEU:HD23	1.74	1.01
1:N:210:PRO:O	1:N:211:LEU:CD1	2.10	0.99
1:L:97:MET:HE1	1:L:100:ARG:HE	1.27	0.98
1:B:196:ARG:HD2	1:O:196:ARG:HE	1.26	0.98
1:F:200:ARG:HG3	1:F:232:MET:HE3	1.47	0.97
1:B:303:LYS:HD2	1:B:303:LYS:N	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:THR:HG23	1:C:121:THR:O	1.66	0.96
1:C:181:ARG:HD2	5:C:533:HOH:O	1.64	0.95
1:J:74:MET:HE3	1:J:75:ILE:HG13	1.47	0.95
1:L:132:LEU:HD11	1:L:164:SER:HA	1.46	0.95
1:M:264:PRO:HB2	1:M:266:LEU:CD1	1.96	0.95
1:J:3:MET:HE1	1:L:106:SER:HB3	1.45	0.94
1:M:127:LEU:HB3	1:N:300:VAL:HG13	1.47	0.94
1:I:152:ILE:HD12	1:K:3:MET:HE3	1.49	0.93
1:J:85:ILE:HG23	1:J:112:ALA:HB3	1.50	0.93
1:K:281:LEU:HG	1:K:285:MET:HE2	1.51	0.93
1:B:303:LYS:H	1:B:303:LYS:CD	1.81	0.93
1:C:291:ALA:N	1:C:292:GLY:HA2	1.81	0.93
1:L:12:ARG:HG3	1:L:12:ARG:NH1	1.68	0.93
1:H:97:MET:HE2	1:H:100:ARG:HG3	1.49	0.93
4:M:606:GOL:H31	5:M:815:HOH:O	1.67	0.92
1:M:97:MET:HE2	1:M:100:ARG:HG3	1.49	0.92
1:O:8:THR:HG22	1:O:155:ASP:OD2	1.70	0.91
1:I:281:LEU:HD11	1:I:285:MET:HE2	1.52	0.91
1:L:11:ARG:NH2	1:L:186:ASP:CG	2.28	0.91
1:P:124:CYS:HB3	1:P:127:LEU:HD23	1.52	0.91
1:F:97:MET:HE1	1:G:62:ILE:HG23	1.51	0.90
1:I:64:THR:HG21	1:L:66:ASN:OD1	1.70	0.90
1:F:203:ILE:HD11	1:F:234:PHE:CD1	2.07	0.90
1:O:300:VAL:CG2	1:P:127:LEU:HD12	2.02	0.89
1:F:212:LEU:CD2	1:F:236:ILE:HB	2.02	0.89
1:P:196:ARG:HH12	1:P:228:GLU:HG2	1.36	0.88
1:N:211:LEU:CD1	1:N:211:LEU:N	2.30	0.88
1:I:62:ILE:HG23	1:L:97:MET:HE3	1.57	0.87
1:M:127:LEU:CD1	1:N:300:VAL:HG11	2.05	0.87
1:L:97:MET:CE	1:L:100:ARG:HE	1.88	0.86
1:G:53:SER:OG	4:G:601:GOL:C3	2.24	0.86
1:L:125:GLY:HA3	1:L:191:GLU:OE2	1.76	0.86
1:B:66:ASN:OD1	1:C:64:THR:HG21	1.76	0.86
1:D:97:MET:HE2	1:D:100:ARG:HG3	1.57	0.85
1:B:97:MET:HE3	1:C:62:ILE:HA	1.58	0.85
1:I:62:ILE:HG23	1:L:97:MET:CE	2.05	0.85
1:L:263:ILE:HG13	1:L:264:PRO:CD	2.06	0.85
1:P:124:CYS:HB3	1:P:127:LEU:CD2	2.07	0.85
1:M:126:HIS:C	1:M:127:LEU:HD23	2.02	0.85
1:C:270:MET:HE2	1:C:274:MET:HE1	1.59	0.84
1:M:133:VAL:CG1	1:M:137:THR:HB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:263:ILE:HG13	1:H:264:PRO:HD2	1.60	0.84
1:E:3:MET:HE3	1:G:152:ILE:HD12	1.57	0.83
1:P:213:LEU:HD11	1:P:215:MET:CE	2.07	0.83
1:N:116:GLU:HG2	5:N:702:HOH:O	1.77	0.83
1:O:127:LEU:HB3	1:P:300:VAL:HG13	1.58	0.83
1:J:271:THR:HG22	1:J:274:MET:H	1.43	0.82
1:K:97:MET:HE2	1:K:97:MET:HA	1.62	0.82
1:F:210:PRO:HA	1:F:235:ARG:HG3	1.62	0.81
1:B:182:ASP:HB3	5:B:679:HOH:O	1.79	0.81
1:M:193:ILE:CG2	1:M:198:MET:HG2	2.09	0.81
1:A:143:ARG:HB3	1:C:291:ALA:O	1.81	0.81
1:L:124:CYS:CB	1:L:127:LEU:HD13	2.09	0.80
1:D:266:LEU:HD22	1:D:270:MET:CE	2.11	0.80
1:M:132:LEU:HD11	1:M:164:SER:HA	1.62	0.80
1:P:97:MET:CE	1:P:97:MET:HA	2.12	0.80
1:P:124:CYS:CB	1:P:127:LEU:HD23	2.12	0.80
1:P:135:THR:O	1:P:139:VAL:HG23	1.81	0.80
1:A:127:LEU:HB3	1:B:300:VAL:HG22	1.62	0.80
1:K:5:THR:CG2	1:K:8:THR:HG23	2.11	0.80
1:H:300:VAL:CG1	1:H:300:VAL:O	2.30	0.80
1:L:10:LEU:O	1:L:14:LEU:CD1	2.29	0.80
1:J:137:THR:O	1:J:140:THR:HB	1.82	0.79
1:P:97:MET:HA	1:P:97:MET:HE2	1.65	0.79
1:C:270:MET:HG3	1:C:274:MET:HE3	1.64	0.79
4:A:605:GOL:H31	5:A:814:HOH:O	1.81	0.79
1:G:12:ARG:HG3	5:G:466:HOH:O	1.81	0.79
1:F:125:GLY:HA2	1:F:130:LYS:HE2	1.64	0.78
1:F:62:ILE:HD11	1:G:96:ILE:HG21	1.64	0.78
1:J:143:ARG:HB3	1:J:183:ALA:HB1	1.65	0.78
1:L:223:SER:O	1:L:224:ILE:HG13	1.83	0.78
1:C:8:THR:CG2	1:C:155:ASP:OD2	2.28	0.78
1:C:29:GLY:N	1:C:74:MET:HE1	1.99	0.78
1:F:196:ARG:HD3	1:F:224:ILE:HG12	1.63	0.78
1:P:300:VAL:O	1:P:300:VAL:CG1	2.31	0.78
1:M:63:CYS:HB2	5:M:572:HOH:O	1.83	0.78
1:L:112:ALA:HB2	1:L:157:VAL:HB	1.66	0.77
1:I:217:GLU:OE2	1:J:266:LEU:HB2	1.85	0.77
1:M:300:VAL:HG12	1:M:301:ASP:N	1.99	0.77
1:I:203:ILE:HD13	1:I:232:MET:O	1.85	0.77
1:N:100:ARG:O	1:N:104:GLN:HG3	1.85	0.77
1:G:127:LEU:HG	1:H:300:VAL:HG13	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:300:VAL:HA	1:P:128:ALA:HB3	1.67	0.76
1:B:203:ILE:HD11	1:B:234:PHE:CE1	2.20	0.76
1:E:97:MET:HE1	1:H:62:ILE:HG23	1.67	0.76
1:M:217:GLU:OE2	1:N:266:LEU:HB2	1.86	0.76
1:E:30:LEU:HD11	1:F:244:LEU:HD11	1.66	0.76
1:K:74:MET:HE3	1:K:75:ILE:HG13	1.68	0.76
1:F:143:ARG:HG3	1:F:183:ALA:HB1	1.67	0.76
1:B:132:LEU:HD11	1:B:164:SER:HA	1.67	0.76
1:N:29:GLY:CA	1:N:74:MET:HE1	2.15	0.76
1:N:87:ASP:OD1	1:N:114:HIS:CE1	2.39	0.76
1:B:97:MET:CE	1:C:62:ILE:HG23	2.16	0.76
1:A:302:LEU:C	1:A:302:LEU:HD23	2.12	0.75
1:K:300:VAL:CB	1:L:127:LEU:HD23	2.16	0.75
1:J:283:GLU:O	1:J:287:VAL:HG23	1.85	0.75
1:O:299:GLY:C	1:O:300:VAL:HG12	2.11	0.75
1:D:64:THR:HG22	1:D:67:ASP:H	1.52	0.75
1:L:11:ARG:NH2	1:L:186:ASP:OD1	2.20	0.75
1:B:125:GLY:HA2	1:B:130:LYS:HE2	1.67	0.75
1:I:215:MET:HE3	1:I:224:ILE:HB	1.68	0.74
1:B:11:ARG:NH2	1:B:149:ARG:HH12	1.84	0.74
1:C:149:ARG:HD2	1:C:156:ILE:O	1.86	0.74
1:A:129:GLY:O	1:A:130:LYS:C	2.30	0.74
1:I:196:ARG:NH1	1:I:228:GLU:OE1	2.20	0.74
1:N:210:PRO:C	1:N:211:LEU:HD13	2.12	0.74
1:D:198:MET:O	1:D:202:VAL:HG23	1.88	0.74
1:A:97:MET:HE3	1:D:62:ILE:HA	1.69	0.74
1:B:196:ARG:HD2	1:O:196:ARG:NE	2.01	0.74
1:L:16:ASN:C	1:L:16:ASN:OD1	2.30	0.74
1:O:127:LEU:HD22	1:P:300:VAL:HG11	1.68	0.74
1:F:33:ARG:HD3	1:F:279:CYS:HA	1.70	0.73
1:O:263:ILE:HG13	1:O:264:PRO:HD2	1.70	0.73
1:F:29:GLY:CA	1:F:74:MET:HE1	2.18	0.73
1:N:252:ARG:O	1:N:256:GLU:HG3	1.88	0.73
1:E:224:ILE:HG21	1:E:232:MET:HE1	1.70	0.73
1:L:97:MET:HE1	1:L:100:ARG:NE	2.02	0.73
1:P:124:CYS:SG	1:P:127:LEU:HD23	2.28	0.73
1:M:300:VAL:CG1	1:M:301:ASP:N	2.52	0.73
1:N:29:GLY:N	1:N:74:MET:HE1	2.03	0.73
1:C:269:GLU:O	1:C:274:MET:HG3	1.88	0.72
1:E:302:LEU:HD11	1:F:126:HIS:O	1.87	0.72
1:C:121:THR:O	1:C:121:THR:CG2	2.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:91:GLY:O	1:N:92:TYR:HB2	1.89	0.72
1:P:300:VAL:O	1:P:300:VAL:HG12	1.88	0.72
1:E:30:LEU:CD1	1:F:244:LEU:CD1	2.67	0.72
1:O:97:MET:HA	1:O:97:MET:HE2	1.71	0.72
1:I:30:LEU:HD21	1:I:275:LEU:HD21	1.70	0.72
1:L:267:ASP:OD1	1:L:269:GLU:HB3	1.90	0.72
1:M:97:MET:CE	1:M:100:ARG:HG3	2.20	0.72
1:D:97:MET:HE2	1:D:97:MET:HA	1.70	0.72
1:L:135:THR:O	1:L:139:VAL:HG23	1.89	0.72
1:M:252:ARG:HD3	5:M:645:HOH:O	1.90	0.72
1:J:256:GLU:HB2	1:J:260:ARG:HH12	1.52	0.72
1:P:29:GLY:N	1:P:74:MET:HE1	2.05	0.72
1:P:102:THR:HG23	1:P:113:PHE:HZ	1.54	0.72
1:M:127:LEU:N	1:M:127:LEU:CD2	2.49	0.71
1:M:264:PRO:HB2	1:M:266:LEU:HD13	1.72	0.71
1:O:246:PRO:HD3	1:P:266:LEU:HD21	1.72	0.71
1:A:41:ASP:HB2	1:I:296:PHE:HA	1.71	0.71
1:D:266:LEU:HD22	1:D:270:MET:HE3	1.72	0.71
1:K:276:PHE:HE1	1:L:127:LEU:HD11	1.55	0.71
1:K:301:ASP:OD2	1:K:301:ASP:N	2.23	0.71
1:B:62:ILE:HG23	1:C:97:MET:HE1	1.72	0.71
1:D:270:MET:HB3	1:D:275:LEU:HD21	1.71	0.71
1:G:62:ILE:HD13	1:G:62:ILE:N	2.05	0.71
1:A:263:ILE:HG13	1:A:264:PRO:HD2	1.72	0.71
1:H:161:ARG:HA	1:H:189:PHE:O	1.89	0.71
1:M:123:ARG:NH1	1:M:128:ALA:O	2.23	0.71
1:C:12:ARG:HG3	5:C:771:HOH:O	1.91	0.71
1:D:64:THR:HG22	1:D:67:ASP:CG	2.16	0.71
1:P:210:PRO:HA	1:P:235:ARG:HG3	1.73	0.70
1:K:11:ARG:NH1	1:K:155:ASP:O	2.23	0.70
1:I:64:THR:HG22	1:I:67:ASP:OD2	1.91	0.70
1:B:213:LEU:HD23	1:B:237:ILE:HD12	1.73	0.70
1:E:300:VAL:HG22	1:F:127:LEU:HB3	1.73	0.70
1:K:8:THR:HG22	1:K:155:ASP:OD2	1.92	0.70
1:M:95:PRO:HD2	1:O:288:ASP:OD1	1.92	0.70
1:P:64:THR:HG23	1:P:66:ASN:H	1.56	0.70
1:F:297:ASP:N	1:F:297:ASP:OD1	2.20	0.70
1:P:196:ARG:HH12	1:P:228:GLU:CG	2.05	0.70
1:F:62:ILE:HG23	1:G:97:MET:HE1	1.74	0.70
1:E:30:LEU:CD1	1:F:244:LEU:HD11	2.21	0.70
1:L:263:ILE:HG13	1:L:264:PRO:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ASP:O	1:C:293:GLY:N	2.20	0.69
1:B:11:ARG:CZ	1:B:149:ARG:HH12	2.06	0.69
1:B:97:MET:HE1	1:C:62:ILE:HG23	1.73	0.69
1:I:7:ALA:HB1	1:I:156:ILE:HA	1.73	0.69
1:H:52:ALA:O	1:H:56:GLY:HA2	1.93	0.69
1:I:62:ILE:HD12	1:L:97:MET:HE3	1.74	0.69
1:N:224:ILE:HD13	1:N:232:MET:HE1	1.74	0.69
1:A:97:MET:CE	1:D:62:ILE:HA	2.21	0.69
1:I:125:GLY:HA2	1:I:130:LYS:HD3	1.74	0.69
1:I:212:LEU:C	1:I:212:LEU:HD23	2.17	0.69
1:L:13:ALA:O	1:L:19:SER:HB2	1.93	0.69
1:B:294:ALA:HB1	1:B:297:ASP:OD2	1.92	0.69
1:C:119:VAL:HG23	1:C:121:THR:HG22	1.76	0.68
1:M:267:ASP:HB2	5:M:560:HOH:O	1.92	0.68
1:H:64:THR:HG22	1:H:67:ASP:H	1.58	0.68
1:B:11:ARG:HH22	1:B:186:ASP:CG	2.00	0.68
1:D:29:GLY:N	1:D:74:MET:HE1	2.09	0.68
1:M:214:ASN:ND2	3:M:501:OAF:O6	2.26	0.68
1:G:149:ARG:HD2	1:G:156:ILE:O	1.93	0.68
1:O:300:VAL:HG23	1:P:127:LEU:HD12	1.76	0.68
1:A:196:ARG:O	1:A:199:ALA:HB3	1.94	0.68
1:D:97:MET:CE	1:D:100:ARG:HG3	2.24	0.68
1:N:149:ARG:HG3	1:N:156:ILE:HG22	1.75	0.68
1:A:112:ALA:HB2	1:A:157:VAL:HB	1.74	0.68
1:A:289:ALA:O	1:A:292:GLY:HA3	1.94	0.68
1:E:30:LEU:HD11	1:F:244:LEU:CD1	2.24	0.68
1:L:213:LEU:HD23	1:L:237:ILE:HG13	1.77	0.68
1:I:52:ALA:O	1:I:56:GLY:HA2	1.94	0.67
1:P:19:SER:O	1:P:235:ARG:NH2	2.24	0.67
1:N:212:LEU:C	1:N:212:LEU:HD23	2.19	0.67
1:E:66:ASN:OD1	1:H:64:THR:HG21	1.95	0.67
1:I:95:PRO:HG3	1:I:140:THR:HG22	1.75	0.67
1:P:102:THR:HG23	1:P:113:PHE:CZ	2.29	0.67
1:K:29:GLY:HA2	1:K:74:MET:HE1	1.77	0.67
1:B:62:ILE:HG23	1:C:97:MET:CE	2.24	0.67
1:I:271:THR:HB	1:I:272:PRO:HD2	1.75	0.67
1:P:76:SER:HA	1:P:84:VAL:HG21	1.77	0.67
1:E:196:ARG:NH1	1:E:228:GLU:OE2	2.27	0.67
1:F:116:GLU:OE2	1:F:122:LYS:NZ	2.26	0.67
1:M:161:ARG:HA	1:M:189:PHE:HB3	1.75	0.67
1:H:294:ALA:O	1:H:297:ASP:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:87:ASP:OD1	1:N:114:HIS:HE1	1.76	0.67
1:M:127:LEU:CD1	1:N:300:VAL:CG1	2.65	0.66
1:C:137:THR:O	1:C:140:THR:HB	1.94	0.66
1:M:66:ASN:OD1	1:M:66:ASN:N	2.28	0.66
1:B:47:GLY:HA3	1:B:87:ASP:OD2	1.95	0.66
1:J:256:GLU:HB2	1:J:260:ARG:NH1	2.10	0.66
1:L:124:CYS:HB3	1:L:127:LEU:CD1	2.13	0.66
1:L:125:GLY:N	3:L:501:OAF:O5	2.24	0.66
1:O:300:VAL:HG21	1:P:127:LEU:HD12	1.77	0.66
1:J:212:LEU:HD23	1:J:212:LEU:C	2.20	0.66
1:L:12:ARG:CG	1:L:12:ARG:NH1	2.38	0.66
1:N:211:LEU:N	1:N:211:LEU:HD13	2.09	0.66
1:F:133:VAL:HG21	1:F:137:THR:HG21	1.76	0.66
1:B:133:VAL:HG21	1:B:137:THR:HG21	1.77	0.66
1:P:275:LEU:O	1:P:278:VAL:HB	1.96	0.66
1:L:29:GLY:N	1:L:74:MET:HE1	2.11	0.66
1:O:11:ARG:NH2	1:O:186:ASP:OD1	2.28	0.66
1:P:196:ARG:NH1	1:P:228:GLU:HG2	2.10	0.66
1:A:181:ARG:HG3	1:A:209:TRP:CE2	2.31	0.65
1:P:116:GLU:OE1	1:P:122:LYS:HD2	1.97	0.65
1:A:130:LYS:H	1:A:166:GLN:NE2	1.93	0.65
1:B:149:ARG:HD2	1:B:156:ILE:O	1.95	0.65
1:I:133:VAL:CG1	1:I:137:THR:HB	2.26	0.65
1:I:244:LEU:HD11	1:J:30:LEU:HD11	1.79	0.65
1:D:11:ARG:NH1	1:D:155:ASP:O	2.27	0.65
1:L:216:VAL:CG2	1:L:240:PRO:HG2	2.27	0.65
1:M:130:LYS:HD2	1:M:163:ASP:HB3	1.76	0.65
1:D:64:THR:CG2	1:D:67:ASP:H	2.09	0.65
1:N:170:TYR:O	1:N:174:VAL:HG23	1.96	0.65
1:A:252:ARG:O	1:A:256:GLU:HG2	1.96	0.65
1:O:275:LEU:HD23	1:P:244:LEU:CD2	2.26	0.65
1:E:95:PRO:HG3	1:E:140:THR:HG22	1.79	0.65
1:E:229:ALA:HA	1:E:232:MET:HE3	1.78	0.65
1:M:149:ARG:HG3	1:M:156:ILE:HG22	1.79	0.65
1:E:11:ARG:HH12	1:E:157:VAL:HA	1.62	0.65
1:C:247:ALA:O	1:C:251:MET:HG3	1.97	0.64
1:C:270:MET:HE2	1:C:274:MET:CE	2.27	0.64
1:L:10:LEU:HG	1:L:14:LEU:HD11	1.79	0.64
1:N:300:VAL:CG1	1:N:300:VAL:O	2.41	0.64
1:N:266:LEU:HD22	1:N:270:MET:HG2	1.79	0.64
1:O:274:MET:HE3	1:O:275:LEU:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:263:ILE:HG13	1:H:264:PRO:CD	2.26	0.64
1:O:273:GLN:NE2	1:O:300:VAL:O	2.29	0.64
1:O:277:ARG:HD3	5:O:595:HOH:O	1.96	0.64
5:E:417:HOH:O	1:H:97:MET:HE1	1.97	0.64
1:E:30:LEU:HD13	1:F:244:LEU:CD1	2.28	0.64
1:B:244:LEU:HD12	1:B:244:LEU:C	2.23	0.64
1:L:46:THR:HG23	1:L:49:GLY:HA3	1.79	0.64
1:B:303:LYS:N	1:B:303:LYS:CD	2.42	0.64
1:C:270:MET:HA	1:C:274:MET:HE3	1.80	0.64
1:H:300:VAL:O	1:H:300:VAL:HG13	1.97	0.64
1:E:199:ALA:O	1:E:202:VAL:HG12	1.98	0.64
1:I:300:VAL:O	1:I:301:ASP:HB2	1.96	0.63
1:K:276:PHE:CE1	1:L:127:LEU:HD11	2.32	0.63
1:L:225:SER:HB2	1:L:228:GLU:H	1.64	0.63
1:O:274:MET:CE	1:O:275:LEU:HG	2.29	0.63
1:K:281:LEU:CG	1:K:285:MET:HE2	2.27	0.63
1:O:48:ALA:HA	1:O:59:ASP:HB2	1.81	0.63
1:A:130:LYS:H	1:A:166:GLN:HE22	1.46	0.63
1:I:8:THR:HG23	1:I:155:ASP:OD2	1.98	0.63
1:I:132:LEU:HD11	1:I:164:SER:HA	1.80	0.63
1:J:3:MET:HE2	1:L:106:SER:HB3	1.78	0.63
1:N:286:LYS:O	1:N:290:GLN:HB2	1.98	0.63
1:C:29:GLY:CA	1:C:74:MET:HE1	2.29	0.63
1:J:112:ALA:HB2	1:J:157:VAL:HB	1.81	0.63
1:L:64:THR:HG23	1:L:66:ASN:H	1.64	0.63
1:M:228:GLU:O	1:M:232:MET:HG3	1.99	0.63
1:N:135:THR:O	1:N:139:VAL:HG23	1.98	0.63
1:A:57:GLN:HG3	1:A:62:ILE:HD13	1.81	0.63
1:E:97:MET:HE3	1:H:62:ILE:HA	1.79	0.63
1:O:301:ASP:O	1:O:302:LEU:CB	2.46	0.63
1:A:199:ALA:O	1:A:202:VAL:HG12	1.99	0.63
1:C:125:GLY:HA2	1:C:130:LYS:HE3	1.81	0.63
1:D:161:ARG:HA	1:D:189:PHE:O	1.99	0.62
1:F:62:ILE:HA	1:G:97:MET:HE3	1.80	0.62
1:F:203:ILE:HD11	1:F:234:PHE:CE1	2.33	0.62
1:B:210:PRO:HB3	1:B:235:ARG:HG3	1.81	0.62
1:K:116:GLU:HB3	1:K:161:ARG:HG2	1.81	0.62
1:M:23:ALA:HB3	1:M:238:ILE:HG22	1.80	0.62
1:H:198:MET:O	1:H:202:VAL:HG23	2.00	0.62
1:A:46:THR:HG23	1:A:49:GLY:HA3	1.81	0.62
1:F:97:MET:CE	1:G:62:ILE:HG23	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:ASP:HB3	5:H:310:HOH:O	1.98	0.62
1:L:223:SER:C	1:L:224:ILE:HG13	2.25	0.62
1:O:26:VAL:O	1:O:46:THR:HG22	1.99	0.62
1:K:24:PRO:HD2	1:K:42:ALA:O	1.99	0.62
1:F:29:GLY:N	1:F:74:MET:HE1	2.15	0.62
1:P:125:GLY:N	3:P:501:OAF:O5	2.27	0.62
1:F:62:ILE:HG23	1:G:97:MET:CE	2.30	0.62
1:G:117:ASP:HB3	1:G:138:TYR:CD1	2.35	0.62
1:H:14:LEU:HD21	1:H:236:ILE:HD11	1.80	0.62
1:L:189:PHE:C	1:L:189:PHE:CD2	2.78	0.61
1:O:135:THR:O	1:O:139:VAL:HG23	2.00	0.61
1:P:299:GLY:HA2	5:P:397:HOH:O	2.00	0.61
1:F:210:PRO:CA	1:F:235:ARG:HG3	2.28	0.61
1:G:20:PHE:CG	1:G:230:LYS:HG3	2.35	0.61
1:K:215:MET:HE3	1:K:224:ILE:HB	1.82	0.61
1:P:125:GLY:HA3	1:P:191:GLU:OE2	2.00	0.61
1:H:21:ILE:HB	1:H:236:ILE:HG12	1.82	0.61
1:F:212:LEU:HD23	1:F:236:ILE:CB	2.22	0.61
1:H:11:ARG:NH1	1:H:155:ASP:O	2.33	0.61
1:P:119:VAL:HG13	1:P:131:ILE:HG22	1.83	0.61
1:C:282:ASP:HB2	5:C:320:HOH:O	2.00	0.61
1:H:215:MET:HE3	1:H:224:ILE:HB	1.82	0.61
1:J:45:MET:HE2	1:J:86:ALA:HB1	1.82	0.61
1:O:29:GLY:HA2	1:O:74:MET:HE1	1.82	0.61
1:E:95:PRO:HG3	1:E:140:THR:CG2	2.31	0.61
1:I:107:ARG:O	1:K:107:ARG:HB3	2.00	0.61
1:J:206:LEU:HD12	1:J:211:LEU:HD21	1.83	0.61
1:L:189:PHE:C	1:L:189:PHE:HD2	2.09	0.61
1:O:299:GLY:O	1:O:300:VAL:HB	1.99	0.61
1:E:64:THR:O	1:E:67:ASP:HB2	2.01	0.61
1:M:152:ILE:HD12	1:O:3:MET:HE3	1.82	0.61
1:O:215:MET:HE3	1:O:224:ILE:HB	1.81	0.61
1:B:29:GLY:CA	1:B:74:MET:HE1	2.31	0.61
1:H:193:ILE:O	1:H:221:THR:HA	2.00	0.61
1:J:21:ILE:HB	1:J:236:ILE:HG13	1.83	0.61
1:E:123:ARG:CG	1:E:127:LEU:HD12	2.31	0.60
1:M:95:PRO:HG3	1:M:140:THR:CG2	2.31	0.60
1:P:213:LEU:CD1	1:P:215:MET:HE2	2.22	0.60
1:I:161:ARG:NH2	3:I:501:OAF:O3	2.32	0.60
1:O:274:MET:HE3	1:O:275:LEU:N	2.16	0.60
1:I:127:LEU:HD22	1:J:300:VAL:HB	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:C	1:B:244:LEU:CD1	2.75	0.60
1:J:170:TYR:O	1:J:174:VAL:HG23	2.01	0.60
1:M:96:ILE:O	1:M:100:ARG:HG2	2.01	0.60
1:O:122:LYS:HD3	1:O:122:LYS:C	2.26	0.60
1:H:161:ARG:HA	1:H:189:PHE:HB3	1.82	0.60
1:P:157:VAL:HG13	1:P:186:ASP:HB2	1.84	0.60
1:I:62:ILE:HG23	1:L:97:MET:HE1	1.81	0.60
1:O:127:LEU:HD22	1:P:300:VAL:CG1	2.31	0.60
1:P:37:SER:HB2	5:P:749:HOH:O	2.00	0.60
1:A:232:MET:HE3	1:A:234:PHE:HE1	1.67	0.60
1:C:161:ARG:HA	1:C:189:PHE:HB3	1.83	0.60
1:O:296:PHE:CZ	1:P:60:LEU:HD22	2.37	0.60
1:O:300:VAL:CG2	1:P:127:LEU:CD1	2.78	0.60
1:B:62:ILE:HA	1:C:97:MET:HE3	1.84	0.60
1:M:215:MET:HE3	1:M:224:ILE:HB	1.83	0.60
1:E:76:SER:HA	1:E:84:VAL:HG21	1.84	0.60
1:I:172:GLU:O	1:I:173:SER:C	2.45	0.60
1:J:29:GLY:HA2	1:J:74:MET:HE1	1.83	0.60
1:C:270:MET:HG3	1:C:274:MET:CE	2.32	0.59
1:N:146:VAL:HG11	1:N:184:GLY:O	2.02	0.59
1:O:274:MET:HE3	1:O:275:LEU:CA	2.32	0.59
1:A:57:GLN:HG3	1:A:62:ILE:CD1	2.33	0.59
1:M:274:MET:O	1:M:278:VAL:HG23	2.01	0.59
1:I:271:THR:HB	1:I:272:PRO:CD	2.32	0.59
1:B:148:ALA:HA	1:B:151:ARG:NH1	2.18	0.59
1:J:212:LEU:HD21	1:J:238:ILE:HG12	1.83	0.59
1:K:19:SER:O	1:K:235:ARG:NH1	2.36	0.59
1:O:161:ARG:HA	1:O:189:PHE:HB3	1.85	0.59
1:F:125:GLY:CA	1:F:130:LYS:HE2	2.32	0.59
1:F:179:ALA:O	1:F:182:ASP:HB3	2.03	0.59
1:I:258:LEU:HD13	1:I:264:PRO:HG3	1.84	0.59
1:M:244:LEU:C	1:M:244:LEU:HD23	2.28	0.59
1:N:44:TYR:OH	1:N:114:HIS:NE2	2.30	0.59
1:N:235:ARG:HB3	1:N:235:ARG:NH1	2.17	0.59
1:A:11:ARG:NH2	1:A:186:ASP:OD1	2.36	0.59
1:F:97:MET:HE3	1:G:62:ILE:HA	1.84	0.59
1:L:281:LEU:O	1:L:285:MET:HB2	2.02	0.59
1:M:97:MET:HE1	1:P:62:ILE:HG23	1.84	0.59
1:K:76:SER:HA	1:K:84:VAL:HG21	1.85	0.59
1:K:161:ARG:HA	1:K:189:PHE:O	2.02	0.59
1:P:270:MET:HG2	1:P:275:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:ASP:O	1:E:132:LEU:HD22	2.03	0.58
1:P:133:VAL:HG21	1:P:137:THR:HB	1.83	0.58
1:C:245:GLY:HA2	1:D:275:LEU:HD11	1.84	0.58
1:J:12:ARG:O	1:J:15:GLU:HB2	2.02	0.58
1:J:149:ARG:HG2	1:J:154:SER:O	2.03	0.58
1:L:76:SER:HA	1:L:84:VAL:HG21	1.85	0.58
1:G:11:ARG:NH2	1:G:186:ASP:OD1	2.36	0.58
1:N:277:ARG:HD3	1:N:282:ASP:OD2	2.03	0.58
1:C:248:VAL:HG22	1:D:30:LEU:HD22	1.86	0.58
1:L:130:LYS:HE3	1:L:166:GLN:HG2	1.86	0.58
1:A:86:ALA:O	1:A:113:PHE:HA	2.03	0.58
1:E:11:ARG:HH22	1:E:186:ASP:CG	2.12	0.58
1:E:16:ASN:O	1:E:235:ARG:NH2	2.37	0.58
1:E:74:MET:HE3	1:E:75:ILE:HG13	1.84	0.58
1:G:190:LEU:HD12	1:G:202:VAL:HG11	1.85	0.58
1:M:125:GLY:O	1:M:130:LYS:HE2	2.04	0.58
1:I:161:ARG:HA	1:I:189:PHE:HB3	1.85	0.58
1:L:100:ARG:O	1:L:101:THR:C	2.45	0.58
1:M:7:ALA:HB1	1:M:156:ILE:HA	1.86	0.58
1:M:133:VAL:HG11	1:M:137:THR:HB	1.85	0.58
1:E:282:ASP:HB2	5:E:375:HOH:O	2.03	0.58
1:H:267:ASP:OD1	1:H:269:GLU:HB3	2.04	0.58
1:I:268:LYS:HA	1:J:218:HIS:CD2	2.39	0.58
1:K:113:PHE:HE2	1:K:156:ILE:HG12	1.69	0.58
1:N:206:LEU:CD2	1:N:209:TRP:HE3	2.16	0.58
1:O:296:PHE:CZ	1:P:60:LEU:CD2	2.87	0.58
1:P:97:MET:HE1	1:P:100:ARG:HE	1.69	0.58
1:A:266:LEU:HD21	1:B:245:GLY:HA3	1.84	0.58
1:C:193:ILE:HG23	1:C:198:MET:HG2	1.86	0.58
1:I:181:ARG:HB2	1:I:209:TRP:CZ2	2.39	0.58
1:M:300:VAL:CG1	1:M:301:ASP:H	2.17	0.58
1:C:291:ALA:N	1:C:292:GLY:CA	2.63	0.58
1:E:149:ARG:NH1	5:E:596:HOH:O	2.35	0.58
1:O:23:ALA:HB3	1:O:238:ILE:HG22	1.86	0.58
1:C:291:ALA:H	1:C:292:GLY:HA2	1.69	0.57
1:E:181:ARG:HG3	1:E:209:TRP:CE2	2.39	0.57
1:I:214:ASN:ND2	3:I:501:OAF:O6	2.37	0.57
1:P:75:ILE:HA	1:P:78:ILE:HD12	1.86	0.57
1:F:212:LEU:CD2	1:F:236:ILE:CB	2.79	0.57
1:E:97:MET:CE	1:H:62:ILE:HG23	2.34	0.57
1:H:285:MET:HG2	1:H:296:PHE:CG	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:196:ARG:HG2	1:L:196:ARG:HH11	1.69	0.57
1:P:197:GLU:HB3	5:P:774:HOH:O	2.05	0.57
1:B:285:MET:HG2	1:B:296:PHE:CG	2.38	0.57
1:M:273:GLN:HG3	1:M:277:ARG:HH12	1.69	0.57
1:D:102:THR:HG23	1:D:113:PHE:CZ	2.40	0.57
1:N:91:GLY:O	1:N:92:TYR:CB	2.52	0.57
1:P:104:GLN:O	1:P:108:SER:HB2	2.04	0.57
1:B:259:LYS:HA	1:I:300:VAL:HG22	1.87	0.57
1:O:8:THR:CG2	1:O:155:ASP:OD2	2.51	0.57
1:P:117:ASP:OD2	1:P:162:THR:HA	2.04	0.57
1:B:96:ILE:HG21	1:C:62:ILE:CD1	2.34	0.57
1:H:300:VAL:O	1:H:300:VAL:HG12	2.03	0.57
1:N:11:ARG:NH2	1:N:186:ASP:OD1	2.37	0.57
1:O:21:ILE:HB	1:O:236:ILE:HG12	1.87	0.57
1:O:90:THR:HG21	1:O:118:GLN:O	2.04	0.57
1:G:203:ILE:HD11	1:G:234:PHE:CE1	2.39	0.57
1:I:200:ARG:O	1:I:204:GLN:HG2	2.04	0.57
1:F:62:ILE:HD12	1:G:97:MET:HE3	1.86	0.57
1:I:30:LEU:HD21	1:I:275:LEU:CD2	2.35	0.57
1:J:174:VAL:O	1:J:177:LEU:N	2.38	0.57
1:P:271:THR:O	1:P:275:LEU:HD23	2.05	0.57
1:D:142:ILE:O	1:D:146:VAL:HG23	2.04	0.57
1:E:64:THR:HG22	1:E:67:ASP:H	1.69	0.57
1:P:124:CYS:SG	1:P:127:LEU:CD2	2.93	0.57
1:A:132:LEU:HD11	1:A:164:SER:HA	1.87	0.56
1:G:128:ALA:HA	1:G:166:GLN:HE22	1.70	0.56
1:H:29:GLY:N	1:H:74:MET:HE1	2.20	0.56
1:J:68:MET:HG3	1:J:92:TYR:OH	2.05	0.56
1:J:152:ILE:HD12	1:J:154:SER:HB2	1.87	0.56
1:L:266:LEU:HB3	1:L:270:MET:HE3	1.87	0.56
1:G:96:ILE:HG12	5:G:516:HOH:O	2.04	0.56
1:I:29:GLY:HA3	1:J:52:ALA:O	2.04	0.56
1:P:130:LYS:CE	1:P:166:GLN:HG2	2.34	0.56
1:A:232:MET:CE	1:A:234:PHE:HE1	2.18	0.56
1:B:149:ARG:HG3	1:B:156:ILE:HG22	1.87	0.56
1:C:163:ASP:OD1	1:C:191:GLU:HG2	2.05	0.56
1:D:281:LEU:HD21	1:D:300:VAL:HG11	1.88	0.56
1:E:11:ARG:NH2	1:E:186:ASP:CG	2.63	0.56
1:F:29:GLY:HA2	1:F:74:MET:HE1	1.87	0.56
1:G:270:MET:HB3	1:G:275:LEU:HD21	1.88	0.56
1:M:45:MET:HG3	1:M:75:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:76:SER:HA	1:O:84:VAL:HG21	1.85	0.56
1:P:132:LEU:HD11	1:P:164:SER:HA	1.87	0.56
1:D:212:LEU:C	1:D:212:LEU:HD23	2.29	0.56
1:M:57:GLN:HG2	1:M:62:ILE:HD12	1.87	0.56
1:C:263:ILE:HG13	1:C:264:PRO:CD	2.35	0.56
1:D:215:MET:HE3	1:D:224:ILE:HB	1.87	0.56
1:M:211:LEU:HB2	5:M:582:HOH:O	2.06	0.56
1:E:263:ILE:HG13	1:E:264:PRO:CD	2.35	0.56
1:G:146:VAL:O	1:G:150:GLN:HG2	2.06	0.56
1:P:132:LEU:HD12	1:P:168:HIS:CE1	2.41	0.56
1:D:266:LEU:HD22	1:D:270:MET:HE1	1.87	0.56
1:G:255:MET:HE3	1:H:35:ALA:HB2	1.87	0.56
1:I:149:ARG:HG2	1:I:156:ILE:HG22	1.87	0.56
1:N:238:ILE:HD12	1:N:240:PRO:HG3	1.87	0.56
1:O:28:ASP:OD2	1:O:28:ASP:C	2.47	0.56
1:P:199:ALA:HB3	1:P:232:MET:HE1	1.86	0.56
1:D:114:HIS:HB3	1:D:159:ILE:HB	1.88	0.56
1:L:273:GLN:O	1:L:277:ARG:HB2	2.06	0.56
1:O:130:LYS:H	1:O:166:GLN:NE2	2.03	0.56
1:B:244:LEU:O	1:B:248:VAL:HG23	2.06	0.56
1:L:12:ARG:N	1:L:12:ARG:CD	2.68	0.56
1:B:147:GLN:HE22	1:D:291:ALA:HA	1.71	0.56
1:B:170:TYR:O	1:B:174:VAL:HG23	2.06	0.56
1:C:198:MET:O	1:C:202:VAL:HG22	2.06	0.56
1:F:181:ARG:CZ	1:F:209:TRP:HB2	2.36	0.56
1:M:203:ILE:HD11	1:M:234:PHE:CD1	2.41	0.56
1:A:203:ILE:HD11	1:A:234:PHE:CE1	2.40	0.55
1:L:91:GLY:HA3	1:L:98:VAL:HG22	1.87	0.55
1:N:86:ALA:O	1:N:113:PHE:HA	2.06	0.55
1:O:299:GLY:O	1:O:300:VAL:CB	2.53	0.55
1:F:170:TYR:O	1:F:174:VAL:HG23	2.06	0.55
1:I:135:THR:O	1:I:139:VAL:HG23	2.06	0.55
1:J:62:ILE:HD13	1:K:97:MET:HE3	1.88	0.55
1:L:112:ALA:CB	1:L:157:VAL:HB	2.36	0.55
1:A:170:TYR:O	1:A:173:SER:HB2	2.06	0.55
1:C:11:ARG:NH2	1:C:186:ASP:OD1	2.39	0.55
1:N:62:ILE:HA	1:O:97:MET:HE3	1.89	0.55
1:C:267:ASP:OD1	1:C:269:GLU:HB3	2.07	0.55
1:D:57:GLN:HG2	1:D:62:ILE:HD12	1.89	0.55
1:I:46:THR:HG23	1:I:49:GLY:HA3	1.86	0.55
1:J:239:PHE:O	1:J:240:PRO:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:271:THR:HB	1:M:272:PRO:CD	2.36	0.55
1:M:127:LEU:HD13	1:N:300:VAL:HG13	1.83	0.55
1:A:29:GLY:N	1:A:74:MET:HE1	2.20	0.55
1:F:16:ASN:O	1:F:235:ARG:NH2	2.39	0.55
1:M:142:ILE:O	1:M:146:VAL:HG22	2.07	0.55
1:O:124:CYS:HB3	1:O:127:LEU:HG	1.89	0.55
1:A:199:ALA:HB1	1:A:232:MET:HE3	1.87	0.55
1:A:300:VAL:HG13	1:A:300:VAL:O	2.07	0.55
1:J:14:LEU:HD21	1:J:236:ILE:HD11	1.88	0.55
1:J:117:ASP:HB3	1:J:138:TYR:CD1	2.41	0.55
1:N:45:MET:HG3	1:N:75:ILE:HD12	1.87	0.55
1:N:235:ARG:HB3	1:N:235:ARG:HH11	1.72	0.55
1:C:14:LEU:O	1:C:235:ARG:NH2	2.40	0.55
1:J:143:ARG:CB	1:J:183:ALA:HB1	2.34	0.55
1:N:62:ILE:HD12	1:O:97:MET:HE3	1.89	0.55
1:O:130:LYS:HD2	1:O:166:GLN:NE2	2.22	0.55
1:G:133:VAL:HG21	1:G:137:THR:HG21	1.88	0.55
1:N:206:LEU:CD2	1:N:209:TRP:CE3	2.90	0.55
1:B:47:GLY:HA2	1:B:68:MET:HE1	1.88	0.54
1:M:275:LEU:HD22	1:N:244:LEU:HD23	1.89	0.54
1:N:29:GLY:HA2	1:N:74:MET:HE1	1.88	0.54
1:D:97:MET:HE1	5:D:756:HOH:O	2.06	0.54
1:M:270:MET:HA	1:M:274:MET:HE3	1.88	0.54
1:N:11:ARG:HH22	1:N:186:ASP:CG	2.15	0.54
1:N:199:ALA:O	1:N:203:ILE:HG13	2.07	0.54
1:O:47:GLY:HA2	1:O:68:MET:HE1	1.87	0.54
1:J:85:ILE:HG23	1:J:112:ALA:CB	2.32	0.54
1:K:190:LEU:HB3	1:K:193:ILE:HD11	1.87	0.54
1:A:89:ASP:OD2	1:A:122:LYS:NZ	2.34	0.54
1:A:266:LEU:HD23	1:A:270:MET:HG3	1.89	0.54
1:B:178:ARG:NH2	1:B:205:ASP:O	2.41	0.54
1:F:168:HIS:CB	1:F:172:GLU:HG2	2.38	0.54
1:L:12:ARG:N	1:L:12:ARG:HD3	2.22	0.54
1:O:125:GLY:HA3	1:O:191:GLU:OE2	2.07	0.54
1:P:132:LEU:HD12	1:P:168:HIS:ND1	2.22	0.54
1:C:300:VAL:HB	1:D:127:LEU:HD22	1.90	0.54
1:K:276:PHE:HE1	1:L:127:LEU:CD1	2.19	0.54
1:P:113:PHE:HE1	1:P:115:ILE:HD11	1.72	0.54
1:P:130:LYS:HE2	1:P:166:GLN:HG2	1.89	0.54
1:G:125:GLY:HA3	1:G:191:GLU:OE2	2.08	0.54
1:N:62:ILE:HG23	1:O:97:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:4:VAL:HG22	1:P:5:THR:H	1.72	0.54
1:A:29:GLY:CA	1:A:74:MET:HE1	2.37	0.54
1:E:57:GLN:HG2	1:E:62:ILE:HD13	1.89	0.54
1:F:285:MET:HG2	1:F:296:PHE:CG	2.43	0.54
1:G:300:VAL:HB	1:H:127:LEU:HD22	1.89	0.54
1:I:224:ILE:HG21	1:I:232:MET:HE1	1.89	0.54
1:J:47:GLY:HA3	1:J:87:ASP:OD2	2.08	0.54
1:B:266:LEU:HD13	1:B:270:MET:SD	2.48	0.54
1:E:228:GLU:O	1:E:232:MET:HE2	2.07	0.54
1:F:97:MET:HE3	1:G:62:ILE:HD12	1.90	0.54
1:I:224:ILE:HG21	1:I:232:MET:CE	2.37	0.54
1:N:76:SER:HA	1:N:84:VAL:HG21	1.89	0.54
1:B:286:LYS:O	1:B:290:GLN:HG3	2.08	0.54
1:K:30:LEU:HD22	1:L:248:VAL:HG22	1.90	0.54
1:N:300:VAL:HG13	1:N:300:VAL:O	2.08	0.54
1:C:64:THR:HG22	1:C:67:ASP:H	1.72	0.53
1:E:268:LYS:HD2	1:F:218:HIS:CE1	2.43	0.53
1:I:281:LEU:O	1:I:285:MET:HG2	2.08	0.53
1:K:113:PHE:CE2	1:K:156:ILE:HG12	2.43	0.53
1:L:20:PHE:CG	1:L:230:LYS:HG3	2.43	0.53
1:N:103:GLU:HB3	1:N:107:ARG:HH12	1.72	0.53
1:P:116:GLU:HA	1:P:161:ARG:O	2.08	0.53
1:B:76:SER:HA	1:B:84:VAL:HG21	1.90	0.53
1:B:178:ARG:HH21	1:B:206:LEU:HD23	1.73	0.53
1:E:151:ARG:NH2	5:E:685:HOH:O	2.33	0.53
1:F:26:VAL:HG11	1:F:32:ALA:HB2	1.90	0.53
1:P:163:ASP:OD1	1:P:191:GLU:HG2	2.09	0.53
1:C:146:VAL:O	1:C:150:GLN:HG2	2.09	0.53
1:E:11:ARG:NH2	1:E:186:ASP:OD1	2.41	0.53
1:G:8:THR:HG22	1:G:12:ARG:HE	1.72	0.53
1:K:116:GLU:CB	1:K:161:ARG:HG2	2.38	0.53
1:A:263:ILE:CG1	1:A:264:PRO:HD2	2.39	0.53
1:P:283:GLU:O	1:P:287:VAL:HG23	2.09	0.53
1:K:53:SER:O	1:L:28:ASP:HB2	2.08	0.53
1:L:63:CYS:SG	1:L:68:MET:HE2	2.48	0.53
1:M:133:VAL:HG12	1:M:137:THR:HB	1.90	0.53
1:F:133:VAL:CG2	1:F:137:THR:HG21	2.38	0.53
1:F:168:HIS:HB3	1:F:172:GLU:HG2	1.90	0.53
1:G:181:ARG:HG3	1:G:209:TRP:CD2	2.43	0.53
1:H:19:SER:O	1:H:235:ARG:NH1	2.41	0.53
1:L:138:TYR:OH	1:L:160:ALA:HB1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:ARG:HD2	5:E:594:HOH:O	2.08	0.53
1:G:189:PHE:C	1:G:189:PHE:CD2	2.87	0.53
1:A:300:VAL:HG22	1:B:127:LEU:HB3	1.91	0.53
1:L:298:GLY:O	1:L:299:GLY:C	2.51	0.53
1:P:97:MET:CE	1:P:100:ARG:HE	2.21	0.53
1:G:22:VAL:HG23	1:G:22:VAL:O	2.07	0.53
1:H:117:ASP:HB3	1:H:138:TYR:CD1	2.44	0.53
1:I:76:SER:HA	1:I:84:VAL:HG21	1.90	0.53
1:B:29:GLY:N	1:B:74:MET:HE1	2.24	0.52
1:B:278:VAL:O	1:B:278:VAL:HG12	2.08	0.52
1:E:190:LEU:HD12	1:E:202:VAL:HG21	1.91	0.52
1:F:193:ILE:O	1:F:221:THR:HA	2.09	0.52
1:J:182:ASP:C	1:J:184:GLY:H	2.16	0.52
1:J:239:PHE:O	1:J:241:PHE:N	2.42	0.52
1:K:23:ALA:HB3	1:K:238:ILE:HG22	1.91	0.52
1:K:28:ASP:OD2	1:L:53:SER:OG	2.23	0.52
1:M:10:LEU:HD23	1:M:157:VAL:HG21	1.90	0.52
1:N:280:GLY:O	1:N:281:LEU:C	2.52	0.52
1:O:274:MET:HE3	1:O:274:MET:C	2.33	0.52
1:D:36:LEU:HD13	1:D:43:LEU:HD21	1.90	0.52
1:G:228:GLU:O	1:G:232:MET:HG3	2.08	0.52
1:H:274:MET:SD	1:H:274:MET:C	2.92	0.52
1:I:21:ILE:H	1:I:21:ILE:HD12	1.75	0.52
1:K:170:TYR:O	1:K:174:VAL:HG23	2.09	0.52
1:J:7:ALA:HB2	1:J:111:ALA:HA	1.90	0.52
1:K:117:ASP:HB3	1:K:138:TYR:CD1	2.44	0.52
1:L:130:LYS:HB2	1:L:166:GLN:NE2	2.25	0.52
1:A:113:PHE:HE1	1:A:115:ILE:HD11	1.74	0.52
1:A:288:ASP:O	1:A:292:GLY:HA2	2.08	0.52
1:E:11:ARG:NH1	1:E:155:ASP:O	2.43	0.52
1:E:271:THR:O	1:E:272:PRO:C	2.52	0.52
1:L:113:PHE:HE1	1:L:115:ILE:HD11	1.75	0.52
1:M:29:GLY:N	1:N:53:SER:O	2.38	0.52
1:N:33:ARG:HD3	1:N:78:ILE:HG21	1.90	0.52
1:B:124:CYS:HB3	1:B:127:LEU:HG	1.92	0.52
1:F:68:MET:HG3	1:F:92:TYR:OH	2.09	0.52
1:A:248:VAL:HG21	1:B:275:LEU:HD12	1.92	0.52
1:J:283:GLU:CD	1:J:283:GLU:H	2.18	0.52
1:K:59:ASP:OD1	1:K:124:CYS:HB2	2.08	0.52
1:L:46:THR:CG2	1:L:49:GLY:HA3	2.40	0.52
1:E:91:GLY:HA3	1:E:98:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:36:LEU:HD23	1:N:78:ILE:HG22	1.91	0.52
1:N:77:ASN:HB2	5:N:748:HOH:O	2.08	0.52
1:A:181:ARG:HG3	1:A:209:TRP:CD2	2.45	0.52
1:H:166:GLN:HG3	1:H:167:THR:N	2.24	0.52
1:P:124:CYS:CB	1:P:127:LEU:CD2	2.81	0.52
1:A:16:ASN:O	1:A:235:ARG:NH2	2.42	0.52
1:C:123:ARG:HG3	1:C:127:LEU:HD12	1.91	0.52
1:G:266:LEU:HD22	1:G:270:MET:HE3	1.92	0.52
1:G:275:LEU:HD12	1:H:244:LEU:HD23	1.92	0.52
1:I:96:ILE:HG21	1:L:62:ILE:HD11	1.92	0.52
4:A:602:GOL:H31	1:C:107:ARG:HH12	1.75	0.52
1:E:89:ASP:OD2	1:E:122:LYS:NZ	2.30	0.51
1:F:103:GLU:O	1:F:106:SER:HB2	2.10	0.51
1:G:133:VAL:HG22	1:G:134:ASP:H	1.74	0.51
1:I:92:TYR:HB3	5:I:548:HOH:O	2.10	0.51
1:K:46:THR:OG1	3:K:501:OAF:O2	2.26	0.51
1:N:154:SER:HB2	1:P:3:MET:HE3	1.91	0.51
1:A:266:LEU:HD23	1:A:270:MET:CG	2.40	0.51
1:B:77:ASN:ND2	1:B:108:SER:O	2.42	0.51
1:C:181:ARG:CD	5:C:533:HOH:O	2.36	0.51
1:E:181:ARG:CZ	1:E:209:TRP:HB2	2.40	0.51
1:I:97:MET:HE3	1:L:62:ILE:HD13	1.92	0.51
1:J:271:THR:CG2	1:J:274:MET:H	2.21	0.51
1:C:64:THR:HG22	1:C:67:ASP:CG	2.35	0.51
1:K:8:THR:CG2	1:K:155:ASP:OD2	2.56	0.51
5:C:531:HOH:O	1:D:266:LEU:HD12	2.11	0.51
1:E:229:ALA:HA	1:E:232:MET:CE	2.40	0.51
1:F:212:LEU:CD2	1:F:236:ILE:CG2	2.89	0.51
1:H:74:MET:HG3	1:H:75:ILE:N	2.25	0.51
1:N:95:PRO:HD2	1:P:288:ASP:OD2	2.10	0.51
1:O:117:ASP:HB3	1:O:138:TYR:CD1	2.46	0.51
1:E:210:PRO:HB3	1:E:235:ARG:HG3	1.93	0.51
1:I:165:LEU:HD21	1:I:194:THR:HG23	1.92	0.51
1:I:165:LEU:CD2	1:I:194:THR:HG23	2.41	0.51
1:K:48:ALA:HA	1:K:59:ASP:HB2	1.91	0.51
1:L:142:ILE:O	1:L:146:VAL:HG23	2.11	0.51
1:P:161:ARG:HA	1:P:189:PHE:O	2.10	0.51
1:G:21:ILE:HB	1:G:236:ILE:HG12	1.93	0.51
1:J:44:TYR:OH	1:J:114:HIS:NE2	2.27	0.51
1:K:7:ALA:HB2	1:K:111:ALA:HA	1.93	0.51
1:L:10:LEU:O	1:L:10:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:NH2	1:B:186:ASP:OD1	2.42	0.51
1:G:189:PHE:C	1:G:189:PHE:HD2	2.19	0.51
1:J:212:LEU:C	1:J:212:LEU:CD2	2.84	0.51
1:P:45:MET:HG3	1:P:75:ILE:HD12	1.93	0.51
1:D:102:THR:HG23	1:D:113:PHE:HZ	1.76	0.50
1:K:86:ALA:O	1:K:113:PHE:HA	2.11	0.50
1:L:189:PHE:CD1	1:L:212:LEU:HD22	2.45	0.50
1:M:4:VAL:HG12	1:M:5:THR:N	2.26	0.50
1:M:128:ALA:HB3	1:N:300:VAL:C	2.35	0.50
1:O:97:MET:HA	1:O:97:MET:CE	2.41	0.50
1:O:191:GLU:OE2	3:O:501:OAF:O6	2.29	0.50
1:A:189:PHE:C	1:A:189:PHE:HD2	2.20	0.50
1:L:64:THR:HG23	1:L:66:ASN:N	2.25	0.50
1:N:239:PHE:O	1:N:240:PRO:C	2.55	0.50
1:B:178:ARG:C	1:B:180:ALA:N	2.69	0.50
1:I:189:PHE:C	1:I:189:PHE:CD2	2.87	0.50
1:I:246:PRO:O	1:I:247:ALA:C	2.54	0.50
1:K:40:PHE:CZ	1:L:258:LEU:HD23	2.46	0.50
1:M:117:ASP:HB3	1:M:138:TYR:CD1	2.46	0.50
1:P:24:PRO:HD2	1:P:42:ALA:O	2.11	0.50
1:G:19:SER:O	1:G:235:ARG:NH1	2.44	0.50
1:I:189:PHE:C	1:I:189:PHE:HD2	2.20	0.50
1:L:130:LYS:HB2	1:L:166:GLN:HE21	1.76	0.50
1:O:196:ARG:O	1:O:199:ALA:HB3	2.11	0.50
1:A:97:MET:HE1	1:D:62:ILE:HG23	1.92	0.50
1:E:123:ARG:HG3	1:E:127:LEU:HD12	1.94	0.50
1:I:10:LEU:HD23	1:I:157:VAL:HG21	1.93	0.50
1:K:27:TYR:CD2	1:K:53:SER:HB2	2.46	0.50
1:M:128:ALA:HB3	1:N:300:VAL:HA	1.92	0.50
1:M:149:ARG:HG3	1:M:156:ILE:CG2	2.41	0.50
1:M:284:SER:O	1:M:287:VAL:HB	2.11	0.50
1:N:25:GLY:HA3	1:N:240:PRO:HA	1.94	0.50
1:O:266:LEU:HB3	1:O:270:MET:HE3	1.92	0.50
1:C:119:VAL:CG2	1:C:121:THR:HG22	2.40	0.50
1:A:129:GLY:O	1:A:130:LYS:O	2.30	0.50
1:A:189:PHE:C	1:A:189:PHE:CD2	2.89	0.50
1:E:300:VAL:O	1:E:300:VAL:HG13	2.12	0.50
1:N:206:LEU:HD22	1:N:209:TRP:CE3	2.47	0.50
1:N:263:ILE:HG13	1:N:264:PRO:CD	2.42	0.50
1:P:215:MET:HE3	1:P:224:ILE:HB	1.94	0.50
1:C:228:GLU:O	1:C:232:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:MET:CE	1:C:274:MET:CE	2.89	0.50
1:E:122:LYS:HD3	1:E:122:LYS:C	2.36	0.50
1:P:89:ASP:HB3	1:P:122:LYS:HD3	1.94	0.50
1:D:64:THR:HG22	1:D:67:ASP:N	2.23	0.50
1:F:228:GLU:O	1:F:232:MET:HG3	2.11	0.50
1:G:244:LEU:O	1:G:248:VAL:HG23	2.11	0.50
1:M:245:GLY:HA3	1:N:266:LEU:HD21	1.92	0.50
1:O:16:ASN:O	1:O:235:ARG:NH2	2.44	0.50
1:P:26:VAL:O	1:P:46:THR:HG22	2.11	0.50
1:P:136:ASP:OD1	1:P:136:ASP:N	2.43	0.50
1:B:210:PRO:CB	1:B:235:ARG:HG3	2.42	0.49
1:I:273:GLN:O	1:I:277:ARG:CG	2.60	0.49
1:I:273:GLN:O	1:I:277:ARG:HG2	2.12	0.49
1:J:19:SER:O	1:J:235:ARG:NH1	2.45	0.49
1:K:252:ARG:HA	1:L:34:VAL:HG13	1.94	0.49
1:M:264:PRO:HB2	1:M:266:LEU:HD11	1.88	0.49
1:N:8:THR:O	1:N:9:SER:C	2.55	0.49
1:G:252:ARG:HB3	1:G:252:ARG:HH11	1.76	0.49
1:K:97:MET:CE	1:K:100:ARG:HD3	2.42	0.49
1:M:189:PHE:CD2	1:M:189:PHE:C	2.89	0.49
1:A:77:ASN:HB2	4:A:602:GOL:H12	1.93	0.49
1:B:181:ARG:HG3	1:B:209:TRP:CE2	2.48	0.49
1:I:172:GLU:HG3	1:I:176:ARG:HD2	1.94	0.49
1:O:261:ASP:O	1:O:263:ILE:HG22	2.11	0.49
1:P:130:LYS:HE2	1:P:166:GLN:OE1	2.13	0.49
1:A:267:ASP:OD2	1:A:269:GLU:HG2	2.12	0.49
1:C:64:THR:CG2	1:C:66:ASN:HB2	2.43	0.49
1:C:123:ARG:HD2	1:C:130:LYS:HG3	1.94	0.49
1:E:5:THR:HG23	5:E:520:HOH:O	2.13	0.49
1:G:62:ILE:N	1:G:62:ILE:CD1	2.75	0.49
1:I:209:TRP:O	1:I:210:PRO:C	2.55	0.49
1:K:29:GLY:CA	1:K:74:MET:HE1	2.42	0.49
1:O:69:ARG:O	1:O:70:ALA:C	2.53	0.49
1:E:96:ILE:HG21	1:H:62:ILE:CD1	2.43	0.49
1:F:90:THR:HB	1:F:141:ARG:NH1	2.28	0.49
1:I:103:GLU:O	1:I:106:SER:HB2	2.13	0.49
1:J:215:MET:HE3	1:J:215:MET:HA	1.93	0.49
1:K:68:MET:HG3	1:K:92:TYR:OH	2.12	0.49
1:N:36:LEU:HD13	1:N:43:LEU:HD11	1.94	0.49
1:N:298:GLY:O	1:N:299:GLY:O	2.30	0.49
1:A:29:GLY:HA2	1:A:74:MET:HE1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:ILE:HD11	1:G:234:PHE:CD1	2.47	0.49
1:I:228:GLU:HG2	1:I:232:MET:HE2	1.94	0.49
1:O:275:LEU:CD2	1:P:244:LEU:CD2	2.91	0.49
1:B:95:PRO:O	1:B:96:ILE:C	2.54	0.49
1:C:224:ILE:HG21	1:C:232:MET:HE2	1.94	0.49
1:F:191:GLU:OE2	3:F:501:OAF:O6	2.31	0.49
1:I:277:ARG:HG3	1:I:277:ARG:HH11	1.77	0.49
1:L:24:PRO:HD2	1:L:42:ALA:O	2.12	0.49
1:N:85:ILE:HG23	1:N:112:ALA:HB3	1.95	0.49
1:A:23:ALA:HB3	1:A:238:ILE:HG22	1.93	0.49
1:D:274:MET:SD	1:D:275:LEU:HD22	2.52	0.49
1:G:20:PHE:HB2	1:G:230:LYS:HE3	1.93	0.49
1:I:97:MET:HE2	1:I:97:MET:HA	1.95	0.49
1:J:3:MET:HE1	1:L:106:SER:CB	2.30	0.49
1:K:214:ASN:HA	1:K:238:ILE:HG12	1.95	0.49
1:M:273:GLN:O	1:M:277:ARG:HG2	2.13	0.49
1:N:149:ARG:HD2	1:N:156:ILE:O	2.13	0.49
1:O:213:LEU:HA	5:O:564:HOH:O	2.13	0.49
1:O:263:ILE:HG13	1:O:264:PRO:CD	2.41	0.49
1:O:276:PHE:HE1	1:P:127:LEU:HD21	1.77	0.49
1:P:274:MET:HE2	1:P:278:VAL:CG2	2.43	0.49
1:D:126:HIS:CE1	1:D:220:ALA:H	2.31	0.49
1:G:124:CYS:HB3	1:G:127:LEU:HD22	1.94	0.49
1:I:112:ALA:HB2	1:I:157:VAL:HB	1.95	0.49
1:F:2:PRO:HB2	1:H:153:GLY:O	2.12	0.48
1:K:195:SER:HB2	1:K:198:MET:H	1.77	0.48
1:O:247:ALA:O	1:O:251:MET:HG3	2.13	0.48
1:P:27:TYR:HD2	1:P:53:SER:HB2	1.78	0.48
1:P:268:LYS:NZ	1:P:268:LYS:H	2.11	0.48
1:A:266:LEU:HD23	1:A:270:MET:CB	2.43	0.48
1:B:269:GLU:HG3	1:B:270:MET:N	2.28	0.48
1:D:215:MET:CE	1:D:224:ILE:H	2.26	0.48
1:O:188:GLY:HA3	1:O:211:LEU:HD23	1.95	0.48
1:O:194:THR:HB	5:O:484:HOH:O	2.14	0.48
1:A:146:VAL:O	1:A:150:GLN:HG3	2.12	0.48
1:F:288:ASP:OD2	1:H:95:PRO:HG2	2.13	0.48
1:H:29:GLY:CA	1:H:74:MET:HE1	2.44	0.48
1:I:118:GLN:NE2	1:I:123:ARG:O	2.43	0.48
1:I:133:VAL:HG12	1:I:137:THR:HB	1.93	0.48
1:K:193:ILE:O	1:K:221:THR:HA	2.13	0.48
1:M:57:GLN:CG	1:M:62:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:112:ALA:CB	1:M:157:VAL:HB	2.43	0.48
1:M:189:PHE:C	1:M:189:PHE:HD2	2.21	0.48
1:M:203:ILE:HD11	1:M:234:PHE:CE1	2.48	0.48
1:L:298:GLY:O	1:L:299:GLY:O	2.30	0.48
1:M:128:ALA:HB3	1:N:300:VAL:CA	2.43	0.48
1:M:159:ILE:HG12	1:M:187:VAL:HB	1.95	0.48
1:F:21:ILE:HG22	1:F:236:ILE:HG23	1.96	0.48
1:K:286:LYS:NZ	1:P:18:ASP:OD2	2.35	0.48
1:K:74:MET:O	1:K:78:ILE:HD12	2.13	0.48
1:K:112:ALA:HB2	1:K:157:VAL:HB	1.95	0.48
1:N:96:ILE:HG21	1:O:62:ILE:HD11	1.95	0.48
1:B:165:LEU:HB3	5:B:658:HOH:O	2.13	0.48
1:C:97:MET:HE2	1:C:100:ARG:HG3	1.95	0.48
1:G:247:ALA:O	1:G:251:MET:HG3	2.14	0.48
1:G:271:THR:O	1:G:275:LEU:HD23	2.13	0.48
1:H:76:SER:HA	1:H:84:VAL:HG21	1.95	0.48
1:N:41:ASP:O	1:N:83:PRO:HD2	2.14	0.48
1:G:23:ALA:HB3	1:G:238:ILE:HG22	1.95	0.48
1:K:155:ASP:O	1:K:156:ILE:C	2.57	0.48
1:L:36:LEU:HD23	1:L:43:LEU:HD11	1.95	0.48
1:A:69:ARG:HG3	1:A:104:GLN:HB3	1.96	0.48
1:K:97:MET:HE1	1:K:100:ARG:HH11	1.79	0.48
1:O:74:MET:HE3	1:O:75:ILE:HG13	1.95	0.48
1:D:161:ARG:NH2	3:D:501:OAF:O3	2.42	0.48
1:E:34:VAL:HG11	1:F:251:MET:HB3	1.95	0.48
1:I:271:THR:O	1:I:274:MET:HB3	2.13	0.48
1:K:301:ASP:C	1:L:128:ALA:HB2	2.39	0.48
1:C:255:MET:HG3	1:D:34:VAL:HG12	1.96	0.47
1:D:210:PRO:HA	1:D:235:ARG:HG3	1.95	0.47
1:F:94:GLY:O	1:F:95:PRO:C	2.57	0.47
1:K:69:ARG:O	1:K:70:ALA:C	2.54	0.47
1:L:64:THR:HG23	1:L:65:LEU:N	2.28	0.47
1:O:7:ALA:HB2	1:O:111:ALA:HA	1.96	0.47
1:O:255:MET:HE3	1:P:243:ALA:HB2	1.96	0.47
1:B:159:ILE:HG12	1:B:187:VAL:HB	1.96	0.47
1:D:125:GLY:HA3	1:D:191:GLU:OE2	2.13	0.47
1:H:129:GLY:H	1:H:166:GLN:HE22	1.62	0.47
1:I:164:SER:O	1:I:168:HIS:N	2.46	0.47
1:M:179:ALA:O	1:M:182:ASP:HB2	2.14	0.47
1:N:96:ILE:HD11	1:P:288:ASP:HB2	1.96	0.47
1:P:117:ASP:OD1	1:P:132:LEU:HD22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:O	1:A:271:THR:N	2.46	0.47
1:C:25:GLY:HA2	1:C:44:TYR:O	2.15	0.47
1:D:112:ALA:HB2	1:D:157:VAL:HB	1.95	0.47
1:E:250:ALA:HB2	1:F:250:ALA:HB2	1.95	0.47
1:I:271:THR:CB	1:I:272:PRO:CD	2.91	0.47
1:F:165:LEU:HB3	5:F:512:HOH:O	2.13	0.47
1:P:300:VAL:HG13	1:P:300:VAL:O	2.13	0.47
1:C:181:ARG:HG3	1:C:209:TRP:CE2	2.49	0.47
1:E:98:VAL:HG11	1:E:141:ARG:O	2.14	0.47
1:H:269:GLU:HB2	5:H:719:HOH:O	2.14	0.47
1:L:97:MET:HE2	1:L:97:MET:HA	1.97	0.47
1:O:11:ARG:O	1:O:15:GLU:HG3	2.13	0.47
1:O:196:ARG:NH1	1:O:224:ILE:HG12	2.29	0.47
1:C:203:ILE:HD11	1:C:234:PHE:CE1	2.49	0.47
1:E:23:ALA:HB3	1:E:238:ILE:HG22	1.97	0.47
1:G:170:TYR:O	1:G:173:SER:HB2	2.14	0.47
1:G:196:ARG:HD3	1:G:228:GLU:OE2	2.14	0.47
1:N:263:ILE:HG13	1:N:264:PRO:HD2	1.97	0.47
1:P:296:PHE:O	1:P:297:ASP:C	2.57	0.47
1:A:277:ARG:HD2	5:A:664:HOH:O	2.15	0.47
1:D:215:MET:HE3	1:D:224:ILE:H	1.80	0.47
1:E:153:GLY:O	1:G:2:PRO:HB2	2.15	0.47
1:E:284:SER:HB2	1:G:96:ILE:HD12	1.95	0.47
1:F:245:GLY:N	1:F:246:PRO:CD	2.78	0.47
1:G:89:ASP:OD1	1:G:122:LYS:HD3	2.15	0.47
1:H:135:THR:O	1:H:139:VAL:HG23	2.14	0.47
1:I:181:ARG:CZ	1:I:209:TRP:HB2	2.45	0.47
1:M:271:THR:HB	1:M:272:PRO:HD2	1.96	0.47
1:N:116:GLU:OE1	1:N:118:GLN:HG3	2.15	0.47
5:N:388:HOH:O	1:P:107:ARG:HG2	2.13	0.47
1:P:20:PHE:CE1	1:P:230:LYS:HA	2.49	0.47
1:P:26:VAL:HB	1:P:31:SER:OG	2.15	0.47
1:P:76:SER:HA	1:P:84:VAL:CG2	2.43	0.47
1:P:118:GLN:HA	1:P:132:LEU:HA	1.96	0.47
1:A:181:ARG:HD3	5:A:423:HOH:O	2.15	0.47
1:B:16:ASN:O	1:B:235:ARG:NH2	2.47	0.47
1:F:62:ILE:CD1	1:G:96:ILE:HG21	2.40	0.47
1:J:161:ARG:HA	1:J:189:PHE:O	2.15	0.47
1:M:27:TYR:CD2	1:M:53:SER:HB2	2.50	0.47
1:K:36:LEU:CD2	1:K:43:LEU:HD11	2.45	0.47
1:L:47:GLY:O	1:L:48:ALA:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:271:THR:HG23	1:N:274:MET:H	1.80	0.47
1:O:214:ASN:HA	1:O:238:ILE:HG13	1.96	0.47
1:C:263:ILE:HG13	1:C:264:PRO:HD2	1.96	0.47
1:J:215:MET:HA	1:J:215:MET:CE	2.45	0.47
1:K:133:VAL:HG21	1:K:141:ARG:NH2	2.30	0.47
1:N:116:GLU:HB3	1:N:161:ARG:HG2	1.97	0.47
1:N:274:MET:O	1:N:278:VAL:HG23	2.15	0.47
1:O:244:LEU:HD23	1:O:248:VAL:HG23	1.97	0.47
1:A:23:ALA:O	1:A:238:ILE:HA	2.15	0.46
1:D:8:THR:O	1:D:12:ARG:HG2	2.15	0.46
1:E:56:GLY:O	1:F:33:ARG:NH1	2.40	0.46
1:G:58:ALA:HA	5:G:670:HOH:O	2.14	0.46
1:J:235:ARG:NH1	1:J:235:ARG:HB3	2.30	0.46
1:N:206:LEU:HD22	1:N:209:TRP:HE3	1.78	0.46
1:D:57:GLN:CG	1:D:62:ILE:HD12	2.46	0.46
1:G:277:ARG:HD2	5:G:575:HOH:O	2.16	0.46
1:H:102:THR:O	1:H:103:GLU:C	2.57	0.46
1:I:95:PRO:HB2	1:K:288:ASP:HA	1.97	0.46
1:I:300:VAL:HG12	1:I:301:ASP:N	2.31	0.46
1:K:130:LYS:H	1:K:166:GLN:NE2	2.13	0.46
1:L:21:ILE:HD13	1:L:236:ILE:HG12	1.97	0.46
1:L:159:ILE:HG12	1:L:187:VAL:HB	1.97	0.46
1:E:28:ASP:OD1	1:E:31:SER:OG	2.32	0.46
1:H:26:VAL:HG11	1:H:32:ALA:HA	1.97	0.46
1:J:11:ARG:O	1:J:15:GLU:HG3	2.16	0.46
1:K:256:GLU:O	1:K:260:ARG:HG3	2.15	0.46
1:L:275:LEU:O	1:L:278:VAL:HB	2.15	0.46
1:M:130:LYS:CD	1:M:163:ASP:HB3	2.44	0.46
1:N:244:LEU:HD12	1:N:244:LEU:N	2.30	0.46
1:O:246:PRO:CD	1:P:266:LEU:HD21	2.42	0.46
1:C:190:LEU:HD12	1:C:202:VAL:HG11	1.97	0.46
1:D:168:HIS:HB3	1:D:172:GLU:HG2	1.97	0.46
1:F:189:PHE:C	1:F:189:PHE:CD2	2.93	0.46
1:G:263:ILE:HG13	1:G:264:PRO:HD2	1.95	0.46
1:I:85:ILE:HG12	1:I:112:ALA:HB3	1.96	0.46
1:J:149:ARG:CG	1:J:154:SER:O	2.63	0.46
1:A:41:ASP:OD1	4:A:605:GOL:H11	2.16	0.46
1:A:297:ASP:C	1:A:297:ASP:OD1	2.57	0.46
1:D:247:ALA:O	1:D:251:MET:HG3	2.15	0.46
1:F:125:GLY:C	1:F:130:LYS:HE2	2.40	0.46
1:G:258:LEU:HD11	1:H:239:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:ARG:HB2	1:I:209:TRP:CH2	2.51	0.46
1:J:63:CYS:HB2	5:J:656:HOH:O	2.16	0.46
1:O:52:ALA:HB1	1:P:30:LEU:HG	1.97	0.46
1:G:172:GLU:O	1:G:176:ARG:HG3	2.15	0.46
1:I:45:MET:HE2	1:I:86:ALA:HB1	1.97	0.46
1:I:275:LEU:HD11	1:J:52:ALA:HB2	1.98	0.46
1:L:88:ALA:O	1:L:89:ASP:C	2.59	0.46
1:M:28:ASP:C	1:M:28:ASP:OD1	2.59	0.46
1:N:49:GLY:HA2	1:N:244:LEU:HD21	1.97	0.46
1:N:209:TRP:O	1:N:211:LEU:HD13	2.15	0.46
1:N:271:THR:CG2	1:N:274:MET:H	2.28	0.46
1:O:127:LEU:CB	1:P:300:VAL:HG13	2.36	0.46
1:O:136:ASP:O	1:O:137:THR:C	2.59	0.46
1:G:130:LYS:HE3	1:G:166:GLN:HG2	1.98	0.46
1:L:10:LEU:HG	1:L:14:LEU:CD1	2.46	0.46
1:O:300:VAL:HG23	1:P:127:LEU:CD1	2.42	0.46
1:A:212:LEU:C	1:A:212:LEU:HD23	2.40	0.46
1:D:161:ARG:HA	1:D:189:PHE:HB3	1.97	0.46
1:D:274:MET:SD	1:D:274:MET:C	2.99	0.46
1:E:243:ALA:HB3	5:E:434:HOH:O	2.15	0.46
1:I:203:ILE:HD11	1:I:234:PHE:CD1	2.51	0.46
1:J:25:GLY:HA3	1:J:240:PRO:HA	1.97	0.46
1:J:161:ARG:HA	1:J:189:PHE:HB3	1.97	0.46
1:O:29:GLY:CA	1:O:74:MET:HE1	2.46	0.46
1:B:300:VAL:O	1:B:300:VAL:HG13	2.15	0.46
1:J:112:ALA:CB	1:J:157:VAL:HB	2.45	0.46
1:K:190:LEU:HD12	1:K:202:VAL:HG11	1.98	0.46
1:P:36:LEU:CD1	1:P:43:LEU:HD21	2.46	0.46
1:P:299:GLY:CA	5:P:397:HOH:O	2.63	0.46
1:A:74:MET:SD	1:A:74:MET:C	2.99	0.46
1:C:19:SER:O	1:C:235:ARG:NH1	2.49	0.46
1:F:122:LYS:HB2	1:F:122:LYS:HE3	1.69	0.46
1:K:218:HIS:HB3	1:L:271:THR:HG22	1.97	0.46
1:L:113:PHE:HD2	1:L:156:ILE:HD11	1.80	0.46
1:M:112:ALA:HB2	1:M:157:VAL:HB	1.97	0.46
1:P:133:VAL:CG2	1:P:137:THR:HB	2.45	0.46
1:E:47:GLY:HA2	1:E:68:MET:HE1	1.98	0.45
1:F:100:ARG:O	1:F:104:GLN:HG3	2.16	0.45
1:L:36:LEU:CD2	1:L:43:LEU:HD11	2.45	0.45
1:L:176:ARG:O	1:L:179:ALA:HB3	2.16	0.45
1:O:281:LEU:CD2	1:O:285:MET:HE2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:GLY:O	1:C:130:LYS:C	2.60	0.45
1:C:170:TYR:CZ	1:C:174:VAL:HG21	2.52	0.45
1:C:189:PHE:C	1:C:189:PHE:CD2	2.94	0.45
1:C:212:LEU:HD21	1:C:238:ILE:HG12	1.97	0.45
1:F:244:LEU:O	1:F:248:VAL:HG23	2.16	0.45
1:H:164:SER:O	1:H:165:LEU:C	2.57	0.45
1:I:97:MET:HE2	1:I:100:ARG:HG3	1.98	0.45
1:L:97:MET:CE	1:L:100:ARG:NE	2.69	0.45
1:M:87:ASP:OD1	1:M:114:HIS:CE1	2.69	0.45
1:O:300:VAL:HA	1:P:128:ALA:CB	2.42	0.45
1:P:133:VAL:HG21	1:P:137:THR:CB	2.46	0.45
1:C:51:ALA:O	1:C:55:HIS:HB2	2.17	0.45
1:C:246:PRO:HD3	1:D:266:LEU:HD21	1.98	0.45
1:H:239:PHE:O	1:H:240:PRO:C	2.60	0.45
1:L:143:ARG:O	1:L:147:GLN:HG3	2.16	0.45
1:A:34:VAL:HG11	1:B:251:MET:HB3	1.98	0.45
1:B:269:GLU:HA	5:B:429:HOH:O	2.17	0.45
1:C:181:ARG:HG3	1:C:209:TRP:CD2	2.51	0.45
1:C:294:ALA:O	1:C:297:ASP:HB2	2.17	0.45
1:I:64:THR:HG21	1:L:66:ASN:CG	2.38	0.45
1:P:21:ILE:HB	1:P:236:ILE:HG12	1.99	0.45
1:P:204:GLN:C	1:P:206:LEU:H	2.25	0.45
1:C:296:PHE:HB2	5:C:738:HOH:O	2.16	0.45
1:E:123:ARG:HG2	1:E:127:LEU:HD12	1.98	0.45
1:F:159:ILE:HG12	1:F:187:VAL:HB	1.98	0.45
1:G:28:ASP:OD1	1:G:31:SER:OG	2.29	0.45
1:L:48:ALA:HA	1:L:59:ASP:HB2	1.97	0.45
1:L:172:GLU:O	1:L:176:ARG:HG3	2.17	0.45
1:N:36:LEU:HD23	1:N:78:ILE:CG2	2.47	0.45
1:N:239:PHE:O	1:N:241:PHE:N	2.50	0.45
1:C:202:VAL:O	1:C:203:ILE:C	2.60	0.45
1:C:264:PRO:HD2	1:D:217:GLU:OE1	2.17	0.45
1:E:89:ASP:O	1:E:115:ILE:HA	2.16	0.45
1:F:212:LEU:HD21	1:F:236:ILE:CG2	2.47	0.45
1:A:191:GLU:OE1	1:A:191:GLU:HA	2.16	0.45
1:J:36:LEU:HD13	1:J:43:LEU:HD11	1.98	0.45
1:J:138:TYR:O	1:J:139:VAL:C	2.60	0.45
1:K:47:GLY:HA2	1:K:68:MET:HE1	1.98	0.45
1:K:130:LYS:HE2	1:K:166:GLN:CD	2.42	0.45
1:P:71:ASN:O	1:P:75:ILE:HG13	2.16	0.45
1:E:62:ILE:O	1:E:62:ILE:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:GLU:OE1	1:G:191:GLU:HA	2.17	0.45
1:I:248:VAL:HG22	1:J:30:LEU:HD22	1.98	0.45
1:J:174:VAL:O	1:J:175:ALA:C	2.60	0.45
1:C:243:ALA:HB2	1:D:255:MET:CE	2.47	0.45
1:D:29:GLY:CA	1:D:74:MET:HE1	2.47	0.45
1:F:189:PHE:C	1:F:189:PHE:HD2	2.24	0.45
1:I:95:PRO:HG3	1:I:140:THR:CG2	2.45	0.45
1:J:100:ARG:O	1:J:104:GLN:HG3	2.17	0.45
1:J:149:ARG:CD	1:J:156:ILE:HG22	2.47	0.45
1:J:202:VAL:CG1	1:J:203:ILE:N	2.79	0.45
1:L:132:LEU:HD11	1:L:164:SER:CA	2.32	0.45
1:L:137:THR:O	1:L:140:THR:HB	2.16	0.45
1:P:165:LEU:HD22	1:P:190:LEU:HD21	1.98	0.45
1:E:97:MET:CE	1:H:62:ILE:HA	2.47	0.45
1:M:177:LEU:O	1:M:178:ARG:C	2.60	0.45
1:N:62:ILE:HG23	1:O:97:MET:HE1	1.99	0.45
1:P:30:LEU:HD23	1:P:30:LEU:HA	1.80	0.45
1:P:251:MET:O	1:P:255:MET:HG2	2.17	0.45
1:A:203:ILE:HD11	1:A:234:PHE:CD1	2.52	0.44
1:G:133:VAL:HG22	1:G:134:ASP:N	2.32	0.44
1:I:29:GLY:N	1:J:53:SER:O	2.50	0.44
1:I:203:ILE:HD13	1:I:232:MET:C	2.41	0.44
1:J:95:PRO:O	1:J:96:ILE:C	2.60	0.44
1:N:68:MET:HE3	1:N:87:ASP:O	2.17	0.44
1:A:94:GLY:H	1:D:121:THR:HG21	1.82	0.44
1:K:176:ARG:O	1:K:179:ALA:HB3	2.17	0.44
1:M:138:TYR:O	1:M:141:ARG:HB2	2.18	0.44
1:O:142:ILE:O	1:O:146:VAL:HG23	2.17	0.44
1:B:64:THR:O	1:B:67:ASP:HB2	2.16	0.44
1:H:36:LEU:HD13	1:H:43:LEU:HD11	1.99	0.44
1:H:69:ARG:HD3	1:H:69:ARG:C	2.42	0.44
1:J:203:ILE:HG21	1:J:233:GLY:HA3	1.99	0.44
1:N:267:ASP:HB3	1:N:270:MET:HE2	1.99	0.44
1:O:189:PHE:C	1:O:189:PHE:CD2	2.95	0.44
1:A:28:ASP:OD2	1:B:53:SER:OG	2.25	0.44
1:B:94:GLY:O	1:B:95:PRO:C	2.61	0.44
1:J:149:ARG:HG3	1:J:154:SER:HB3	1.98	0.44
1:O:187:VAL:HG12	1:O:188:GLY:N	2.33	0.44
1:P:69:ARG:HG3	1:P:104:GLN:HB3	1.99	0.44
1:P:79:SER:HA	1:P:80:PRO:HD3	1.85	0.44
1:P:126:HIS:C	1:P:127:LEU:HD22	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:172:GLU:O	1:P:176:ARG:HG3	2.17	0.44
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.76	0.44
1:B:146:VAL:HG21	1:B:183:ALA:O	2.17	0.44
1:D:16:ASN:O	1:D:235:ARG:NH2	2.50	0.44
1:E:57:GLN:CG	1:E:62:ILE:HD13	2.47	0.44
1:N:209:TRP:O	1:N:211:LEU:CD1	2.65	0.44
1:A:11:ARG:HH22	1:A:186:ASP:CG	2.25	0.44
1:A:142:ILE:O	1:A:146:VAL:HG23	2.18	0.44
1:A:200:ARG:HG2	1:A:232:MET:HG2	1.99	0.44
1:C:138:TYR:O	1:C:141:ARG:HB2	2.18	0.44
1:E:250:ALA:CB	1:F:250:ALA:HB2	2.48	0.44
1:M:91:GLY:HA3	1:M:98:VAL:HG22	1.99	0.44
1:N:300:VAL:O	1:N:300:VAL:HG12	2.12	0.44
1:O:198:MET:O	1:O:199:ALA:C	2.60	0.44
1:A:95:PRO:HG3	1:A:140:THR:HG23	2.00	0.44
1:I:93:GLY:HA3	1:I:97:MET:HG3	1.99	0.44
1:J:241:PHE:O	1:J:242:ALA:C	2.59	0.44
1:K:272:PRO:HA	1:K:275:LEU:HD23	1.99	0.44
1:L:64:THR:HG22	1:L:67:ASP:H	1.83	0.44
1:M:164:SER:O	1:M:165:LEU:C	2.61	0.44
1:O:273:GLN:H	1:O:273:GLN:HG2	1.40	0.44
1:P:193:ILE:HD12	1:P:213:LEU:HD23	1.99	0.44
1:A:145:ALA:O	1:A:149:ARG:HB2	2.18	0.44
1:B:34:VAL:O	1:B:35:ALA:C	2.60	0.44
1:F:151:ARG:NH2	5:F:596:HOH:O	2.43	0.44
1:G:155:ASP:O	1:G:156:ILE:C	2.60	0.44
1:H:27:TYR:HD2	1:H:53:SER:HB2	1.82	0.44
1:I:27:TYR:CD2	1:I:53:SER:HB2	2.53	0.44
1:K:8:THR:HG22	1:K:155:ASP:HB2	1.99	0.44
1:M:48:ALA:HA	1:M:59:ASP:HB2	2.00	0.44
1:P:45:MET:HG3	1:P:75:ILE:CD1	2.48	0.44
1:A:59:ASP:O	1:A:60:LEU:HD23	2.17	0.44
1:A:112:ALA:CB	1:A:157:VAL:HB	2.45	0.44
1:C:16:ASN:OD1	1:C:16:ASN:C	2.60	0.44
1:D:64:THR:HG23	1:D:66:ASN:N	2.33	0.44
1:E:268:LYS:HD2	1:F:218:HIS:HE1	1.83	0.44
1:I:28:ASP:C	1:I:74:MET:HE1	2.43	0.44
1:I:64:THR:HG22	1:I:67:ASP:CG	2.42	0.44
1:I:74:MET:HE3	1:I:75:ILE:HG13	1.99	0.44
1:N:30:LEU:C	1:N:32:ALA:N	2.75	0.44
1:N:161:ARG:HA	1:N:189:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:105:TYR:O	1:O:110:VAL:HB	2.17	0.44
1:O:300:VAL:O	1:O:300:VAL:HG22	2.17	0.44
1:J:3:MET:HE3	1:L:154:SER:CB	2.48	0.43
1:J:24:PRO:HD2	1:J:42:ALA:O	2.18	0.43
1:K:97:MET:HE1	1:K:100:ARG:HD3	2.00	0.43
1:L:258:LEU:HD12	1:L:263:ILE:C	2.43	0.43
1:L:271:THR:O	1:L:272:PRO:C	2.61	0.43
1:N:137:THR:O	1:N:140:THR:HB	2.18	0.43
1:B:122:LYS:HE3	1:B:122:LYS:HB2	1.69	0.43
1:C:7:ALA:HB1	1:C:155:ASP:C	2.43	0.43
1:C:129:GLY:H	1:C:166:GLN:HE22	1.66	0.43
1:F:210:PRO:CB	1:F:235:ARG:HG3	2.47	0.43
1:I:241:PHE:HD1	1:I:244:LEU:HD22	1.84	0.43
1:J:45:MET:CE	1:J:86:ALA:HB1	2.47	0.43
1:J:182:ASP:C	1:J:184:GLY:N	2.76	0.43
1:K:159:ILE:HG12	1:K:187:VAL:HB	2.01	0.43
1:O:34:VAL:O	1:O:35:ALA:C	2.62	0.43
1:P:11:ARG:HH22	1:P:149:ARG:NH1	2.16	0.43
1:C:41:ASP:O	1:C:83:PRO:HD2	2.18	0.43
1:F:47:GLY:HA3	1:F:87:ASP:OD2	2.18	0.43
1:F:209:TRP:CD1	1:F:210:PRO:HD2	2.53	0.43
1:I:62:ILE:O	1:I:62:ILE:HG22	2.17	0.43
1:J:69:ARG:HG3	1:J:104:GLN:HB3	2.00	0.43
1:J:252:ARG:O	1:J:256:GLU:HG2	2.17	0.43
1:M:45:MET:HG3	1:M:75:ILE:CD1	2.47	0.43
1:N:149:ARG:HG2	1:N:154:SER:O	2.18	0.43
1:P:66:ASN:OD1	1:P:66:ASN:N	2.52	0.43
1:D:123:ARG:HE	1:D:123:ARG:HB2	1.56	0.43
1:I:244:LEU:O	1:I:248:VAL:HG23	2.17	0.43
1:N:49:GLY:CA	1:N:244:LEU:HD21	2.48	0.43
1:N:79:SER:HA	1:N:80:PRO:HD3	1.76	0.43
1:N:270:MET:HE2	1:N:270:MET:HB2	1.97	0.43
1:P:271:THR:O	1:P:272:PRO:C	2.54	0.43
1:C:68:MET:HG3	1:C:92:TYR:OH	2.17	0.43
1:E:7:ALA:HB1	1:E:156:ILE:HA	2.00	0.43
1:H:15:GLU:O	1:H:17:PRO:HD3	2.18	0.43
1:H:191:GLU:OE2	3:H:501:OAF:O6	2.36	0.43
1:J:236:ILE:HG22	1:J:237:ILE:N	2.32	0.43
1:K:69:ARG:HG3	1:K:104:GLN:HB3	2.01	0.43
1:M:30:LEU:HD21	1:M:275:LEU:CD1	2.47	0.43
1:M:78:ILE:HD11	1:N:56:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:198:MET:HB2	1:M:198:MET:HE3	1.52	0.43
1:P:54:VAL:HG12	1:P:55:HIS:CD2	2.54	0.43
1:P:190:LEU:HD22	1:P:193:ILE:HG12	2.01	0.43
1:A:11:ARG:NH2	1:A:186:ASP:CG	2.76	0.43
1:B:65:LEU:O	1:B:66:ASN:C	2.62	0.43
1:B:161:ARG:HA	1:B:189:PHE:HB3	1.99	0.43
1:C:28:ASP:OD1	1:C:28:ASP:C	2.62	0.43
1:H:8:THR:HG23	1:H:155:ASP:OD2	2.18	0.43
1:H:125:GLY:HA3	1:H:191:GLU:OE2	2.18	0.43
1:H:266:LEU:HD22	1:H:270:MET:HE3	2.00	0.43
1:K:26:VAL:O	1:K:46:THR:HG22	2.18	0.43
1:L:75:ILE:HA	1:L:78:ILE:HD12	2.00	0.43
1:M:224:ILE:HG21	1:M:232:MET:HE2	2.00	0.43
1:G:274:MET:SD	1:G:274:MET:C	3.01	0.43
1:H:18:ASP:O	1:H:19:SER:C	2.61	0.43
1:H:215:MET:HE3	1:H:224:ILE:H	1.84	0.43
1:L:122:LYS:H	1:L:122:LYS:HG3	1.62	0.43
1:M:181:ARG:NH1	1:M:209:TRP:HB2	2.34	0.43
1:N:74:MET:HA	5:N:748:HOH:O	2.18	0.43
1:O:33:ARG:HD3	1:O:78:ILE:HG21	2.01	0.43
1:O:112:ALA:HB2	1:O:157:VAL:HB	2.00	0.43
1:B:29:GLY:HA2	1:B:74:MET:HE1	2.00	0.43
1:G:97:MET:HA	1:G:100:ARG:HG3	2.01	0.43
1:G:190:LEU:HD12	1:G:202:VAL:CG1	2.49	0.43
1:I:68:MET:HG3	1:I:92:TYR:OH	2.18	0.43
1:P:200:ARG:HA	1:P:203:ILE:HD12	2.00	0.43
1:B:96:ILE:HG21	1:C:62:ILE:HD11	2.01	0.43
1:C:123:ARG:NH1	1:C:129:GLY:HA3	2.34	0.43
1:G:252:ARG:HB3	1:G:252:ARG:NH1	2.33	0.43
1:I:170:TYR:O	1:I:173:SER:HB2	2.18	0.43
1:M:127:LEU:CB	1:N:300:VAL:HG13	2.34	0.43
1:P:161:ARG:HD2	1:P:189:PHE:CE1	2.53	0.43
1:A:20:PHE:CG	1:A:230:LYS:HG3	2.53	0.43
1:B:96:ILE:HG21	1:C:62:ILE:HD12	2.01	0.43
1:B:178:ARG:O	1:B:179:ALA:C	2.62	0.43
1:C:96:ILE:O	1:C:100:ARG:HG2	2.19	0.43
1:C:269:GLU:O	1:C:269:GLU:HG2	2.15	0.43
1:D:263:ILE:HG12	1:D:264:PRO:HD2	2.01	0.43
1:F:161:ARG:HA	1:F:189:PHE:HB3	2.01	0.43
1:K:126:HIS:ND1	1:K:219:GLY:HA3	2.34	0.43
1:M:76:SER:HA	1:M:84:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:146:VAL:HG12	1:M:158:VAL:HG21	2.01	0.43
1:M:274:MET:HB2	5:M:807:HOH:O	2.18	0.43
1:O:189:PHE:C	1:O:189:PHE:HD2	2.27	0.43
1:P:27:TYR:CD2	1:P:53:SER:HB2	2.53	0.43
1:D:191:GLU:OE2	3:D:501:OAF:O6	2.37	0.42
1:E:117:ASP:HB3	1:E:138:TYR:CD1	2.54	0.42
1:G:266:LEU:HD21	1:H:246:PRO:HD3	2.00	0.42
1:I:29:GLY:HA2	1:I:74:MET:HE1	2.00	0.42
1:J:224:ILE:HD13	1:J:232:MET:HE1	2.00	0.42
1:B:157:VAL:HG13	1:B:186:ASP:HB2	2.00	0.42
1:D:123:ARG:HG2	1:D:127:LEU:HB2	2.01	0.42
1:D:210:PRO:HB3	1:D:235:ARG:HG3	2.01	0.42
1:H:266:LEU:HD22	1:H:270:MET:CE	2.49	0.42
1:I:300:VAL:CG1	1:I:301:ASP:N	2.83	0.42
1:J:168:HIS:HB3	1:J:172:GLU:HG2	2.01	0.42
1:J:174:VAL:O	1:J:178:ARG:N	2.49	0.42
1:K:37:SER:C	1:K:39:GLY:N	2.77	0.42
1:K:224:ILE:HG21	1:K:232:MET:HE2	2.01	0.42
1:L:113:PHE:HE1	1:L:115:ILE:CD1	2.31	0.42
1:N:138:TYR:C	1:N:140:THR:N	2.75	0.42
1:O:3:MET:HE2	1:O:3:MET:HB3	1.95	0.42
1:P:21:ILE:CD1	1:P:236:ILE:HG12	2.48	0.42
1:P:196:ARG:HH12	1:P:228:GLU:CD	2.26	0.42
1:B:123:ARG:O	1:B:124:CYS:C	2.62	0.42
1:C:26:VAL:O	1:C:45:MET:HA	2.20	0.42
1:H:203:ILE:HD11	1:H:234:PHE:CE1	2.54	0.42
1:O:275:LEU:HD23	1:P:244:LEU:HD23	2.01	0.42
1:P:113:PHE:O	1:P:159:ILE:HB	2.19	0.42
1:A:41:ASP:CB	1:I:296:PHE:HA	2.45	0.42
1:B:244:LEU:HD12	1:B:244:LEU:O	2.19	0.42
1:B:244:LEU:CD1	1:B:244:LEU:O	2.66	0.42
1:C:189:PHE:C	1:C:189:PHE:HD2	2.27	0.42
1:D:215:MET:CE	1:D:224:ILE:HB	2.49	0.42
1:G:271:THR:HB	1:G:272:PRO:HD2	2.01	0.42
1:H:52:ALA:O	1:H:56:GLY:CA	2.66	0.42
1:H:196:ARG:NH1	1:H:228:GLU:OE1	2.53	0.42
1:I:59:ASP:OD1	1:I:124:CYS:HB2	2.20	0.42
1:M:146:VAL:HG11	1:M:184:GLY:O	2.19	0.42
1:O:14:LEU:HD23	1:O:14:LEU:HA	1.65	0.42
1:P:157:VAL:HG13	1:P:186:ASP:CB	2.48	0.42
1:B:16:ASN:OD1	1:B:17:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:MET:SD	1:C:274:MET:C	3.02	0.42
1:F:217:GLU:O	1:F:218:HIS:HB2	2.19	0.42
1:G:199:ALA:O	1:G:202:VAL:HG23	2.19	0.42
1:J:23:ALA:HA	1:J:24:PRO:HD2	1.92	0.42
1:K:130:LYS:HG3	1:K:166:GLN:NE2	2.34	0.42
1:C:46:THR:HG23	1:C:49:GLY:HA3	2.00	0.42
1:D:64:THR:HG23	1:D:66:ASN:H	1.84	0.42
1:D:193:ILE:O	1:D:221:THR:HA	2.19	0.42
1:F:131:ILE:HD13	1:F:131:ILE:HA	1.91	0.42
1:F:186:ASP:O	1:F:210:PRO:HG2	2.20	0.42
1:L:16:ASN:OD1	1:L:17:PRO:N	2.51	0.42
1:L:116:GLU:OE2	1:L:122:LYS:HE3	2.20	0.42
1:L:122:LYS:HE2	1:L:122:LYS:HB2	1.94	0.42
1:M:59:ASP:OD1	1:M:124:CYS:HB2	2.19	0.42
1:N:65:LEU:HD13	1:N:101:THR:OG1	2.19	0.42
1:N:73:GLU:HB2	1:N:108:SER:HB3	2.02	0.42
1:O:197:GLU:C	1:O:197:GLU:OE2	2.62	0.42
1:P:149:ARG:NH1	1:P:186:ASP:OD2	2.52	0.42
1:A:10:LEU:O	1:A:11:ARG:C	2.62	0.42
1:B:86:ALA:O	1:B:113:PHE:HA	2.19	0.42
1:B:143:ARG:HA	1:B:146:VAL:HG22	2.01	0.42
1:F:251:MET:O	1:F:255:MET:HG2	2.19	0.42
1:G:27:TYR:CD2	1:G:53:SER:HB2	2.55	0.42
1:H:189:PHE:C	1:H:189:PHE:CD2	2.96	0.42
1:J:96:ILE:H	1:J:96:ILE:HG12	1.25	0.42
1:J:226:ALA:O	1:J:227:ALA:C	2.62	0.42
1:L:50:THR:O	1:L:54:VAL:HB	2.20	0.42
1:L:251:MET:O	1:L:255:MET:HG2	2.20	0.42
1:L:263:ILE:HG13	1:L:264:PRO:HD3	1.95	0.42
1:M:225:SER:O	1:M:226:ALA:C	2.62	0.42
1:O:90:THR:O	1:O:141:ARG:HD3	2.19	0.42
1:P:7:ALA:HB1	1:P:156:ILE:N	2.34	0.42
1:A:17:PRO:HA	1:A:235:ARG:HE	1.85	0.42
1:B:137:THR:O	1:B:140:THR:HB	2.19	0.42
1:C:95:PRO:HG3	1:C:140:THR:CG2	2.50	0.42
1:E:14:LEU:HA	1:E:235:ARG:NH2	2.35	0.42
1:F:119:VAL:CG1	1:F:120:GLN:N	2.83	0.42
1:F:132:LEU:HD12	1:F:168:HIS:CE1	2.55	0.42
1:G:255:MET:HE2	1:H:243:ALA:HB2	2.01	0.42
1:G:267:ASP:OD1	1:G:269:GLU:HB3	2.19	0.42
1:G:300:VAL:HA	1:H:128:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:LEU:HD11	1:H:198:MET:HE1	2.01	0.42
1:L:121:THR:HG22	5:L:763:HOH:O	2.20	0.42
1:P:105:TYR:CD2	1:P:110:VAL:HG21	2.55	0.42
1:F:155:ASP:O	1:F:156:ILE:C	2.63	0.42
1:G:246:PRO:HD3	1:H:266:LEU:HD21	2.01	0.42
1:G:282:ASP:HB2	5:G:405:HOH:O	2.20	0.42
1:H:82:THR:HA	1:H:83:PRO:HD2	1.90	0.42
1:H:280:GLY:O	1:H:281:LEU:C	2.61	0.42
1:K:5:THR:CG2	1:K:8:THR:CG2	2.93	0.42
1:M:4:VAL:CG1	1:M:5:THR:N	2.83	0.42
1:M:30:LEU:HA	1:M:30:LEU:HD23	1.81	0.42
1:O:24:PRO:HD2	1:O:42:ALA:O	2.20	0.42
1:O:224:ILE:HG21	1:O:232:MET:HE2	2.01	0.42
1:P:273:GLN:CD	1:P:273:GLN:H	2.28	0.42
4:A:602:GOL:H32	1:C:103:GLU:OE1	2.20	0.42
1:D:10:LEU:N	5:D:752:HOH:O	2.53	0.42
1:D:74:MET:HG3	1:D:75:ILE:N	2.35	0.42
1:E:69:ARG:O	1:E:70:ALA:C	2.60	0.42
1:F:130:LYS:H	1:F:166:GLN:NE2	2.17	0.42
1:H:4:VAL:HG12	1:H:5:THR:N	2.35	0.42
1:I:49:GLY:O	1:I:52:ALA:HB3	2.20	0.42
1:L:63:CYS:CB	1:L:68:MET:HE2	2.50	0.42
1:M:62:ILE:O	1:M:62:ILE:HG22	2.18	0.42
1:M:99:ALA:O	1:M:100:ARG:C	2.62	0.42
1:B:121:THR:HG21	1:C:94:GLY:H	1.85	0.41
1:C:130:LYS:HE2	1:C:163:ASP:HB3	2.01	0.41
1:C:136:ASP:O	1:C:137:THR:C	2.62	0.41
1:D:143:ARG:HG3	1:D:183:ALA:HB1	2.01	0.41
1:D:252:ARG:HH11	1:D:252:ARG:HB3	1.83	0.41
1:F:58:ALA:HA	5:F:529:HOH:O	2.18	0.41
1:I:24:PRO:HG3	1:I:40:PHE:CD1	2.55	0.41
1:K:17:PRO:HA	1:K:235:ARG:NH2	2.35	0.41
1:K:165:LEU:HB2	1:K:190:LEU:HD21	2.02	0.41
1:M:28:ASP:C	1:M:74:MET:HE1	2.45	0.41
1:M:162:THR:HG22	1:M:177:LEU:HD21	2.02	0.41
1:M:273:GLN:OE1	1:M:273:GLN:CA	2.67	0.41
1:N:45:MET:HE2	1:N:86:ALA:HB1	2.02	0.41
1:O:296:PHE:HZ	1:P:60:LEU:HD22	1.82	0.41
1:P:166:GLN:HG3	1:P:167:THR:N	2.35	0.41
1:P:200:ARG:H	1:P:200:ARG:HG3	1.61	0.41
1:B:168:HIS:HB3	1:B:172:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLN:O	1:C:274:MET:C	2.60	0.41
1:D:143:ARG:NH1	5:D:690:HOH:O	2.53	0.41
1:E:23:ALA:HA	1:E:24:PRO:HD2	1.97	0.41
1:J:68:MET:O	1:J:69:ARG:C	2.63	0.41
1:J:193:ILE:H	1:J:193:ILE:HG12	1.66	0.41
1:K:34:VAL:O	1:K:35:ALA:C	2.61	0.41
1:M:152:ILE:HG13	1:M:154:SER:HB3	2.02	0.41
1:N:11:ARG:O	1:N:15:GLU:HG3	2.20	0.41
1:N:152:ILE:HD12	1:P:3:MET:HE1	2.01	0.41
1:P:119:VAL:O	1:P:120:GLN:C	2.62	0.41
1:P:142:ILE:O	1:P:146:VAL:HG23	2.19	0.41
1:P:170:TYR:O	1:P:174:VAL:HG23	2.21	0.41
1:A:45:MET:HG3	1:A:75:ILE:CD1	2.51	0.41
1:B:209:TRP:HA	1:B:210:PRO:HD3	1.94	0.41
1:D:159:ILE:HG12	1:D:187:VAL:HB	2.02	0.41
1:L:274:MET:HE2	1:L:278:VAL:CG2	2.50	0.41
1:M:263:ILE:O	1:M:263:ILE:CG2	2.69	0.41
1:M:266:LEU:HB3	1:M:270:MET:SD	2.60	0.41
1:N:224:ILE:HD13	1:N:232:MET:CE	2.47	0.41
1:O:296:PHE:HZ	1:P:60:LEU:CD2	2.33	0.41
1:P:89:ASP:O	1:P:115:ILE:HA	2.19	0.41
1:P:97:MET:HA	1:P:97:MET:HE3	1.99	0.41
1:B:203:ILE:HD11	1:B:234:PHE:CD1	2.54	0.41
1:B:212:LEU:HA	1:B:236:ILE:O	2.19	0.41
1:D:190:LEU:HD13	1:D:193:ILE:HG12	2.01	0.41
1:D:263:ILE:HA	1:D:264:PRO:HD3	1.93	0.41
1:E:203:ILE:HD11	1:E:234:PHE:CE1	2.56	0.41
1:I:181:ARG:NH2	1:I:209:TRP:HB2	2.35	0.41
1:M:45:MET:SD	1:M:71:ASN:HB3	2.60	0.41
1:M:88:ALA:O	1:M:89:ASP:HB2	2.20	0.41
1:O:26:VAL:HG11	1:O:32:ALA:HB2	2.01	0.41
1:P:274:MET:HE2	1:P:278:VAL:HG21	2.03	0.41
1:A:95:PRO:HG3	1:A:140:THR:CG2	2.49	0.41
1:A:294:ALA:O	1:A:295:ALA:C	2.59	0.41
1:E:123:ARG:HD2	1:E:130:LYS:HG2	2.00	0.41
1:E:263:ILE:HG13	1:E:264:PRO:HD3	2.00	0.41
1:F:170:TYR:O	1:F:173:SER:HB2	2.20	0.41
1:G:275:LEU:HD12	1:H:244:LEU:CD2	2.51	0.41
1:H:116:GLU:HB3	1:H:161:ARG:HD3	2.01	0.41
1:J:41:ASP:O	1:J:83:PRO:HD2	2.21	0.41
1:J:117:ASP:OD2	1:J:176:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:117:ASP:OD2	1:K:176:ARG:NH1	2.54	0.41
1:K:194:THR:HA	1:K:220:ALA:O	2.21	0.41
1:M:30:LEU:HD22	1:N:248:VAL:CG2	2.51	0.41
1:B:278:VAL:O	1:B:278:VAL:CG1	2.68	0.41
1:C:122:LYS:NZ	5:C:309:HOH:O	2.38	0.41
1:C:302:LEU:HD12	1:C:302:LEU:HA	1.97	0.41
1:J:148:ALA:HA	1:J:151:ARG:NH1	2.35	0.41
1:J:257:LYS:O	1:J:261:ASP:N	2.48	0.41
1:K:110:VAL:HG12	1:K:112:ALA:H	1.85	0.41
1:N:177:LEU:HD21	1:N:189:PHE:H	1.85	0.41
1:C:244:LEU:HD23	1:D:275:LEU:HD12	2.02	0.41
1:H:73:GLU:O	1:H:77:ASN:ND2	2.48	0.41
1:H:221:THR:HA	1:H:222:PRO:HD3	1.91	0.41
1:J:133:VAL:HG22	1:J:137:THR:HB	2.02	0.41
1:L:170:TYR:CD2	1:L:170:TYR:C	2.99	0.41
1:L:215:MET:HA	1:L:215:MET:HE2	2.01	0.41
1:N:162:THR:HG23	1:N:190:LEU:HD23	2.02	0.41
1:O:57:GLN:HG2	1:O:62:ILE:HD13	2.02	0.41
1:O:300:VAL:CA	1:P:128:ALA:HB3	2.44	0.41
1:P:65:LEU:HD12	1:P:65:LEU:O	2.20	0.41
1:P:82:THR:HA	1:P:83:PRO:HD3	1.79	0.41
1:C:232:MET:HE3	1:C:234:PHE:HE1	1.85	0.41
1:F:200:ARG:HG3	1:F:232:MET:CE	2.33	0.41
1:H:69:ARG:HG3	1:H:104:GLN:HB3	2.01	0.41
1:H:203:ILE:HD11	1:H:234:PHE:CD1	2.56	0.41
1:K:212:LEU:HD23	1:K:212:LEU:C	2.46	0.41
1:L:30:LEU:HD23	1:L:30:LEU:HA	1.94	0.41
1:M:300:VAL:HG13	1:M:301:ASP:H	1.83	0.41
1:N:24:PRO:HD2	1:N:42:ALA:O	2.20	0.41
1:O:130:LYS:H	1:O:166:GLN:HE21	1.68	0.41
1:O:165:LEU:HD12	1:O:165:LEU:HA	1.88	0.41
1:A:91:GLY:HA3	1:A:98:VAL:HG22	2.03	0.41
1:A:232:MET:CE	1:A:234:PHE:CE1	2.99	0.41
1:A:235:ARG:HA	1:A:235:ARG:HD2	1.73	0.41
1:A:252:ARG:HH21	1:B:274:MET:CE	2.33	0.41
1:A:256:GLU:HG2	1:A:256:GLU:H	1.74	0.41
1:B:130:LYS:H	1:B:166:GLN:NE2	2.18	0.41
1:B:193:ILE:O	1:B:221:THR:HA	2.20	0.41
1:B:198:MET:HA	1:B:201:GLN:HB2	2.02	0.41
1:D:23:ALA:HA	1:D:24:PRO:HD3	1.83	0.41
1:D:110:VAL:O	1:D:156:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:THR:HG23	1:D:190:LEU:HD23	2.02	0.41
1:E:16:ASN:OD1	1:E:16:ASN:C	2.64	0.41
1:E:107:ARG:HG2	1:G:107:ARG:O	2.20	0.41
1:E:259:LYS:HD2	1:E:259:LYS:HA	1.66	0.41
1:E:271:THR:O	1:E:275:LEU:HD23	2.21	0.41
1:F:122:LYS:H	1:F:122:LYS:HG3	1.70	0.41
1:F:266:LEU:HB3	1:F:270:MET:HE3	2.02	0.41
1:I:138:TYR:O	1:I:141:ARG:N	2.50	0.41
1:I:270:MET:HG2	1:J:245:GLY:CA	2.51	0.41
1:J:149:ARG:HD2	1:J:156:ILE:HG22	2.03	0.41
1:J:283:GLU:CD	1:J:283:GLU:N	2.78	0.41
1:K:113:PHE:CD2	1:K:113:PHE:N	2.89	0.41
1:K:214:ASN:HA	1:K:238:ILE:CG1	2.51	0.41
1:L:196:ARG:HH11	1:L:196:ARG:CG	2.32	0.41
1:N:62:ILE:HG23	1:O:97:MET:HE3	2.02	0.41
1:A:23:ALA:HA	1:A:24:PRO:HD2	1.88	0.41
1:A:143:ARG:CB	1:C:291:ALA:O	2.62	0.41
1:B:181:ARG:CZ	1:B:209:TRP:HB2	2.51	0.41
1:F:76:SER:HA	1:F:84:VAL:HG21	2.03	0.41
1:J:179:ALA:O	1:J:182:ASP:HB2	2.21	0.41
1:K:21:ILE:HB	1:K:236:ILE:HG12	2.03	0.41
1:L:99:ALA:O	1:L:103:GLU:HG3	2.21	0.41
1:M:85:ILE:HG12	1:M:112:ALA:HB3	2.02	0.41
1:B:140:THR:HA	1:D:291:ALA:O	2.21	0.40
1:D:123:ARG:O	1:D:124:CYS:C	2.63	0.40
1:E:110:VAL:HG12	1:E:156:ILE:HD11	2.03	0.40
1:F:253:GLU:OE1	1:F:253:GLU:HA	2.21	0.40
1:G:124:CYS:SG	1:G:125:GLY:N	2.94	0.40
1:G:137:THR:O	1:G:140:THR:HB	2.21	0.40
1:I:4:VAL:CG1	1:I:5:THR:N	2.84	0.40
1:J:202:VAL:HG13	1:J:203:ILE:N	2.36	0.40
1:M:97:MET:HE3	1:P:62:ILE:HD13	2.03	0.40
1:N:8:THR:HG23	1:N:155:ASP:OD2	2.21	0.40
1:P:90:THR:HG21	1:P:118:GLN:O	2.22	0.40
1:B:210:PRO:HA	1:B:235:ARG:HG3	2.03	0.40
1:E:189:PHE:CE2	1:E:214:ASN:HB2	2.56	0.40
1:G:181:ARG:HG3	1:G:209:TRP:CG	2.56	0.40
1:J:302:LEU:HA	1:J:302:LEU:HD12	1.51	0.40
1:L:12:ARG:HD3	1:L:12:ARG:H	1.84	0.40
1:A:198:MET:O	1:A:199:ALA:C	2.65	0.40
1:F:118:GLN:HA	1:F:132:LEU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ASP:HB2	1:H:276:PHE:CE2	2.57	0.40
1:I:251:MET:O	1:I:255:MET:HB2	2.21	0.40
1:K:149:ARG:HG3	1:K:154:SER:O	2.21	0.40
1:L:164:SER:OG	1:L:173:SER:HA	2.21	0.40
1:L:285:MET:HG2	1:L:296:PHE:CG	2.56	0.40
1:O:165:LEU:HB2	1:O:190:LEU:HD21	2.03	0.40
1:A:47:GLY:HA2	1:A:68:MET:HE1	2.02	0.40
1:B:275:LEU:O	1:B:278:VAL:HB	2.22	0.40
1:D:76:SER:HA	1:D:84:VAL:HG21	2.03	0.40
1:F:11:ARG:NH2	1:F:186:ASP:OD1	2.51	0.40
1:G:198:MET:O	1:G:202:VAL:HG22	2.21	0.40
1:J:66:ASN:OD1	1:K:64:THR:HG21	2.21	0.40
1:K:11:ARG:HH22	1:K:186:ASP:CG	2.28	0.40
1:L:102:THR:HG23	1:L:113:PHE:CZ	2.56	0.40
1:M:100:ARG:HG2	1:M:100:ARG:H	1.76	0.40
1:O:69:ARG:HG3	1:O:104:GLN:HB3	2.03	0.40
1:O:281:LEU:O	1:O:284:SER:HB2	2.22	0.40
1:A:209:TRP:HA	1:A:210:PRO:HD3	2.00	0.40
1:B:210:PRO:CA	1:B:235:ARG:HG3	2.50	0.40
1:F:273:GLN:O	1:F:277:ARG:HG3	2.21	0.40
1:M:47:GLY:HA3	1:M:87:ASP:OD2	2.21	0.40
1:M:57:GLN:HG2	1:M:62:ILE:CD1	2.49	0.40
1:N:152:ILE:HD12	1:P:3:MET:CE	2.51	0.40
1:O:274:MET:HE2	1:O:275:LEU:HG	2.04	0.40
1:P:59:ASP:C	1:P:59:ASP:OD1	2.64	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	299/302 (99%)	278 (93%)	20 (7%)	1 (0%)	36 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	300/302 (99%)	284 (95%)	15 (5%)	1 (0%)	36	58
1	C	299/302 (99%)	286 (96%)	11 (4%)	2 (1%)	18	38
1	D	299/302 (99%)	289 (97%)	8 (3%)	2 (1%)	18	38
1	E	299/302 (99%)	279 (93%)	20 (7%)	0	100	100
1	F	299/302 (99%)	279 (93%)	19 (6%)	1 (0%)	36	58
1	G	299/302 (99%)	282 (94%)	15 (5%)	2 (1%)	18	38
1	H	299/302 (99%)	284 (95%)	14 (5%)	1 (0%)	36	58
1	I	298/302 (99%)	271 (91%)	24 (8%)	3 (1%)	12	28
1	J	288/302 (95%)	260 (90%)	27 (9%)	1 (0%)	36	58
1	K	298/302 (99%)	275 (92%)	20 (7%)	3 (1%)	12	28
1	L	298/302 (99%)	268 (90%)	22 (7%)	8 (3%)	4	7
1	M	298/302 (99%)	270 (91%)	26 (9%)	2 (1%)	18	38
1	N	288/302 (95%)	266 (92%)	18 (6%)	4 (1%)	9	19
1	O	299/302 (99%)	268 (90%)	28 (9%)	3 (1%)	12	28
1	P	299/302 (99%)	262 (88%)	32 (11%)	5 (2%)	7	15
All	All	4759/4832 (98%)	4401 (92%)	319 (7%)	39 (1%)	16	34

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	MET
1	C	299	GLY
1	I	295	ALA
1	J	242	ALA
1	L	151	ARG
1	L	299	GLY
1	O	300	VAL
1	D	297	ASP
1	K	268	LYS
1	L	72	ALA
1	M	242	ALA
1	M	295	ALA
1	N	9	SER
1	N	92	TYR
1	N	242	ALA
1	O	268	LYS
1	P	87	ASP

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Mol	Chain	Res	Type
1	P	89	ASP
1	B	179	ALA
1	L	87	ASP
1	L	205	ASP
1	P	205	ASP
1	P	268	LYS
1	D	300	VAL
1	G	289	ALA
1	H	297	ASP
1	I	259	LYS
1	L	71	ASN
1	L	89	ASP
1	G	89	ASP
1	I	173	SER
1	N	8	THR
1	P	266	LEU
1	C	203	ILE
1	F	106	SER
1	K	264	PRO
1	O	199	ALA
1	K	298	GLY
1	L	156	ILE

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/228 (99%)	201 (89%)	24 (11%)	6	14
1	B	226/228 (99%)	202 (89%)	24 (11%)	6	14
1	C	227/228 (100%)	201 (88%)	26 (12%)	5	11
1	D	226/228 (99%)	199 (88%)	27 (12%)	5	10
1	E	227/228 (100%)	197 (87%)	30 (13%)	4	8
1	F	226/228 (99%)	197 (87%)	29 (13%)	4	8
1	G	227/228 (100%)	201 (88%)	26 (12%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	227/228 (100%)	196 (86%)	31 (14%)	3	7
1	I	225/228 (99%)	200 (89%)	25 (11%)	6	12
1	J	220/228 (96%)	192 (87%)	28 (13%)	4	9
1	K	225/228 (99%)	202 (90%)	23 (10%)	7	15
1	L	224/228 (98%)	193 (86%)	31 (14%)	3	7
1	M	226/228 (99%)	199 (88%)	27 (12%)	5	10
1	N	220/228 (96%)	181 (82%)	39 (18%)	2	3
1	O	222/228 (97%)	196 (88%)	26 (12%)	5	11
1	P	226/228 (99%)	196 (87%)	30 (13%)	4	8
All	All	3599/3648 (99%)	3153 (88%)	446 (12%)	4	9

All (446) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	19	SER
1	A	36	LEU
1	A	46	THR
1	A	57	GLN
1	A	74	MET
1	A	100	ARG
1	A	115	ILE
1	A	122	LYS
1	A	140	THR
1	A	173	SER
1	A	189	PHE
1	A	190	LEU
1	A	196	ARG
1	A	197	GLU
1	A	204	GLN
1	A	206	LEU
1	A	212	LEU
1	A	232	MET
1	A	253	GLU
1	A	256	GLU
1	A	269	GLU
1	A	300	VAL
1	A	302	LEU
1	B	21	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	26	VAL
1	B	36	LEU
1	B	46	THR
1	B	115	ILE
1	B	119	VAL
1	B	122	LYS
1	B	131	ILE
1	B	133	VAL
1	B	134	ASP
1	B	143	ARG
1	B	166	GLN
1	B	167	THR
1	B	173	SER
1	B	190	LEU
1	B	193	ILE
1	B	223	SER
1	B	244	LEU
1	B	266	LEU
1	B	269	GLU
1	B	275	LEU
1	B	283	GLU
1	B	300	VAL
1	B	303	LYS
1	C	12	ARG
1	C	16	ASN
1	C	22	VAL
1	C	30	LEU
1	C	36	LEU
1	C	46	THR
1	C	64	THR
1	C	74	MET
1	C	100	ARG
1	C	121	THR
1	C	123	ARG
1	C	133	VAL
1	C	140	THR
1	C	178	ARG
1	C	190	LEU
1	C	196	ARG
1	C	202	VAL
1	C	204	GLN
1	C	256	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	259	LYS
1	C	263	ILE
1	C	266	LEU
1	C	268	LYS
1	C	269	GLU
1	C	270	MET
1	C	290	GLN
1	D	3	MET
1	D	4	VAL
1	D	9	SER
1	D	21	ILE
1	D	36	LEU
1	D	43	LEU
1	D	46	THR
1	D	62	ILE
1	D	64	THR
1	D	122	LYS
1	D	133	VAL
1	D	143	ARG
1	D	151	ARG
1	D	167	THR
1	D	181	ARG
1	D	190	LEU
1	D	194	THR
1	D	200	ARG
1	D	204	GLN
1	D	212	LEU
1	D	244	LEU
1	D	252	ARG
1	D	268	LYS
1	D	284	SER
1	D	300	VAL
1	D	301	ASP
1	D	302	LEU
1	E	2	PRO
1	E	5	THR
1	E	11	ARG
1	E	19	SER
1	E	31	SER
1	E	34	VAL
1	E	36	LEU
1	E	46	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	64	THR
1	E	74	MET
1	E	120	GLN
1	E	122	LYS
1	E	127	LEU
1	E	132	LEU
1	E	146	VAL
1	E	166	GLN
1	E	171	GLU
1	E	190	LEU
1	E	196	ARG
1	E	197	GLU
1	E	206	LEU
1	E	232	MET
1	E	252	ARG
1	E	253	GLU
1	E	259	LYS
1	E	263	ILE
1	E	268	LYS
1	E	269	GLU
1	E	297	ASP
1	E	300	VAL
1	F	4	VAL
1	F	21	ILE
1	F	46	THR
1	F	74	MET
1	F	78	ILE
1	F	95	PRO
1	F	100	ARG
1	F	115	ILE
1	F	122	LYS
1	F	133	VAL
1	F	140	THR
1	F	166	GLN
1	F	167	THR
1	F	172	GLU
1	F	173	SER
1	F	189	PHE
1	F	190	LEU
1	F	193	ILE
1	F	197	GLU
1	F	201	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	211	LEU
1	F	212	LEU
1	F	223	SER
1	F	259	LYS
1	F	269	GLU
1	F	275	LEU
1	F	286	LYS
1	F	297	ASP
1	F	300	VAL
1	G	11	ARG
1	G	12	ARG
1	G	36	LEU
1	G	57	GLN
1	G	62	ILE
1	G	65	LEU
1	G	74	MET
1	G	100	ARG
1	G	116	GLU
1	G	132	LEU
1	G	140	THR
1	G	143	ARG
1	G	167	THR
1	G	181	ARG
1	G	182	ASP
1	G	189	PHE
1	G	190	LEU
1	G	200	ARG
1	G	202	VAL
1	G	204	GLN
1	G	252	ARG
1	G	259	LYS
1	G	268	LYS
1	G	269	GLU
1	G	281	LEU
1	G	286	LYS
1	H	9	SER
1	H	18	ASP
1	H	36	LEU
1	H	46	THR
1	H	62	ILE
1	H	64	THR
1	H	66	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	115	ILE
1	H	122	LYS
1	H	133	VAL
1	H	151	ARG
1	H	166	GLN
1	H	167	THR
1	H	173	SER
1	H	181	ARG
1	H	190	LEU
1	H	194	THR
1	H	202	VAL
1	H	206	LEU
1	H	212	LEU
1	H	215	MET
1	H	224	ILE
1	H	231	GLU
1	H	252	ARG
1	H	253	GLU
1	H	263	ILE
1	H	275	LEU
1	H	277	ARG
1	H	283	GLU
1	H	297	ASP
1	H	300	VAL
1	I	5	THR
1	I	8	THR
1	I	9	SER
1	I	22	VAL
1	I	57	GLN
1	I	69	ARG
1	I	74	MET
1	I	100	ARG
1	I	115	ILE
1	I	122	LYS
1	I	124	CYS
1	I	134	ASP
1	I	166	GLN
1	I	186	ASP
1	I	189	PHE
1	I	212	LEU
1	I	218	HIS
1	I	231	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	244	LEU
1	I	252	ARG
1	I	259	LYS
1	I	267	ASP
1	I	274	MET
1	I	277	ARG
1	I	301	ASP
1	J	11	ARG
1	J	26	VAL
1	J	36	LEU
1	J	46	THR
1	J	79	SER
1	J	96	ILE
1	J	115	ILE
1	J	116	GLU
1	J	131	ILE
1	J	146	VAL
1	J	152	ILE
1	J	156	ILE
1	J	167	THR
1	J	190	LEU
1	J	193	ILE
1	J	204	GLN
1	J	212	LEU
1	J	213	LEU
1	J	215	MET
1	J	218	HIS
1	J	223	SER
1	J	256	GLU
1	J	266	LEU
1	J	268	LYS
1	J	271	THR
1	J	277	ARG
1	J	301	ASP
1	J	302	LEU
1	K	19	SER
1	K	26	VAL
1	K	36	LEU
1	K	37	SER
1	K	74	MET
1	K	78	ILE
1	K	96	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	115	ILE
1	K	122	LYS
1	K	131	ILE
1	K	133	VAL
1	K	149	ARG
1	K	161	ARG
1	K	190	LEU
1	K	195	SER
1	K	200	ARG
1	K	202	VAL
1	K	223	SER
1	K	225	SER
1	K	256	GLU
1	K	266	LEU
1	K	267	ASP
1	K	301	ASP
1	L	4	VAL
1	L	12	ARG
1	L	34	VAL
1	L	36	LEU
1	L	64	THR
1	L	67	ASP
1	L	96	ILE
1	L	100	ARG
1	L	115	ILE
1	L	122	LYS
1	L	127	LEU
1	L	131	ILE
1	L	140	THR
1	L	173	SER
1	L	174	VAL
1	L	189	PHE
1	L	196	ARG
1	L	197	GLU
1	L	213	LEU
1	L	225	SER
1	L	231	GLU
1	L	237	ILE
1	L	239	PHE
1	L	252	ARG
1	L	253	GLU
1	L	263	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	269	GLU
1	L	283	GLU
1	L	286	LYS
1	L	300	VAL
1	L	301	ASP
1	M	12	ARG
1	M	37	SER
1	M	66	ASN
1	M	78	ILE
1	M	82	THR
1	M	122	LYS
1	M	127	LEU
1	M	134	ASP
1	M	137	THR
1	M	143	ARG
1	M	151	ARG
1	M	158	VAL
1	M	167	THR
1	M	190	LEU
1	M	195	SER
1	M	198	MET
1	M	204	GLN
1	M	211	LEU
1	M	228	GLU
1	M	231	GLU
1	M	259	LYS
1	M	269	GLU
1	M	273	GLN
1	M	274	MET
1	M	277	ARG
1	M	285	MET
1	M	301	ASP
1	N	3	MET
1	N	4	VAL
1	N	5	THR
1	N	8	THR
1	N	9	SER
1	N	11	ARG
1	N	12	ARG
1	N	28	ASP
1	N	36	LEU
1	N	45	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	N	74	MET
1	N	76	SER
1	N	78	ILE
1	N	79	SER
1	N	81	SER
1	N	82	THR
1	N	100	ARG
1	N	115	ILE
1	N	119	VAL
1	N	121	THR
1	N	140	THR
1	N	166	GLN
1	N	190	LEU
1	N	193	ILE
1	N	201	GLN
1	N	202	VAL
1	N	204	GLN
1	N	206	LEU
1	N	211	LEU
1	N	223	SER
1	N	231	GLU
1	N	253	GLU
1	N	266	LEU
1	N	269	GLU
1	N	270	MET
1	N	271	THR
1	N	275	LEU
1	N	296	PHE
1	N	300	VAL
1	O	9	SER
1	O	16	ASN
1	O	31	SER
1	O	36	LEU
1	O	46	THR
1	O	60	LEU
1	O	62	ILE
1	O	100	ARG
1	O	122	LYS
1	O	131	ILE
1	O	167	THR
1	O	173	SER
1	O	190	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	197	GLU
1	O	223	SER
1	O	225	SER
1	O	244	LEU
1	O	252	ARG
1	O	261	ASP
1	O	267	ASP
1	O	273	GLN
1	O	274	MET
1	O	281	LEU
1	O	286	LYS
1	O	290	GLN
1	O	300	VAL
1	P	9	SER
1	P	15	GLU
1	P	22	VAL
1	P	36	LEU
1	P	46	THR
1	P	54	VAL
1	P	64	THR
1	P	76	SER
1	P	96	ILE
1	P	97	MET
1	P	108	SER
1	P	122	LYS
1	P	127	LEU
1	P	137	THR
1	P	154	SER
1	P	166	GLN
1	P	171	GLU
1	P	174	VAL
1	P	200	ARG
1	P	204	GLN
1	P	205	ASP
1	P	217	GLU
1	P	228	GLU
1	P	256	GLU
1	P	268	LYS
1	P	269	GLU
1	P	270	MET
1	P	275	LEU
1	P	277	ARG

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Mol	Chain	Res	Type
1	P	300	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	104	GLN
1	A	166	GLN
1	B	120	GLN
1	B	147	GLN
1	B	166	GLN
1	C	57	GLN
1	D	104	GLN
1	D	120	GLN
1	E	104	GLN
1	E	120	GLN
1	E	168	HIS
1	F	77	ASN
1	F	150	GLN
1	F	166	GLN
1	F	168	HIS
1	F	201	GLN
1	G	57	GLN
1	G	290	GLN
1	H	150	GLN
1	H	166	GLN
1	H	290	GLN
1	I	104	GLN
1	I	147	GLN
1	J	16	ASN
1	J	118	GLN
1	J	147	GLN
1	K	166	GLN
1	K	168	HIS
1	K	204	GLN
1	L	147	GLN
1	L	166	GLN
1	N	71	ASN
1	O	71	ASN
1	O	166	GLN
1	O	290	GLN
1	P	204	GLN

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Mol	Chain	Res	Type
1	P	273	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 16 are monoatomic - leaving 19 for Mogul analysis.

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
3	OAF	G	501	2	10,11,11	1.91	2 (20%)	13,18,18	1.15	1 (7%)
3	OAF	F	501	2	10,11,11	1.41	1 (10%)	13,18,18	2.49	6 (46%)
3	OAF	D	501	2	10,11,11	2.46	3 (30%)	13,18,18	3.26	5 (38%)
4	GOL	A	602	-	5,5,5	0.95	0	5,5,5	1.70	2 (40%)
3	OAF	K	501	2	10,11,11	1.29	1 (10%)	13,18,18	1.43	3 (23%)
3	OAF	B	501	2	10,11,11	1.12	0	13,18,18	2.10	5 (38%)
3	OAF	C	501	2	10,11,11	1.76	3 (30%)	13,18,18	1.40	3 (23%)
4	GOL	A	605	-	5,5,5	0.52	0	5,5,5	1.08	0
4	GOL	M	606	-	5,5,5	0.52	0	5,5,5	0.98	0
3	OAF	E	501	2	10,11,11	1.80	2 (20%)	13,18,18	1.76	6 (46%)
3	OAF	P	501	2	10,11,11	2.54	3 (30%)	13,18,18	3.28	6 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	G	601	-	5,5,5	0.91	0	5,5,5	1.85	2 (40%)
3	OAF	O	501	2	10,11,11	1.58	2 (20%)	13,18,18	2.38	6 (46%)
3	OAF	I	501	2	10,11,11	1.22	2 (20%)	13,18,18	1.59	4 (30%)
4	GOL	E	604	-	5,5,5	0.72	0	5,5,5	0.77	0
3	OAF	A	501	2	10,11,11	1.80	2 (20%)	13,18,18	1.79	3 (23%)
3	OAF	M	501	2	10,11,11	1.47	1 (10%)	13,18,18	1.68	3 (23%)
3	OAF	H	501	2	10,11,11	1.71	1 (10%)	13,18,18	1.83	4 (30%)
3	OAF	L	501	2	10,11,11	1.83	3 (30%)	13,18,18	3.14	3 (23%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OAF	G	501	2	-	6/14/21/21	-
3	OAF	F	501	2	-	5/14/21/21	-
3	OAF	D	501	2	-	3/14/21/21	-
4	GOL	A	602	-	-	2/4/4/4	-
3	OAF	K	501	2	-	7/14/21/21	-
3	OAF	B	501	2	-	5/14/21/21	-
3	OAF	C	501	2	-	4/14/21/21	-
4	GOL	A	605	-	-	3/4/4/4	-
4	GOL	M	606	-	-	2/4/4/4	-
3	OAF	E	501	2	-	5/14/21/21	-
3	OAF	P	501	2	-	6/14/21/21	-
4	GOL	G	601	-	-	4/4/4/4	-
3	OAF	O	501	2	-	6/14/21/21	-
3	OAF	I	501	2	-	5/14/21/21	-
4	GOL	E	604	-	-	0/4/4/4	-
3	OAF	A	501	2	-	3/14/21/21	-
3	OAF	M	501	2	-	1/14/21/21	-
3	OAF	H	501	2	-	4/14/21/21	-
3	OAF	L	501	2	-	1/14/21/21	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	OAF	C3-C4	-6.62	1.45	1.54
3	P	501	OAF	C3-C4	5.01	1.62	1.54
3	P	501	OAF	O3-C2	4.65	1.46	1.39
3	H	501	OAF	C3-C4	-4.37	1.48	1.54
3	G	501	OAF	C3-C2	-4.29	1.50	1.54
3	A	501	OAF	C3-C4	-3.94	1.49	1.54
3	L	501	OAF	O3-C2	3.94	1.45	1.39
3	P	501	OAF	O4-C2	3.34	1.44	1.39
3	C	501	OAF	O4-C2	3.11	1.44	1.39
3	E	501	OAF	O3-C2	3.10	1.44	1.39
3	C	501	OAF	C3-C2	-3.10	1.51	1.54
3	E	501	OAF	O4-C2	3.05	1.44	1.39
3	M	501	OAF	C3-C2	3.04	1.56	1.54
3	F	501	OAF	O4-C2	2.87	1.44	1.39
3	O	501	OAF	C3-C4	-2.61	1.51	1.54
3	L	501	OAF	O4-C2	2.46	1.43	1.39
3	O	501	OAF	C3-C2	-2.44	1.51	1.54
3	L	501	OAF	C3-C4	2.43	1.58	1.54
3	D	501	OAF	O5-C4	-2.37	1.21	1.30
3	D	501	OAF	C3-C2	-2.35	1.52	1.54
3	K	501	OAF	O4-C2	2.33	1.43	1.39
3	G	501	OAF	O4-C2	2.19	1.43	1.39
3	I	501	OAF	O3-C2	2.18	1.43	1.39
3	I	501	OAF	O5-C4	-2.15	1.22	1.30
3	A	501	OAF	O3-C2	2.05	1.42	1.39
3	C	501	OAF	O2-C1	-2.01	1.23	1.30

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	OAF	F2-C3-C2	-9.78	97.81	109.32
3	P	501	OAF	F2-C3-C2	-9.26	98.42	109.32
3	D	501	OAF	F1-C3-C2	7.48	118.12	109.32
3	D	501	OAF	F2-C3-C2	-7.06	101.01	109.32
3	F	501	OAF	F1-C3-C2	6.18	116.60	109.32
3	O	501	OAF	F1-C3-C2	-5.10	103.31	109.32
3	L	501	OAF	F1-C3-C2	4.09	114.14	109.32
3	O	501	OAF	F1-C3-C4	-3.83	101.60	110.37
3	P	501	OAF	F2-C3-F1	3.80	116.22	106.56
3	M	501	OAF	O3-C2-C3	3.59	115.28	107.18
3	A	501	OAF	C2-C3-C4	-3.43	107.70	114.16
3	D	501	OAF	F1-C3-C4	-3.36	102.66	110.37
3	H	501	OAF	F1-C3-C2	3.30	113.21	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	OAF	F1-C3-C4	-3.30	102.82	110.37
3	I	501	OAF	F1-C3-C4	-3.29	102.83	110.37
3	F	501	OAF	F1-C3-C4	-3.29	102.83	110.37
3	B	501	OAF	F2-C3-C2	-3.15	105.61	109.32
3	M	501	OAF	C2-C3-C4	-3.12	108.28	114.16
3	P	501	OAF	F1-C3-C2	3.09	112.96	109.32
3	O	501	OAF	F2-C3-F1	3.05	114.34	106.56
3	E	501	OAF	C2-C3-C4	-2.97	108.56	114.16
3	I	501	OAF	O3-C2-C3	2.87	113.67	107.18
3	B	501	OAF	O3-C2-C3	2.84	113.59	107.18
3	F	501	OAF	F2-C3-C2	-2.84	105.98	109.32
3	B	501	OAF	F2-C3-F1	2.83	113.76	106.56
3	K	501	OAF	O5-C4-C3	2.82	119.28	112.50
3	F	501	OAF	O5-C4-C3	2.81	119.24	112.50
3	D	501	OAF	F2-C3-F1	2.74	113.53	106.56
3	K	501	OAF	F1-C3-C2	-2.73	106.11	109.32
3	O	501	OAF	O5-C4-C3	2.72	119.05	112.50
3	A	501	OAF	F2-C3-C2	2.72	112.52	109.32
3	B	501	OAF	O5-C4-C3	2.71	119.00	112.50
3	C	501	OAF	F1-C3-C4	-2.70	104.19	110.37
3	O	501	OAF	O4-C2-C3	2.66	113.18	107.18
3	P	501	OAF	O4-C2-C3	2.66	113.17	107.18
4	A	602	GOL	O2-C2-C3	2.65	120.15	109.18
3	L	501	OAF	O5-C4-C3	2.58	118.71	112.50
4	G	601	GOL	O1-C1-C2	2.54	121.81	110.38
3	E	501	OAF	F1-C3-C4	2.53	116.16	110.37
3	E	501	OAF	F2-C3-F1	-2.52	100.14	106.56
3	A	501	OAF	O3-C2-C3	2.49	112.80	107.18
3	E	501	OAF	O5-C4-C3	2.49	118.47	112.50
3	K	501	OAF	O3-C2-C3	2.44	112.68	107.18
3	H	501	OAF	O5-C4-C3	2.39	118.25	112.50
3	P	501	OAF	O5-C4-C3	2.39	118.25	112.50
3	H	501	OAF	O3-C2-C3	2.39	112.57	107.18
3	P	501	OAF	F1-C3-C4	-2.31	105.07	110.37
4	G	601	GOL	O3-C3-C2	-2.24	100.30	110.38
3	C	501	OAF	F2-C3-C4	2.22	115.45	110.37
3	H	501	OAF	O6-C4-C3	-2.20	114.28	119.57
3	F	501	OAF	F2-C3-C4	2.20	115.40	110.37
3	C	501	OAF	O5-C4-C3	2.18	117.74	112.50
3	G	501	OAF	O5-C4-C3	2.17	117.72	112.50
3	M	501	OAF	F1-C3-C2	2.15	111.85	109.32
3	I	501	OAF	F2-C3-C4	2.12	115.23	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	501	OAF	C2-C3-C4	-2.11	110.19	114.16
3	O	501	OAF	O6-C4-C3	-2.10	114.53	119.57
3	E	501	OAF	F1-C3-C2	2.09	111.79	109.32
3	E	501	OAF	O6-C4-C3	-2.09	114.54	119.57
4	A	602	GOL	O2-C2-C1	2.08	117.77	109.18
3	D	501	OAF	O3-C2-C3	2.08	111.87	107.18
3	F	501	OAF	C2-C3-C4	-2.07	110.27	114.16

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	501	OAF	O3-C2-C3-F1
3	G	501	OAF	O4-C2-C3-F1
3	G	501	OAF	O4-C2-C3-F2
3	G	501	OAF	O3-C2-C3-F1
3	I	501	OAF	O2-C1-C2-O3
3	K	501	OAF	O2-C1-C2-O3
3	K	501	OAF	O1-C1-C2-O4
3	K	501	OAF	O1-C1-C2-O3
3	K	501	OAF	O3-C2-C3-F1
3	O	501	OAF	O2-C1-C2-O4
3	O	501	OAF	O4-C2-C3-F2
3	O	501	OAF	O3-C2-C3-F1
3	P	501	OAF	O4-C2-C3-F2
4	A	605	GOL	O1-C1-C2-O2
4	A	605	GOL	O1-C1-C2-C3
4	G	601	GOL	O1-C1-C2-C3
4	G	601	GOL	C1-C2-C3-O3
4	M	606	GOL	O1-C1-C2-C3
4	M	606	GOL	O1-C1-C2-O2
4	A	602	GOL	O1-C1-C2-O2
4	A	602	GOL	O2-C2-C3-O3
4	G	601	GOL	O1-C1-C2-O2
4	G	601	GOL	O2-C2-C3-O3
3	D	501	OAF	O3-C2-C3-F2
3	E	501	OAF	O4-C2-C3-F1
3	F	501	OAF	O3-C2-C3-F1
3	O	501	OAF	O4-C2-C3-F1
3	O	501	OAF	O3-C2-C3-F2
3	H	501	OAF	O3-C2-C3-F1
3	I	501	OAF	O3-C2-C3-F1

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Mol	Chain	Res	Type	Atoms
3	K	501	OAF	O4-C2-C3-F1
3	P	501	OAF	O3-C2-C3-F1
4	A	605	GOL	O2-C2-C3-O3
3	B	501	OAF	O4-C2-C3-F2
3	B	501	OAF	O3-C2-C3-F1
3	B	501	OAF	O3-C2-C3-F2
3	C	501	OAF	O4-C2-C3-F1
3	C	501	OAF	O3-C2-C3-F1
3	D	501	OAF	O3-C2-C3-F1
3	H	501	OAF	O4-C2-C3-F2
3	H	501	OAF	O3-C2-C3-F2
3	I	501	OAF	O3-C2-C3-F2
3	K	501	OAF	O4-C2-C3-F2
3	P	501	OAF	O4-C2-C3-F1
3	P	501	OAF	O3-C2-C3-F2
3	A	501	OAF	O1-C1-C2-O4
3	E	501	OAF	O1-C1-C2-O4
3	G	501	OAF	O1-C1-C2-O4
3	I	501	OAF	O1-C1-C2-O4
3	I	501	OAF	O1-C1-C2-O3
3	M	501	OAF	O1-C1-C2-O4
3	A	501	OAF	O2-C1-C2-O4
3	B	501	OAF	O2-C1-C2-O4
3	B	501	OAF	O2-C1-C2-O3
3	C	501	OAF	O2-C1-C2-O4
3	D	501	OAF	O2-C1-C2-O4
3	E	501	OAF	O2-C1-C2-O4
3	F	501	OAF	O2-C1-C2-O4
3	G	501	OAF	O2-C1-C2-O4
3	H	501	OAF	O2-C1-C2-O4
3	L	501	OAF	O2-C1-C2-O4
3	O	501	OAF	O2-C1-C2-O3
3	P	501	OAF	F1-C3-C4-O5
3	P	501	OAF	F1-C3-C4-O6
3	F	501	OAF	O4-C2-C3-F1
3	F	501	OAF	O4-C2-C3-F2
3	F	501	OAF	O3-C2-C3-F2
3	A	501	OAF	O3-C2-C3-F1
3	C	501	OAF	O4-C2-C3-F2
3	E	501	OAF	O4-C2-C3-F2
3	G	501	OAF	O3-C2-C3-F2
3	K	501	OAF	O3-C2-C3-F2

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	OAF	1	0
3	D	501	OAF	2	0
4	A	602	GOL	3	0
3	K	501	OAF	1	0
4	A	605	GOL	3	0
4	M	606	GOL	1	0
3	P	501	OAF	1	0
4	G	601	GOL	2	0
3	O	501	OAF	1	0
3	I	501	OAF	2	0
3	M	501	OAF	1	0
3	H	501	OAF	1	0
3	L	501	OAF	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	301/302 (99%)	-1.73	0 100 100	33, 37, 40, 44	0
1	B	302/302 (100%)	-1.72	0 100 100	33, 37, 42, 44	0
1	C	301/302 (99%)	-1.74	0 100 100	31, 37, 41, 44	0
1	D	301/302 (99%)	-1.75	0 100 100	33, 37, 41, 45	0
1	E	301/302 (99%)	-1.74	0 100 100	33, 37, 41, 44	0
1	F	301/302 (99%)	-1.72	0 100 100	32, 37, 41, 45	0
1	G	301/302 (99%)	-1.72	0 100 100	33, 37, 40, 45	0
1	H	301/302 (99%)	-1.73	0 100 100	32, 37, 41, 44	0
1	I	300/302 (99%)	-1.71	0 100 100	32, 38, 41, 46	0
1	J	292/302 (96%)	-1.70	0 100 100	33, 38, 42, 46	0
1	K	300/302 (99%)	-1.73	0 100 100	33, 38, 42, 48	0
1	L	300/302 (99%)	-1.65	0 100 100	33, 38, 44, 48	0
1	M	300/302 (99%)	-1.72	0 100 100	32, 37, 42, 47	0
1	N	292/302 (96%)	-1.69	0 100 100	32, 38, 42, 48	0
1	O	301/302 (99%)	-1.72	0 100 100	33, 38, 42, 46	0
1	P	301/302 (99%)	-1.68	0 100 100	34, 38, 43, 47	0
All	All	4795/4832 (99%)	-1.72	0 100 100	31, 37, 42, 48	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	OAF	B	501	12/12	0.99	0.03	28,32,36,36	0
3	OAF	I	501	12/12	0.99	0.03	35,36,38,41	0
3	OAF	L	501	12/12	0.99	0.04	38,41,43,44	0
3	OAF	P	501	12/12	0.99	0.03	37,40,42,42	0
4	GOL	A	602	6/6	0.99	0.04	33,35,39,40	0
4	GOL	A	605	6/6	0.99	0.03	36,39,41,42	0
4	GOL	E	604	6/6	0.99	0.04	37,40,41,43	0
4	GOL	M	606	6/6	0.99	0.04	35,38,39,41	0
2	MN	I	401	1/1	1.00	0.02	39,39,39,39	0
2	MN	J	401	1/1	1.00	0.02	43,43,43,43	0
2	MN	K	401	1/1	1.00	0.02	38,38,38,38	0
2	MN	L	401	1/1	1.00	0.03	41,41,41,41	0
2	MN	M	401	1/1	1.00	0.02	38,38,38,38	0
2	MN	N	401	1/1	1.00	0.02	43,43,43,43	0
2	MN	O	401	1/1	1.00	0.02	39,39,39,39	0
2	MN	P	401	1/1	1.00	0.03	42,42,42,42	0
3	OAF	A	501	12/12	1.00	0.04	33,35,36,37	0
2	MN	A	401	1/1	1.00	0.02	33,33,33,33	0
3	OAF	C	501	12/12	1.00	0.03	32,34,35,36	0
3	OAF	D	501	12/12	1.00	0.02	30,31,33,34	0
3	OAF	E	501	12/12	1.00	0.02	28,32,34,34	0
3	OAF	F	501	12/12	1.00	0.03	32,33,35,35	0
3	OAF	G	501	12/12	1.00	0.02	31,34,37,38	0
3	OAF	H	501	12/12	1.00	0.02	33,36,36,39	0
2	MN	B	401	1/1	1.00	0.02	37,37,37,37	0
3	OAF	K	501	12/12	1.00	0.03	33,36,38,39	0
2	MN	C	401	1/1	1.00	0.02	35,35,35,35	0
3	OAF	M	501	12/12	1.00	0.02	29,34,36,37	0
3	OAF	O	501	12/12	1.00	0.02	30,35,37,38	0
2	MN	D	401	1/1	1.00	0.01	36,36,36,36	0
2	MN	E	401	1/1	1.00	0.03	36,36,36,36	0
2	MN	F	401	1/1	1.00	0.02	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	G	401	1/1	1.00	0.02	34,34,34,34	0
4	GOL	G	601	6/6	1.00	0.03	31,35,37,38	0
2	MN	H	401	1/1	1.00	0.03	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.