



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 10:38 am GMT

PDB ID : 3HWX  
Title : Crystal structure of menaquinone synthesis protein MenD from E. coli in complex with ThDP  
Authors : Priyadarshi, A.; Hwang, K.Y.  
Deposited on : 2009-06-19  
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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

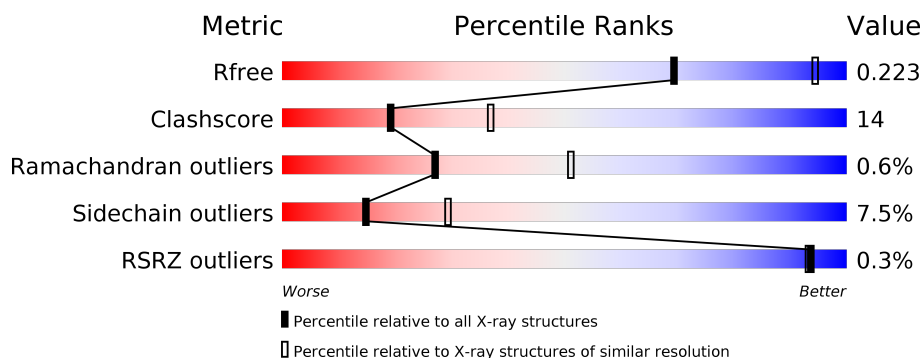
# 1 Overall quality at a glance

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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	556	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>.</div> </div> </div>
1	A	556	<div> <div>66%</div> <div>30%</div> <div>.</div> </div>
1	B	556	<div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	I	556	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>.</div> </div> </div>
1	J	556	<div> <div>68%</div> <div>29%</div> <div>.</div> </div>
1	R	556	<div> <div>70%</div> <div>27%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	S	556	<div><div>%</div><div><div></div><div>68%</div><div>28%</div><div></div></div><div></div></div>
1	Z	556	<div><div></div><div>65%</div><div>30%</div><div></div></div> <div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35302 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-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4323	2742	780	786	15			
1	B	556	Total	C	N	O	S	0	0	0
			4332	2747	781	789	15			
1	I	554	Total	C	N	O	S	0	0	0
			4319	2740	779	785	15			
1	J	556	Total	C	N	O	S	0	0	0
			4332	2747	781	789	15			
1	R	554	Total	C	N	O	S	0	0	0
			4319	2740	779	785	15			
1	S	556	Total	C	N	O	S	0	0	0
			4332	2747	781	789	15			
1	Z	554	Total	C	N	O	S	0	0	0
			4319	2740	779	785	15			
1	1	556	Total	C	N	O	S	0	0	0
			4332	2747	781	789	15			

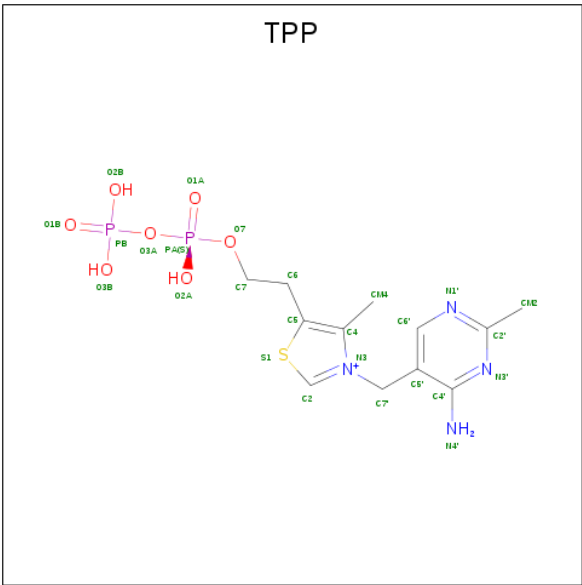
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	LEU	PRO	ENGINEERED	UNP P17109
B	36	LEU	PRO	ENGINEERED	UNP P17109
I	36	LEU	PRO	ENGINEERED	UNP P17109
J	36	LEU	PRO	ENGINEERED	UNP P17109
R	36	LEU	PRO	ENGINEERED	UNP P17109
S	36	LEU	PRO	ENGINEERED	UNP P17109
Z	36	LEU	PRO	ENGINEERED	UNP P17109
1	36	LEU	PRO	ENGINEERED	UNP P17109

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	I	3	Total Na 3 3	0	0
2	Z	2	Total Na 2 2	0	0
2	A	2	Total Na 2 2	0	0
2	R	3	Total Na 3 3	0	0
2	S	3	Total Na 3 3	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 26 12 4 7 2 1	0	0
3	B	1	Total C N O P S 26 12 4 7 2 1	0	0
3	I	1	Total C N O P S 26 12 4 7 2 1	0	0
3	J	1	Total C N O P S 26 12 4 7 2 1	0	0
3	R	1	Total C N O P S 26 12 4 7 2 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	S	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
3	Z	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
3	1	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Mg	0	0
			1	1		
4	1	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	Z	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	R	1	Total	Mg	0	0
			1	1		
4	S	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			6	3	3		
5	1	1	Total	C	O	0	0
			6	3	3		

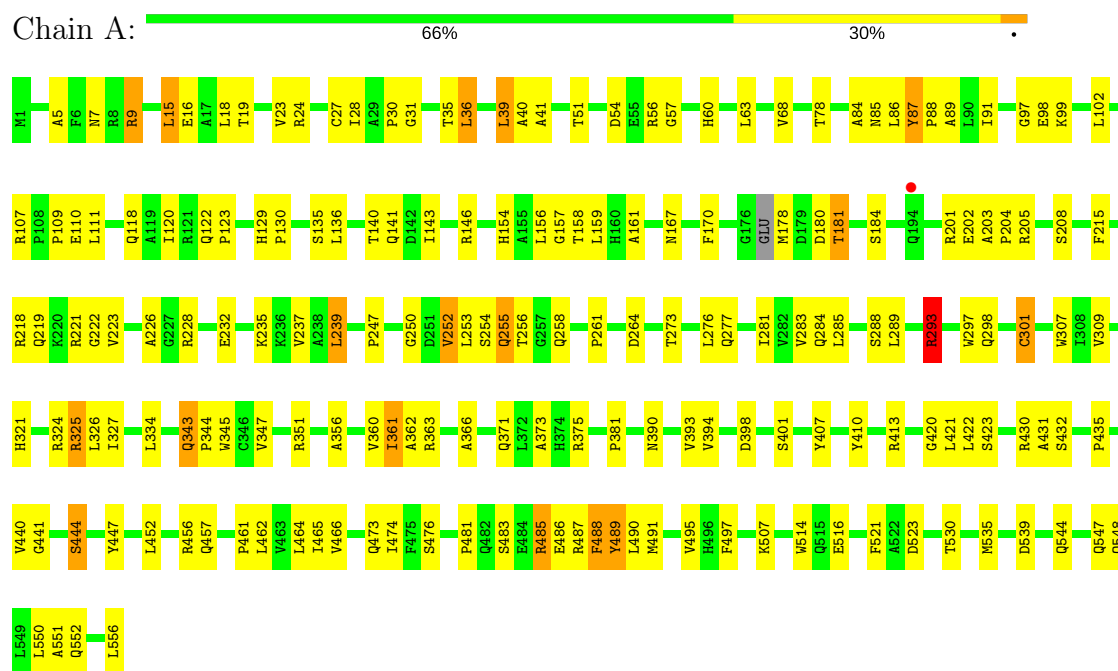
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total	O	0	0
			50	50		
6	B	56	Total	O	0	0
			56	56		
6	I	53	Total	O	0	0
			53	53		
6	J	43	Total	O	0	0
			43	43		
6	R	55	Total	O	0	0
			55	55		
6	S	76	Total	O	0	0
			76	76		
6	Z	55	Total	O	0	0
			55	55		
6	1	63	Total	O	0	0
			63	63		

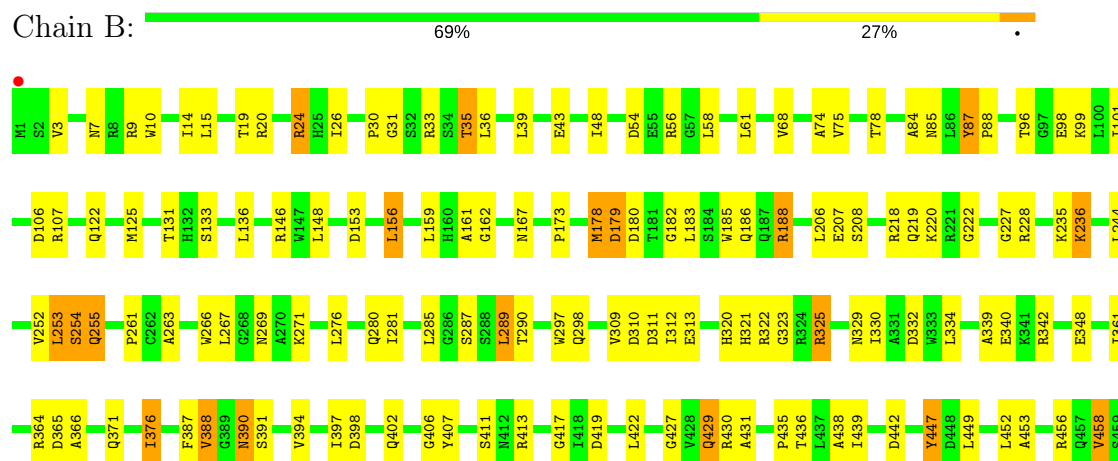
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

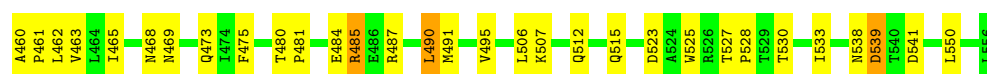
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



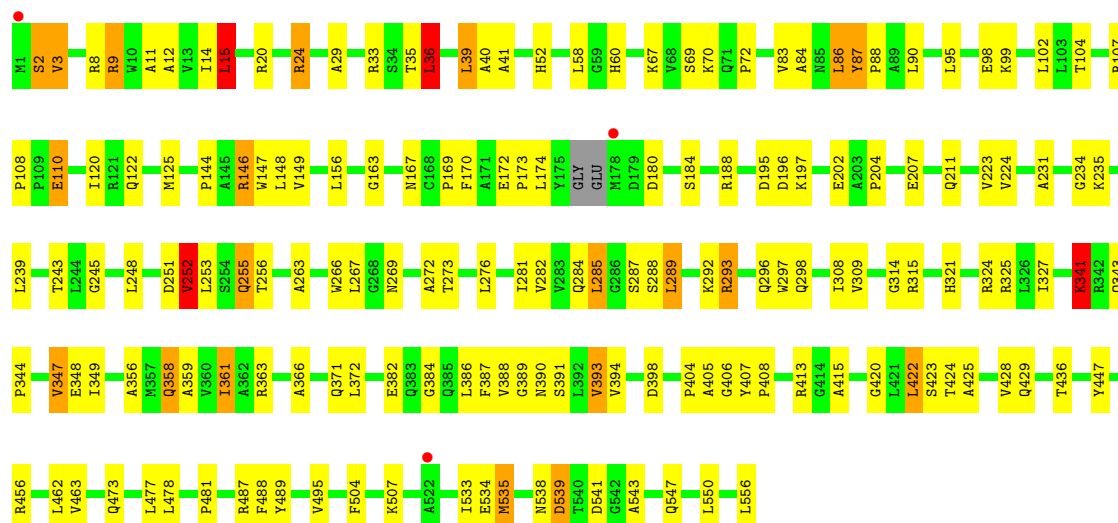
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



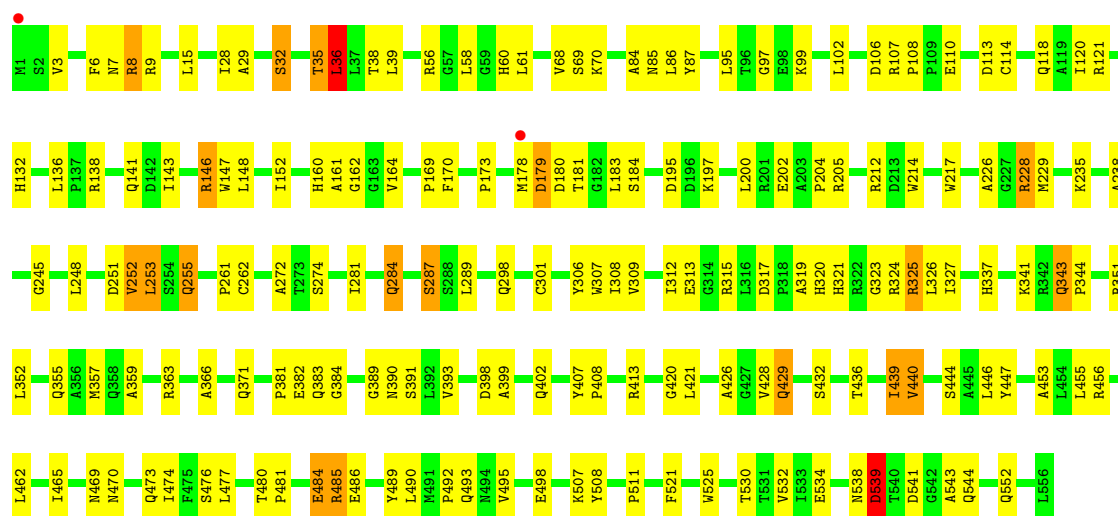




• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

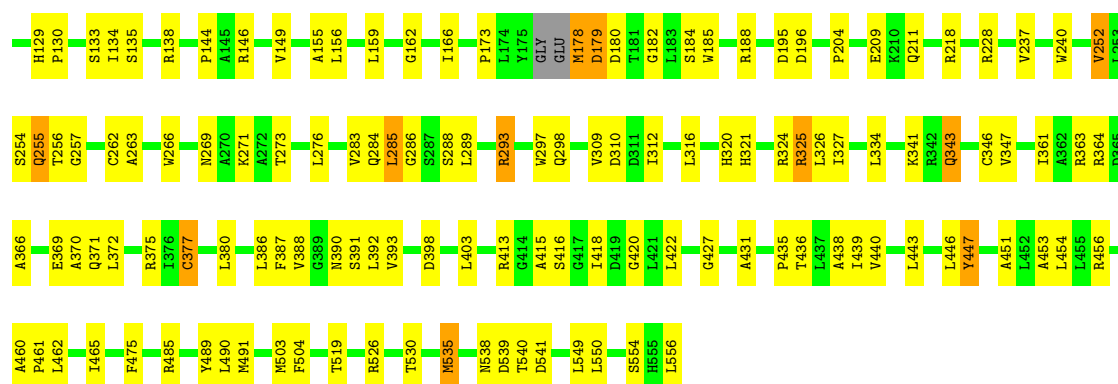


• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

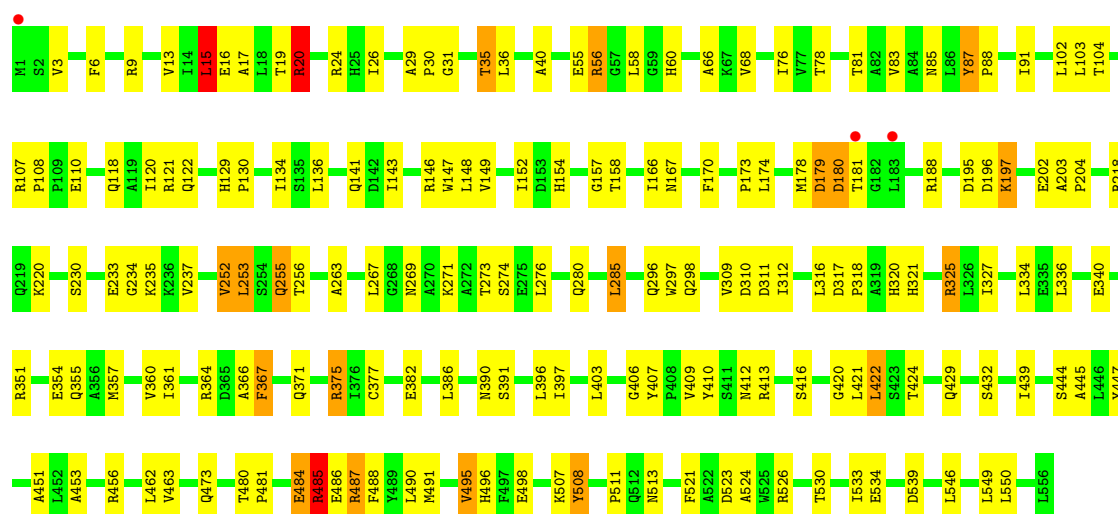


• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

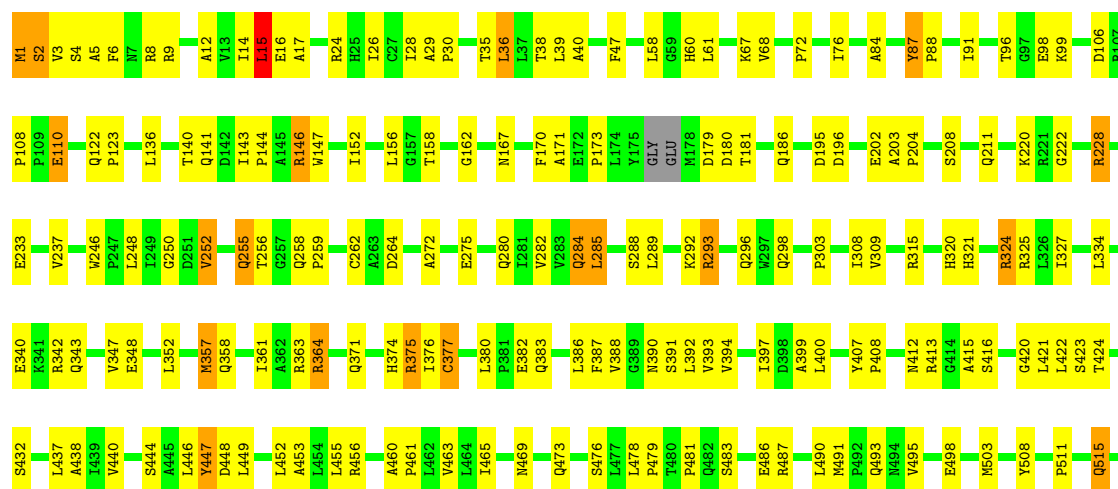




• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

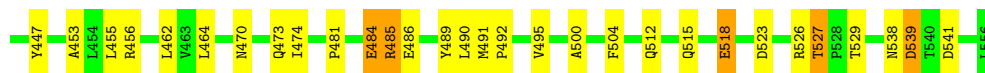
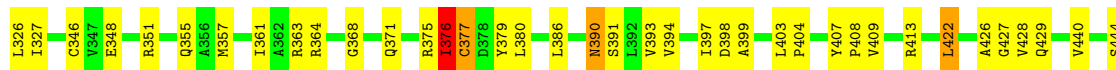
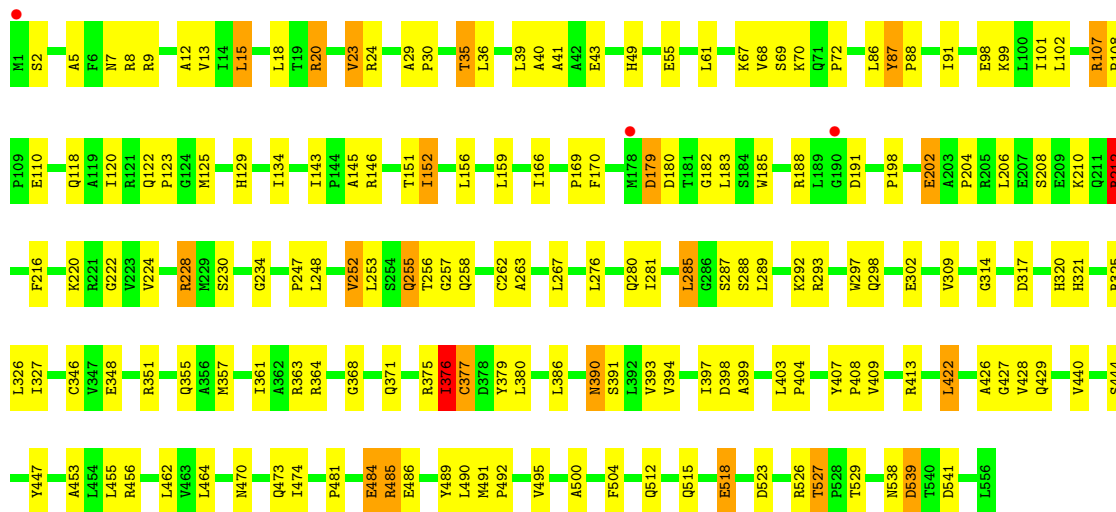


• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase





- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.35Å 90.46Å 169.17Å 75.99° 83.00° 64.15°	Depositor
Resolution (Å)	47.69 – 2.60 47.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	83.5 (47.69-2.60) 83.5 (47.69-2.60)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.26	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.197 , 0.253 0.201 , 0.223	Depositor DCC
$R_{free}$ test set	6053 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,-k+1	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	35302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, TPP, NA

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	1	0.80	0/4439	0.87	4/6053 (0.1%)
1	A	0.83	2/4429 (0.0%)	0.89	5/6038 (0.1%)
1	B	0.79	2/4439 (0.0%)	0.89	7/6053 (0.1%)
1	I	0.79	3/4425 (0.1%)	0.87	6/6033 (0.1%)
1	J	0.72	0/4439	0.85	4/6053 (0.1%)
1	R	0.80	3/4425 (0.1%)	0.87	5/6033 (0.1%)
1	S	0.78	0/4439	0.87	7/6053 (0.1%)
1	Z	0.73	1/4425 (0.0%)	0.86	4/6033 (0.1%)
All	All	0.78	11/35460 (0.0%)	0.87	42/48349 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	347	VAL	CB-CG1	-7.42	1.37	1.52
1	R	346	CYS	CB-SG	-7.32	1.69	1.82
1	I	348	GLU	CB-CG	-6.70	1.39	1.52
1	A	489	TYR	CD1-CE1	-6.66	1.29	1.39
1	A	488	PHE	CE1-CZ	-6.51	1.25	1.37
1	R	347	VAL	CB-CG2	-5.95	1.40	1.52
1	B	33	ARG	CZ-NH1	-5.67	1.25	1.33
1	I	348	GLU	CG-CD	-5.58	1.43	1.51
1	I	347	VAL	CB-CG2	-5.52	1.41	1.52
1	B	31	GLY	C-O	-5.31	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	479	PRO	N-CD	5.04	1.54	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	Z	36	LEU	CA-CB-CG	-10.65	90.80	115.30
1	A	9	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	R	538	ASN	CB-CA-C	7.60	125.59	110.40
1	B	153	ASP	CB-CG-OD1	7.39	124.95	118.30
1	S	146	ARG	NE-CZ-NH2	7.07	123.84	120.30
1	Z	478	LEU	CB-CA-C	6.79	123.10	110.20
1	I	15	LEU	CA-CB-CG	-6.61	100.10	115.30
1	R	541	ASP	CB-CG-OD1	6.47	124.13	118.30
1	S	180	ASP	CB-CG-OD2	-6.41	112.54	118.30
1	1	390	ASN	CB-CA-C	6.33	123.07	110.40
1	I	239	LEU	CA-CB-CG	6.28	129.75	115.30
1	1	228	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	1	15	LEU	CA-CB-CG	-6.25	100.93	115.30
1	A	36	LEU	CA-CB-CG	-6.15	101.15	115.30
1	I	422	LEU	CA-CB-CG	6.07	129.27	115.30
1	S	15	LEU	CA-CB-CG	-5.98	101.55	115.30
1	J	36	LEU	CA-CB-CG	-5.95	101.62	115.30
1	B	390	ASN	CB-CA-C	5.90	122.19	110.40
1	S	20	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	1	422	LEU	CA-CB-CG	5.78	128.60	115.30
1	J	15	LEU	CA-CB-CG	-5.76	102.05	115.30
1	Z	228	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	490	LEU	CA-CB-CG	5.62	128.24	115.30
1	R	218	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	J	228	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	293	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	228	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	J	107	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	153	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	R	15	LEU	CA-CB-CG	-5.29	103.13	115.30
1	S	146	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	S	56	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	Z	15	LEU	CA-CB-CG	-5.08	103.62	115.30
1	I	36	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	B	156	LEU	CA-CB-CG	-5.06	103.67	115.30
1	I	86	LEU	CA-CB-CG	5.04	126.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	239	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	R	443	LEU	CA-CB-CG	5.01	126.83	115.30
1	I	239	LEU	CB-CG-CD1	5.01	119.52	111.00
1	S	390	ASN	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	485	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4332	0	4302	137	0
1	A	4323	0	4295	146	0
1	B	4332	0	4302	128	0
1	I	4319	0	4292	123	0
1	J	4332	0	4302	132	0
1	R	4319	0	4292	114	0
1	S	4332	0	4302	112	0
1	Z	4319	0	4292	141	0
2	1	1	0	0	0	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	I	3	0	0	0	0
2	R	3	0	0	0	0
2	S	3	0	0	0	0
2	Z	2	0	0	0	0
3	1	26	0	16	1	0
3	A	26	0	16	1	0
3	B	26	0	16	7	0
3	I	26	0	16	1	0
3	J	26	0	16	1	0
3	R	26	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	26	0	16	1	0
3	Z	26	0	16	2	0
4	1	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	Z	1	0	0	0	0
5	1	6	0	8	0	0
5	J	6	0	8	0	0
6	1	63	0	0	5	0
6	A	50	0	0	4	0
6	B	56	0	0	5	0
6	I	53	0	0	3	0
6	J	43	0	0	4	0
6	R	55	0	0	3	0
6	S	76	0	0	6	0
6	Z	55	0	0	8	0
All	All	35302	0	34523	956	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 14.

All (956) 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)
1:1:7:ASN:HB3	1:1:36:LEU:CD1	1.80	1.12
1:Z:264:ASP:O	1:Z:293:ARG:HG3	1.47	1.12
1:R:293:ARG:HH11	1:R:293:ARG:HG2	1.12	1.12
1:R:39:LEU:HD21	1:S:481:PRO:HG2	1.28	1.12
1:A:39:LEU:HD21	1:B:481:PRO:HG3	1.21	1.11
1:Z:293:ARG:HH11	1:Z:293:ARG:CG	1.68	1.07
1:Z:108:PRO:HB2	1:Z:110:GLU:OE1	1.51	1.06
1:I:24:ARG:HG2	1:I:24:ARG:NH1	1.65	1.03
1:1:7:ASN:HB3	1:1:36:LEU:HD13	1.41	1.02
1:I:39:LEU:HD21	1:J:481:PRO:HG3	1.38	1.02
1:1:35:THR:HG22	1:1:36:LEU:HD23	1.43	1.01
1:Z:348:GLU:HB2	6:Z:686:HOH:O	1.60	1.00
1:R:252:VAL:HG22	1:R:398:ASP:HB2	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:293:ARG:NH1	1:Z:293:ARG:HG2	1.54	1.00
1:I:24:ARG:CG	1:I:24:ARG:HH11	1.73	0.99
1:I:24:ARG:HG2	1:I:24:ARG:HH11	1.13	0.99
1:B:24:ARG:NH2	1:B:48:ILE:HD11	1.79	0.97
1:A:7:ASN:HB3	1:A:36:LEU:HD13	1.48	0.95
1:I:489:TYR:HE2	1:J:35:THR:OG1	1.51	0.94
1:1:9:ARG:HH21	1:1:180:ASP:HA	1.34	0.93
1:B:219:GLN:HG2	1:B:342:ARG:NH2	1.84	0.92
1:Z:293:ARG:HG2	1:Z:293:ARG:HH11	0.77	0.92
1:Z:36:LEU:HD13	1:Z:170:PHE:CD1	2.05	0.90
1:A:252:VAL:HG13	1:A:398:ASP:HA	1.55	0.88
1:S:36:LEU:H	1:S:36:LEU:HD22	1.39	0.88
1:I:489:TYR:CE2	1:J:35:THR:OG1	2.26	0.87
1:A:204:PRO:HG3	1:I:327:ILE:HD13	1.54	0.87
1:R:134:ILE:HD11	1:R:155:ALA:HB2	1.58	0.85
1:A:68:VAL:HG11	1:A:432:SER:HB3	1.59	0.84
1:B:78:THR:HG22	6:B:871:HOH:O	1.77	0.84
1:1:9:ARG:NH2	1:1:180:ASP:HA	1.92	0.83
1:S:325:ARG:HB3	1:1:202:GLU:HB2	1.60	0.83
1:J:383:GLN:OE1	1:J:383:GLN:HA	1.79	0.83
1:J:108:PRO:HB2	1:J:110:GLU:OE2	1.78	0.83
1:S:16:GLU:O	1:S:19:THR:HB	1.79	0.83
1:S:269:ASN:OD1	1:S:271:LYS:HB2	1.77	0.83
1:B:252:VAL:HG13	1:B:398:ASP:HA	1.62	0.82
1:A:255:GLN:HG2	1:A:407:TYR:O	1.80	0.82
1:J:3:VAL:HB	1:J:173:PRO:HD2	1.62	0.81
1:B:43:GLU:HG3	6:B:814:HOH:O	1.79	0.80
1:Z:465:ILE:HD11	1:Z:521:PHE:HZ	1.46	0.80
1:Z:29:ALA:HB2	1:Z:58:LEU:HD22	1.63	0.80
1:R:293:ARG:NH1	1:R:293:ARG:HG2	1.89	0.79
1:Z:195:ASP:CG	1:Z:196:ASP:H	1.85	0.79
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.48	0.78
1:A:440:VAL:CG1	1:A:444:SER:HB2	2.13	0.78
1:A:36:LEU:HD12	1:A:170:PHE:CD1	2.17	0.78
1:A:264:ASP:O	1:A:293:ARG:HG3	1.82	0.78
1:J:359:ALA:HB1	1:J:552:GLN:NE2	1.97	0.78
1:R:90:LEU:HD21	1:R:130:PRO:HG3	1.65	0.78
1:J:29:ALA:HB2	1:J:58:LEU:HD22	1.66	0.78
1:Z:421:LEU:HD12	1:Z:444:SER:HB3	1.66	0.77
1:Z:14:ILE:HG23	1:Z:152:ILE:HD11	1.67	0.77
1:I:372:LEU:HD22	1:I:535:MET:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:195:ASP:OD1	1:Z:196:ASP:N	2.17	0.76
1:A:440:VAL:HG13	1:A:444:SER:HB2	1.68	0.76
1:1:7:ASN:HB3	1:1:36:LEU:HD11	1.64	0.75
1:I:436:THR:HB	1:I:462:LEU:HD12	1.67	0.75
1:J:309:VAL:HG22	1:J:326:LEU:HB2	1.68	0.75
1:A:363:ARG:NH2	1:A:548:GLN:OE1	2.20	0.74
1:J:359:ALA:HB1	1:J:552:GLN:HE22	1.53	0.74
1:Z:24:ARG:NH1	6:Z:567:HOH:O	2.20	0.74
1:1:252:VAL:HG13	1:1:398:ASP:HA	1.69	0.74
1:R:293:ARG:CG	1:R:293:ARG:HH11	1.96	0.73
1:Z:220:LYS:HD2	1:Z:280:GLN:OE1	1.88	0.73
1:Z:30:PRO:HD3	1:1:491:MET:SD	2.28	0.73
1:I:481:PRO:HG3	1:J:39:LEU:HD21	1.69	0.73
1:Z:498:GLU:HG3	1:Z:508:TYR:CE2	2.23	0.73
1:A:491:MET:SD	1:B:30:PRO:HD3	2.29	0.73
1:I:293:ARG:CG	1:I:293:ARG:HH11	2.02	0.72
1:B:453:ALA:HA	1:B:456:ARG:HD2	1.71	0.72
1:I:35:THR:HG22	1:I:39:LEU:HD22	1.71	0.72
1:R:327:ILE:HD13	1:Z:204:PRO:HG3	1.68	0.72
1:R:387:PHE:HB3	1:R:438:ALA:HB2	1.71	0.72
1:R:252:VAL:HG22	1:R:398:ASP:CB	2.18	0.72
1:Z:60:HIS:CD2	1:Z:420:GLY:HA3	2.24	0.72
1:A:481:PRO:HG3	1:B:39:LEU:HD21	1.71	0.72
1:R:391:SER:HG	3:R:601:TPP:PB	2.12	0.72
1:I:372:LEU:HD22	1:I:535:MET:HE3	1.70	0.71
1:1:99:LYS:HD3	1:1:159:LEU:HD23	1.72	0.71
1:S:36:LEU:HD21	1:S:174:LEU:HD22	1.73	0.71
1:Z:15:LEU:HD13	1:Z:40:ALA:HB3	1.73	0.71
1:I:293:ARG:HG2	1:I:293:ARG:HH11	1.56	0.71
1:J:351:ARG:HG2	1:J:355:GLN:NE2	2.05	0.70
1:I:292:LYS:O	1:I:296:GLN:HG3	1.91	0.70
1:B:14:ILE:CG1	1:B:148:LEU:HD21	2.22	0.70
1:R:252:VAL:CG2	1:R:398:ASP:HB2	2.18	0.70
1:R:390:ASN:O	1:R:393:VAL:HG12	1.92	0.70
1:A:507:LYS:CE	1:A:523:ASP:OD2	2.40	0.70
1:J:148:LEU:O	1:J:152:ILE:HD12	1.91	0.70
1:I:535:MET:HA	6:I:902:HOH:O	1.92	0.70
1:1:35:THR:HG22	1:1:36:LEU:CD2	2.21	0.69
1:R:16:GLU:O	1:R:19:THR:HB	1.92	0.69
1:A:293:ARG:NH1	1:A:293:ARG:HG2	2.06	0.69
1:Z:361:ILE:O	1:Z:364:ARG:CG	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:386:LEU:HD23	1:1:409:VAL:HG22	1.73	0.69
1:S:143:ILE:HG12	1:Z:110:GLU:CG	2.21	0.69
1:B:252:VAL:HG11	1:B:397:ILE:HG22	1.73	0.69
1:J:99:LYS:HA	1:J:162:GLY:O	1.93	0.69
1:Z:465:ILE:HD11	1:Z:521:PHE:CZ	2.28	0.69
1:B:429:GLN:HG2	1:B:458:VAL:HG12	1.75	0.69
1:I:456:ARG:NH2	1:J:493:GLN:O	2.23	0.69
1:Z:361:ILE:O	1:Z:364:ARG:HG3	1.94	0.68
1:B:320:HIS:CE1	1:J:147:TRP:HD1	2.11	0.68
1:B:429:GLN:HG3	1:B:430:ARG:N	2.08	0.68
1:S:473:GLN:HG3	1:S:539:ASP:O	1.93	0.68
1:1:134:ILE:HD12	1:1:166:ILE:HG12	1.75	0.68
1:1:212:ARG:HH11	1:1:212:ARG:CG	2.06	0.68
1:A:39:LEU:HD21	1:B:481:PRO:CG	2.12	0.68
1:R:30:PRO:HD3	1:S:491:MET:SD	2.32	0.68
1:A:97:GLY:HA2	1:A:161:ALA:HB1	1.76	0.68
1:I:9:ARG:NH2	1:I:180:ASP:HA	2.08	0.68
1:R:491:MET:SD	1:S:30:PRO:HD3	2.33	0.68
1:Z:211:GLN:OE1	1:Z:324:ARG:HD3	1.93	0.68
1:J:511:PRO:HD2	1:J:534:GLU:O	1.93	0.68
1:B:26:ILE:HG13	1:B:74:ALA:HB3	1.75	0.67
1:Z:255:GLN:HG2	1:Z:407:TYR:O	1.94	0.67
1:A:293:ARG:CG	1:A:293:ARG:HH11	2.07	0.67
1:I:108:PRO:HB2	1:I:110:GLU:OE1	1.95	0.67
1:Z:39:LEU:HD11	1:1:481:PRO:HG3	1.76	0.67
1:Z:108:PRO:HD3	1:Z:170:PHE:O	1.94	0.67
1:I:243:THR:HG23	1:I:341:LYS:HG3	1.77	0.67
1:S:204:PRO:HG3	1:1:327:ILE:HD13	1.76	0.67
1:1:228:ARG:HB2	1:1:253:LEU:HD23	1.75	0.66
1:B:253:LEU:HD21	1:B:413:ARG:HG3	1.77	0.66
1:J:36:LEU:H	1:J:36:LEU:CD1	2.08	0.66
1:R:325:ARG:HB3	1:Z:202:GLU:HB2	1.76	0.66
1:A:129:HIS:N	1:A:130:PRO:HD2	2.10	0.66
1:A:87:TYR:O	1:A:91:ILE:HG13	1.96	0.66
1:1:351:ARG:HG2	1:1:355:GLN:NE2	2.10	0.66
1:I:293:ARG:NH1	1:I:293:ARG:HG2	2.09	0.66
1:I:366:ALA:HB3	1:I:371:GLN:NE2	2.11	0.66
1:S:422:LEU:HB2	1:S:451:ALA:HB3	1.77	0.66
1:R:228:ARG:NH2	1:R:288:SER:OG	2.29	0.66
1:R:439:ILE:HG12	1:R:465:ILE:HD12	1.78	0.66
1:1:41:ALA:O	1:1:49:HIS:NE2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ALA:HA	1:A:178:MET:HG3	1.78	0.65
1:B:252:VAL:CG1	1:B:398:ASP:HA	2.26	0.65
1:Z:9:ARG:NH2	1:Z:180:ASP:HA	2.12	0.65
1:J:343:GLN:NE2	1:J:344:PRO:HD2	2.12	0.65
1:A:252:VAL:CG1	1:A:398:ASP:HA	2.25	0.65
1:Z:108:PRO:HG3	1:Z:171:ALA:HA	1.78	0.65
1:A:327:ILE:N	1:A:327:ILE:HD12	2.12	0.65
1:I:36:LEU:HD11	1:I:170:PHE:CE1	2.32	0.65
1:Z:315:ARG:NH1	1:Z:320:HIS:ND1	2.43	0.65
1:S:179:ASP:OD1	1:S:181:THR:N	2.30	0.65
1:S:143:ILE:HG12	1:Z:110:GLU:HG3	1.79	0.64
1:J:36:LEU:HD12	1:J:36:LEU:H	1.63	0.64
1:Z:84:ALA:HB1	1:I:87:TYR:HB3	1.79	0.64
1:I:512:GLN:HB2	6:I:898:HOH:O	1.97	0.64
1:A:60:HIS:CD2	1:A:420:GLY:HA3	2.32	0.64
1:R:237:VAL:HG22	1:R:334:LEU:HD11	1.80	0.64
1:S:147:TRP:HD1	1:I:320:HIS:CE1	2.15	0.64
6:Z:617:HOH:O	1:I:43:GLU:CG	2.46	0.63
1:J:465:ILE:HD11	1:J:521:PHE:HZ	1.63	0.63
1:S:255:GLN:HG2	1:S:407:TYR:O	1.98	0.63
1:I:255:GLN:HG2	1:I:407:TYR:O	1.98	0.63
1:B:329:ASN:HB3	1:B:332:ASP:OD2	1.98	0.63
1:I:285:LEU:HD13	1:I:309:VAL:HB	1.80	0.63
1:J:262:CYS:HA	1:J:399:ALA:O	1.98	0.63
1:S:386:LEU:HD23	1:S:409:VAL:HG22	1.78	0.63
1:I:485:ARG:O	1:I:489:TYR:HB2	1.99	0.63
1:R:184:SER:O	1:R:188:ARG:HG2	1.99	0.63
1:S:276:LEU:HD13	1:S:297:TRP:CE2	2.33	0.63
1:S:421:LEU:HD12	1:S:444:SER:HB3	1.79	0.63
1:J:327:ILE:HD12	1:J:327:ILE:N	2.14	0.63
1:B:14:ILE:HG12	1:B:148:LEU:HD21	1.81	0.63
1:I:393:VAL:HG13	1:I:394:VAL:H	1.63	0.63
1:R:84:ALA:HB1	1:S:87:TYR:HB3	1.81	0.63
1:A:481:PRO:CG	1:B:39:LEU:HD21	2.29	0.62
1:R:159:LEU:HD11	1:R:162:GLY:O	1.99	0.62
1:I:247:PRO:HG3	1:I:346:CYS:SG	2.39	0.62
1:A:440:VAL:HG12	1:A:441:GLY:O	1.99	0.62
1:A:136:LEU:HB2	1:A:167:ASN:O	1.99	0.62
1:J:8:ARG:HG2	1:J:8:ARG:HH21	1.64	0.62
1:B:276:LEU:HD13	1:B:297:TRP:CE2	2.35	0.62
1:S:523:ASP:OD1	1:S:526:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:320:HIS:HB2	1:Z:146:ARG:HG3	1.81	0.62
1:I:481:PRO:CG	1:J:39:LEU:HD21	2.29	0.61
1:I:36:LEU:HD11	1:I:170:PHE:CD1	2.35	0.61
1:Z:14:ILE:HG23	1:Z:152:ILE:CD1	2.29	0.61
1:Z:39:LEU:CD2	1:1:484:GLU:HG3	2.30	0.61
1:Z:72:PRO:HA	1:Z:99:LYS:HB2	1.83	0.61
1:1:228:ARG:HA	1:1:253:LEU:O	2.01	0.61
6:Z:617:HOH:O	1:1:43:GLU:HG3	2.00	0.61
1:1:538:ASN:HB2	1:1:541:ASP:OD2	1.99	0.61
1:A:31:GLY:HA3	1:A:78:THR:HB	1.83	0.61
1:J:343:GLN:HG3	6:J:571:HOH:O	2.00	0.61
1:J:366:ALA:O	1:J:371:GLN:HG2	2.01	0.61
1:R:26:ILE:HG13	1:R:74:ALA:HB3	1.82	0.61
1:I:235:LYS:HE2	1:I:406:GLY:HA3	1.82	0.60
1:S:480:THR:O	1:S:485:ARG:NH1	2.34	0.60
1:B:388:VAL:HG13	1:B:411:SER:HB3	1.83	0.60
1:Z:377:CYS:HA	1:Z:380:LEU:HG	1.84	0.60
1:J:351:ARG:HG2	1:J:355:GLN:HE22	1.66	0.60
1:Z:250:GLY:O	1:Z:258:GLN:HG2	2.01	0.60
1:1:379:TYR:HE1	1:1:518:GLU:HG3	1.67	0.59
1:J:9:ARG:NH2	1:J:180:ASP:HA	2.16	0.59
1:B:322:ARG:NH2	1:J:195:ASP:OD2	2.35	0.59
1:R:415:ALA:O	1:R:416:SER:HB2	2.01	0.59
1:S:220:LYS:NZ	1:S:280:GLN:HE22	2.00	0.59
1:B:14:ILE:HG13	1:B:148:LEU:HD21	1.85	0.59
1:A:30:PRO:HG2	3:B:601:TPP:HM43	1.84	0.59
1:I:393:VAL:HG13	1:I:394:VAL:N	2.16	0.59
1:Z:315:ARG:HH12	1:Z:320:HIS:CE1	2.19	0.59
1:J:284:GLN:HG2	1:J:308:ILE:HG23	1.83	0.59
1:S:157:GLY:HA3	1:S:202:GLU:O	2.03	0.59
1:1:276:LEU:HD13	1:1:297:TRP:CE2	2.38	0.59
1:R:285:LEU:HD13	1:R:309:VAL:HB	1.84	0.59
1:1:298:GLN:O	1:1:321:HIS:HE1	1.85	0.59
1:A:466:VAL:HG11	1:A:497:PHE:CE1	2.37	0.59
1:S:252:VAL:HG13	6:S:847:HOH:O	2.01	0.59
1:1:325:ARG:NH1	1:1:326:LEU:O	2.36	0.59
1:A:39:LEU:CD2	1:B:481:PRO:HG3	2.14	0.59
1:A:36:LEU:HD12	1:A:170:PHE:CG	2.37	0.59
1:A:9:ARG:HH22	1:A:180:ASP:HA	1.68	0.59
1:A:9:ARG:NH2	1:A:180:ASP:HA	2.17	0.59
1:R:453:ALA:HA	1:R:456:ARG:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:20:ARG:HG2	1:S:197:LYS:O	2.02	0.59
1:Z:498:GLU:HG3	1:Z:508:TYR:CD2	2.37	0.59
1:1:252:VAL:HG11	1:1:397:ILE:HG22	1.83	0.58
1:1:69:SER:O	1:1:70:LYS:HB2	2.02	0.58
1:B:68:VAL:HB	1:B:431:ALA:HB3	1.84	0.58
1:R:387:PHE:O	1:R:438:ALA:HA	2.03	0.58
1:J:214:TRP:CD1	1:J:337:HIS:HB3	2.39	0.58
1:J:6:PHE:CE1	1:J:141:GLN:HG3	2.37	0.58
3:A:601:TPP:HM43	1:B:30:PRO:HB2	1.86	0.58
1:Z:195:ASP:CG	1:Z:196:ASP:N	2.56	0.58
1:A:258:GLN:O	1:A:261:PRO:HD3	2.03	0.58
1:B:480:THR:HB	1:B:481:PRO:HD2	1.86	0.58
1:1:474:ILE:O	1:1:474:ILE:HG13	2.03	0.58
1:A:489:TYR:OH	1:B:35:THR:OG1	2.21	0.58
1:A:9:ARG:HH21	1:A:180:ASP:C	2.08	0.58
1:S:121:ARG:NH1	6:S:877:HOH:O	2.35	0.58
1:B:68:VAL:HB	1:B:431:ALA:CB	2.34	0.57
1:1:292:LYS:HD3	1:1:293:ARG:NH1	2.19	0.57
1:I:415:ALA:O	1:J:118:GLN:HG3	2.05	0.57
1:R:27:CYS:O	1:R:75:VAL:HA	2.04	0.57
1:Z:233:GLU:O	1:Z:237:VAL:HG23	2.04	0.57
1:Z:252:VAL:CG1	1:Z:397:ILE:HG22	2.35	0.57
1:I:67:LYS:HG3	1:I:98:GLU:OE2	2.04	0.57
1:Z:361:ILE:O	1:Z:364:ARG:HG2	2.05	0.57
1:J:287:SER:HB2	6:J:765:HOH:O	2.04	0.57
1:J:390:ASN:OD1	1:J:413:ARG:HD2	2.05	0.57
1:Z:358:GLN:HA	1:Z:361:ILE:HG12	1.85	0.57
1:Z:292:LYS:O	1:Z:296:GLN:HG3	2.05	0.57
1:1:2:SER:HB3	1:1:5:ALA:HB3	1.85	0.57
1:1:7:ASN:CB	1:1:36:LEU:HD13	2.26	0.57
1:A:435:PRO:HB3	1:A:461:PRO:HG2	1.85	0.57
1:I:356:ALA:O	1:I:359:ALA:HB3	2.05	0.57
1:J:138:ARG:NH1	6:J:872:HOH:O	2.36	0.57
1:J:8:ARG:NH1	1:J:39:LEU:HD13	2.20	0.57
1:R:276:LEU:HD13	1:R:297:TRP:CE2	2.40	0.57
1:I:538:ASN:HB2	1:I:541:ASP:OD2	2.05	0.56
1:1:220:LYS:HD3	1:1:280:GLN:NE2	2.20	0.56
1:A:489:TYR:HH	1:B:35:THR:HG1	1.54	0.56
1:I:14:ILE:HG12	1:I:148:LEU:HD11	1.86	0.56
1:I:15:LEU:HD22	1:I:41:ALA:HB2	1.86	0.56
1:R:418:ILE:HD13	3:R:601:TPP:H72	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:98:GLU:O	1:R:162:GLY:HA2	2.05	0.56
1:B:222:GLY:HA2	1:B:281:ILE:O	2.05	0.56
1:J:315:ARG:HH12	1:J:320:HIS:CE1	2.24	0.56
1:B:9:ARG:HH21	1:B:180:ASP:HA	1.68	0.56
1:S:220:LYS:HZ3	1:S:280:GLN:HE22	1.51	0.56
1:R:286:GLY:HA2	1:R:310:ASP:OD2	2.05	0.56
1:B:473:GLN:NE2	1:B:539:ASP:HB2	2.20	0.56
1:I:11:ALA:HB2	1:I:36:LEU:HD12	1.88	0.56
1:S:108:PRO:HD3	1:S:170:PHE:O	2.05	0.56
1:I:35:THR:HG23	1:J:489:TYR:OH	2.05	0.56
1:I:86:LEU:HD13	1:I:102:LEU:HD13	1.88	0.56
1:A:36:LEU:CD1	1:A:170:PHE:CD1	2.89	0.56
1:S:36:LEU:H	1:S:36:LEU:CD2	2.16	0.56
1:R:312:ILE:HD11	1:R:316:LEU:HD21	1.88	0.56
1:Z:16:GLU:O	1:Z:17:ALA:C	2.42	0.56
1:I:252:VAL:HG22	1:I:398:ASP:HB2	1.87	0.56
1:I:487:ARG:HD3	1:I:488:PHE:CZ	2.41	0.56
1:J:382:GLU:O	1:J:383:GLN:HB2	2.06	0.56
1:R:15:LEU:HD22	1:R:41:ALA:HB2	1.88	0.56
1:I:24:ARG:CB	1:I:24:ARG:HH11	2.20	0.55
1:Z:9:ARG:HH21	1:Z:180:ASP:HA	1.69	0.55
1:1:210:LYS:HB3	1:1:212:ARG:NH1	2.21	0.55
1:J:146:ARG:HD3	6:J:564:HOH:O	2.06	0.55
1:S:143:ILE:HG12	1:Z:110:GLU:HG2	1.85	0.55
1:1:224:VAL:HG12	1:1:248:LEU:CD1	2.36	0.55
1:A:309:VAL:HG22	1:A:326:LEU:HD12	1.88	0.55
1:Z:282:VAL:HG23	1:Z:303:PRO:HG3	1.87	0.55
1:I:391:SER:OG	3:I:601:TPP:O2B	2.25	0.55
1:R:462:LEU:O	1:R:530:THR:HA	2.05	0.55
1:Z:99:LYS:HA	1:Z:162:GLY:O	2.07	0.55
1:1:285:LEU:HD23	1:1:309:VAL:HB	1.88	0.55
1:B:469:ASN:HB2	1:B:539:ASP:HA	1.89	0.55
1:I:9:ARG:HH21	1:I:180:ASP:HA	1.70	0.55
1:B:146:ARG:HG3	1:J:320:HIS:HB2	1.88	0.55
1:R:422:LEU:HB2	1:R:451:ALA:HB3	1.88	0.55
1:S:120:ILE:HG13	1:S:122:GLN:HG3	1.89	0.55
1:A:18:LEU:HB3	1:A:23:VAL:HG21	1.89	0.55
1:B:298:GLN:O	1:B:321:HIS:HE1	1.90	0.55
1:S:371:GLN:O	1:S:375:ARG:HG2	2.07	0.55
1:Z:473:GLN:O	1:Z:476:SER:HB2	2.07	0.55
1:1:86:LEU:HD13	1:1:102:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ALA:O	1:B:371:GLN:HG2	2.06	0.54
1:R:366:ALA:O	1:R:371:GLN:HG2	2.08	0.54
1:Z:285:LEU:HD13	1:Z:309:VAL:HB	1.89	0.54
1:A:15:LEU:HD13	1:A:40:ALA:HB3	1.90	0.54
1:A:56:ARG:HA	1:A:85:ASN:O	2.07	0.54
1:I:487:ARG:HD3	1:I:488:PHE:CE2	2.41	0.54
1:S:285:LEU:HD23	1:S:309:VAL:HB	1.89	0.54
1:A:440:VAL:HG11	1:A:444:SER:HB2	1.88	0.54
1:J:7:ASN:HB3	1:J:36:LEU:HD22	1.89	0.54
1:Z:146:ARG:HD3	6:Z:619:HOH:O	2.07	0.54
1:A:226:ALA:HB3	1:A:250:GLY:HA2	1.88	0.54
1:R:372:LEU:HD22	1:R:535:MET:HE2	1.90	0.54
1:S:218:ARG:CZ	1:S:340:GLU:HB2	2.38	0.54
1:I:144:PRO:HB2	1:I:146:ARG:HG2	1.90	0.54
1:J:179:ASP:OD1	1:J:180:ASP:N	2.41	0.54
1:R:7:ASN:HB3	1:R:36:LEU:HG	1.88	0.54
1:S:255:GLN:HA	6:S:733:HOH:O	2.07	0.54
1:Z:387:PHE:O	1:Z:438:ALA:HA	2.07	0.54
1:B:390:ASN:OD1	1:B:413:ARG:HD2	2.08	0.54
1:Z:237:VAL:HG22	1:Z:334:LEU:HD11	1.89	0.54
1:Z:486:GLU:HA	1:Z:490:LEU:HD12	1.89	0.54
1:A:120:ILE:HG13	1:A:122:GLN:HG3	1.89	0.54
1:A:507:LYS:HE3	1:A:523:ASP:OD2	2.07	0.54
1:R:15:LEU:HD13	1:R:40:ALA:HB3	1.89	0.54
1:S:60:HIS:CD2	1:S:420:GLY:HA3	2.43	0.54
1:Z:298:GLN:O	1:Z:321:HIS:HE1	1.90	0.54
1:I:234:GLY:O	1:I:256:THR:HG22	2.08	0.54
1:R:144:PRO:HB2	1:R:146:ARG:HG2	1.89	0.54
1:S:298:GLN:O	1:S:321:HIS:HE1	1.90	0.54
1:B:236:LYS:HB3	1:B:334:LEU:HD12	1.90	0.53
1:I:266:TRP:CZ3	1:I:349:ILE:HG12	2.43	0.53
1:B:220:LYS:HD3	1:B:280:GLN:NE2	2.23	0.53
1:R:65:LEU:HD23	1:R:427:GLY:O	2.08	0.53
1:I:327:ILE:N	1:I:327:ILE:HD12	2.24	0.53
1:I:255:GLN:HG2	1:I:407:TYR:O	2.08	0.53
1:J:235:LYS:O	1:J:238:ALA:HB3	2.09	0.53
1:R:320:HIS:CE1	1:Z:147:TRP:HD1	2.26	0.53
1:I:35:THR:O	1:I:39:LEU:HG	2.09	0.53
1:Z:390:ASN:OD1	1:Z:413:ARG:HD2	2.08	0.53
1:S:320:HIS:HB2	1:I:146:ARG:HG3	1.90	0.53
1:B:325:ARG:HB3	1:J:202:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ASN:HB3	1:B:36:LEU:HD13	1.90	0.53
1:B:429:GLN:HG3	1:B:430:ARG:H	1.74	0.53
1:I:298:GLN:O	1:I:321:HIS:HE1	1.91	0.53
1:J:69:SER:O	1:J:70:LYS:HB2	2.08	0.53
1:R:195:ASP:CG	1:R:196:ASP:H	2.11	0.53
1:S:495:VAL:HG13	1:S:496:HIS:N	2.22	0.53
1:I:8:ARG:HG3	1:I:36:LEU:HD22	1.91	0.53
1:J:480:THR:O	1:J:485:ARG:NH1	2.41	0.53
1:R:91:ILE:HG12	1:R:129:HIS:ND1	2.23	0.53
1:S:26:ILE:HD11	1:S:76:ILE:HD11	1.91	0.53
1:Z:9:ARG:NH2	1:Z:179:ASP:O	2.41	0.53
1:I:293:ARG:NH1	1:I:293:ARG:CG	2.66	0.52
1:S:36:LEU:N	1:S:36:LEU:HD22	2.18	0.52
1:S:68:VAL:HG22	1:S:410:TYR:CE1	2.44	0.52
1:I:169:PRO:HD2	6:I:570:HOH:O	2.08	0.52
1:I:20:ARG:HD2	1:I:197:LYS:O	2.09	0.52
1:I:453:ALA:HA	1:I:456:ARG:HD2	1.90	0.52
1:A:430:ARG:NH2	1:A:457:GLN:HB2	2.24	0.52
1:A:201:ARG:NH2	1:I:324:ARG:NH1	2.58	0.52
1:B:436:THR:O	1:B:462:LEU:HA	2.08	0.52
1:I:276:LEU:HD13	1:I:297:TRP:CE2	2.45	0.52
1:A:485:ARG:O	1:A:489:TYR:HB2	2.09	0.52
1:B:3:VAL:HB	1:B:173:PRO:HD2	1.91	0.52
1:I:473:GLN:OE1	1:I:473:GLN:HA	2.09	0.52
1:A:430:ARG:HH21	1:A:457:GLN:HB2	1.74	0.52
1:I:284:GLN:HB3	1:I:308:ILE:HG12	1.92	0.52
1:I:60:HIS:CD2	1:I:420:GLY:HA3	2.45	0.52
1:R:269:ASN:OD1	1:R:271:LYS:HB2	2.09	0.52
1:B:208:SER:HA	1:J:204:PRO:HA	1.92	0.52
1:R:257:GLY:HA2	1:R:403:LEU:O	2.10	0.52
1:A:129:HIS:H	1:A:130:PRO:HD2	1.73	0.52
1:B:538:ASN:HB2	1:B:541:ASP:OD2	2.10	0.52
1:R:138:ARG:HG2	1:R:138:ARG:HH11	1.74	0.52
1:Z:264:ASP:O	1:Z:293:ARG:CG	2.40	0.52
1:Z:422:LEU:HG	1:Z:448:ASP:HB3	1.92	0.52
1:I:14:ILE:HG13	1:I:148:LEU:HD21	1.91	0.52
1:I:456:ARG:HD2	1:I:504:PHE:HB3	1.92	0.52
1:R:387:PHE:HB3	1:R:438:ALA:CB	2.39	0.52
1:I:216:PHE:HE1	1:I:220:LYS:HZ2	1.57	0.51
1:Z:179:ASP:HB2	1:Z:181:THR:OG1	2.09	0.51
1:A:366:ALA:O	1:A:371:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLN:HG2	1:B:342:ARG:HH21	1.70	0.51
1:J:298:GLN:O	1:J:321:HIS:HE1	1.93	0.51
1:A:390:ASN:O	1:A:393:VAL:HG12	2.09	0.51
1:J:252:VAL:HG13	1:J:398:ASP:HA	1.90	0.51
1:Z:515:GLN:O	1:Z:519:THR:OG1	2.27	0.51
1:J:381:PRO:HG2	1:J:384:GLY:HA3	1.92	0.51
1:Z:68:VAL:HG11	1:Z:432:SER:HB3	1.91	0.51
1:I:390:ASN:OD1	1:I:413:ARG:HD2	2.10	0.51
1:I:543:ALA:O	1:I:547:GLN:HG3	2.10	0.51
1:J:226:ALA:HB2	1:J:248:LEU:HD11	1.93	0.51
1:I:120:ILE:HG22	1:J:95:LEU:HD11	1.93	0.51
1:R:298:GLN:O	1:R:321:HIS:CE1	2.64	0.51
1:S:486:GLU:HA	1:S:490:LEU:HD12	1.93	0.51
1:Z:437:LEU:HD13	1:Z:463:VAL:HB	1.92	0.51
1:A:60:HIS:CG	1:A:420:GLY:HA3	2.45	0.51
1:A:84:ALA:HB1	1:B:87:TYR:HB3	1.92	0.51
1:A:63:LEU:HD12	1:A:98:GLU:HG2	1.92	0.51
1:R:377:CYS:HA	1:R:380:LEU:HG	1.92	0.51
1:S:6:PHE:CE1	1:S:141:GLN:HG3	2.46	0.51
1:A:284:GLN:C	1:A:285:LEU:HD23	2.31	0.51
1:I:87:TYR:HB3	1:J:84:ALA:HB1	1.93	0.51
1:S:253:LEU:HD21	1:S:413:ARG:HG3	1.93	0.51
1:Z:259:PRO:HD2	6:Z:653:HOH:O	2.11	0.51
1:I:364:ARG:O	1:I:375:ARG:NH2	2.35	0.50
1:I:384:GLY:O	1:I:408:PRO:HD2	2.11	0.50
1:S:60:HIS:O	1:S:424:THR:HA	2.10	0.50
1:I:29:ALA:HB1	1:I:30:PRO:HD2	1.93	0.50
1:A:516:GLU:HG2	6:I:559:HOH:O	2.10	0.50
1:J:480:THR:OG1	1:J:485:ARG:HD3	2.10	0.50
1:A:154:HIS:CE1	1:I:314:GLY:HA2	2.46	0.50
1:R:178:MET:HG3	1:R:179:ASP:N	2.27	0.50
1:R:3:VAL:HB	1:R:173:PRO:HG2	1.92	0.50
1:Z:264:ASP:HB3	1:Z:399:ALA:CB	2.41	0.50
1:I:298:GLN:O	1:I:321:HIS:CE1	2.64	0.50
1:R:27:CYS:N	1:R:74:ALA:O	2.44	0.50
1:I:426:ALA:HB2	1:I:455:LEU:CD2	2.42	0.50
1:B:24:ARG:HH21	1:B:48:ILE:HD11	1.74	0.50
1:J:390:ASN:OD1	1:J:413:ARG:CD	2.59	0.50
1:S:68:VAL:HG11	1:S:432:SER:HB3	1.93	0.50
1:A:146:ARG:HD3	6:A:799:HOH:O	2.11	0.50
1:B:506:LEU:HD22	1:B:530:THR:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:361:ILE:HG23	1:S:364:ARG:HD2	1.94	0.50
1:I:252:VAL:CG2	1:I:398:ASP:HB2	2.42	0.50
1:J:476:SER:OG	1:J:490:LEU:HD21	2.11	0.50
1:S:107:ARG:NH2	1:S:118:GLN:HB3	2.27	0.50
1:I:9:ARG:HG3	1:I:182:GLY:HA3	1.93	0.50
1:Z:481:PRO:HG3	1:I:39:LEU:HD11	1.92	0.50
1:B:365:ASP:HB2	6:B:861:HOH:O	2.10	0.50
1:B:56:ARG:HA	1:B:85:ASN:O	2.11	0.50
1:B:99:LYS:HB3	1:B:159:LEU:HD21	1.94	0.50
1:J:469:ASN:HB2	1:J:539:ASP:HA	1.92	0.50
1:S:195:ASP:OD1	1:S:196:ASP:N	2.45	0.50
1:B:323:GLY:O	1:J:200:LEU:HA	2.12	0.49
1:I:195:ASP:CG	1:I:196:ASP:H	2.15	0.49
1:I:263:ALA:O	1:I:267:LEU:HD12	2.11	0.49
1:J:390:ASN:O	1:J:393:VAL:HG12	2.12	0.49
1:Z:340:GLU:O	1:Z:342:ARG:HG2	2.12	0.49
1:J:359:ALA:CB	1:J:552:GLN:NE2	2.72	0.49
1:S:31:GLY:HA3	1:S:78:THR:HB	1.94	0.49
1:S:396:LEU:O	1:S:397:ILE:C	2.48	0.49
1:S:29:ALA:HB2	1:S:58:LEU:HD22	1.94	0.49
1:B:312:ILE:CG1	1:B:313:GLU:H	2.25	0.49
1:J:28:ILE:HG21	1:J:38:THR:HG23	1.94	0.49
1:S:136:LEU:HB2	1:S:167:ASN:O	2.12	0.49
1:A:123:PRO:HB3	1:A:135:SER:OG	2.11	0.49
1:B:391:SER:OG	3:B:601:TPP:O2B	2.30	0.49
1:J:97:GLY:HA2	1:J:161:ALA:HB1	1.93	0.49
1:J:56:ARG:HA	1:J:85:ASN:O	2.12	0.49
1:I:223:VAL:HB	1:I:282:VAL:HG13	1.94	0.49
1:I:224:VAL:CG1	1:I:248:LEU:HD13	2.42	0.49
1:A:223:VAL:HG13	1:A:247:PRO:HG2	1.94	0.49
1:A:222:GLY:HA2	1:A:281:ILE:O	2.12	0.49
1:B:99:LYS:HA	1:B:162:GLY:O	2.13	0.49
1:J:36:LEU:HD13	1:J:170:PHE:CD2	2.47	0.49
1:I:107:ARG:HB3	1:I:108:PRO:HD2	1.93	0.49
1:B:227:GLY:O	1:B:254:SER:HA	2.11	0.49
1:I:263:ALA:O	1:I:267:LEU:HD12	2.13	0.49
1:A:16:GLU:O	1:A:19:THR:HB	2.13	0.49
1:B:218:ARG:CZ	1:B:340:GLU:HB2	2.42	0.49
1:R:475:PHE:HB2	1:R:490:LEU:HD23	1.95	0.49
1:R:503:MET:HG2	1:R:504:PHE:CD2	2.48	0.49
1:R:80:GLY:O	1:R:83:VAL:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:617:HOH:O	1:1:43:GLU:HG2	2.12	0.49
1:B:387:PHE:O	1:B:438:ALA:HA	2.13	0.49
1:B:96:THR:OG1	1:B:98:GLU:OE1	2.28	0.49
1:S:179:ASP:OD1	1:S:180:ASP:N	2.46	0.49
1:Z:284:GLN:HG2	1:Z:308:ILE:HG23	1.95	0.49
1:1:212:ARG:NH1	1:1:212:ARG:CG	2.72	0.49
1:J:132:HIS:O	1:J:164:VAL:HA	2.13	0.49
1:R:298:GLN:O	1:R:321:HIS:HE1	1.96	0.49
1:1:212:ARG:HH11	1:1:212:ARG:HG3	1.77	0.48
1:B:88:PRO:HB3	1:B:419:ASP:OD2	2.13	0.48
1:I:35:THR:HG22	1:I:39:LEU:CD2	2.42	0.48
1:I:358:GLN:HA	1:I:361:ILE:HG23	1.93	0.48
1:J:3:VAL:HB	1:J:173:PRO:CD	2.39	0.48
1:R:364:ARG:HH21	1:R:364:ARG:HG3	1.77	0.48
1:R:60:HIS:CD2	1:R:420:GLY:HA3	2.48	0.48
1:S:129:HIS:N	1:S:130:PRO:HD2	2.28	0.48
1:Z:453:ALA:HA	1:Z:456:ARG:HD2	1.93	0.48
1:A:440:VAL:CG1	1:A:441:GLY:N	2.76	0.48
1:R:283:VAL:HG12	1:R:285:LEU:HD22	1.95	0.48
1:Z:26:ILE:HG22	1:Z:47:PHE:HB3	1.95	0.48
1:A:99:LYS:HD3	1:A:159:LEU:HD23	1.95	0.48
1:B:435:PRO:HA	1:B:461:PRO:O	2.13	0.48
1:R:439:ILE:HG23	1:R:465:ILE:HB	1.96	0.48
1:B:255:GLN:HG2	1:B:407:TYR:O	2.14	0.48
1:B:61:LEU:HD12	1:B:427:GLY:CA	2.44	0.48
1:I:287:SER:O	1:I:288:SER:HB2	2.13	0.48
1:Z:108:PRO:HB2	1:Z:110:GLU:CD	2.31	0.48
1:Z:298:GLN:O	1:Z:321:HIS:CE1	2.67	0.48
1:1:363:ARG:C	6:1:698:HOH:O	2.52	0.48
1:1:473:GLN:HG3	1:1:539:ASP:O	2.13	0.48
1:B:376:ILE:HD11	1:B:439:ILE:HD11	1.95	0.48
1:S:230:SER:OG	1:S:233:GLU:HG3	2.14	0.48
1:Z:363:ARG:NH2	1:Z:548:GLN:OE1	2.45	0.48
1:A:283:VAL:HG12	1:A:285:LEU:HD21	1.96	0.48
1:B:101:ILE:HD12	1:B:156:LEU:HD11	1.95	0.48
1:Z:9:ARG:HD3	1:Z:186:GLN:OE1	2.13	0.48
1:Z:264:ASP:HB3	1:Z:399:ALA:HB2	1.95	0.48
1:1:224:VAL:HG12	1:1:248:LEU:HD13	1.96	0.48
1:A:27:CYS:C	1:A:28:ILE:HG13	2.33	0.48
1:J:429:GLN:HG2	1:J:462:LEU:HD12	1.95	0.48
1:Z:87:TYR:O	1:Z:91:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLY:HA2	3:B:601:TPP:N3'	2.29	0.48
1:J:462:LEU:O	1:J:530:THR:HA	2.13	0.48
1:A:486:GLU:HA	1:A:490:LEU:HD12	1.96	0.48
1:B:261:PRO:HG3	1:B:402:GLN:NE2	2.29	0.48
1:B:460:ALA:O	1:B:461:PRO:C	2.53	0.48
1:I:36:LEU:CD1	1:I:170:PHE:CE1	2.97	0.48
1:S:129:HIS:N	1:S:130:PRO:CD	2.77	0.48
1:Z:412:ASN:O	1:Z:416:SER:HA	2.13	0.48
1:B:285:LEU:HD23	1:B:309:VAL:HB	1.96	0.47
1:S:508:TYR:CD2	1:S:508:TYR:C	2.87	0.47
1:1:188:ARG:HA	1:1:188:ARG:HD2	1.63	0.47
1:1:317:ASP:OD1	1:1:317:ASP:C	2.52	0.47
1:1:486:GLU:HA	1:1:490:LEU:HD12	1.95	0.47
1:B:26:ILE:HG13	1:B:74:ALA:CB	2.41	0.47
1:I:252:VAL:HG13	1:I:398:ASP:HA	1.95	0.47
1:I:29:ALA:HB2	1:I:58:LEU:HD22	1.95	0.47
1:I:69:SER:O	1:I:70:LYS:HB2	2.14	0.47
1:J:68:VAL:CG2	1:J:428:VAL:HG13	2.45	0.47
1:J:486:GLU:HA	1:J:490:LEU:HD12	1.96	0.47
1:1:179:ASP:OD1	1:1:180:ASP:N	2.46	0.47
1:I:245:GLY:O	1:I:344:PRO:HA	2.15	0.47
1:J:68:VAL:HG11	1:J:432:SER:HB3	1.96	0.47
1:J:439:ILE:HG23	1:J:465:ILE:HB	1.95	0.47
1:R:391:SER:OG	3:R:601:TPP:PB	2.71	0.47
1:S:56:ARG:HG3	1:S:88:PRO:HG2	1.96	0.47
1:S:204:PRO:HB2	1:1:206:LEU:CD1	2.45	0.47
1:B:146:ARG:HD3	6:B:631:HOH:O	2.13	0.47
1:B:188:ARG:HB3	6:B:666:HOH:O	2.14	0.47
1:R:372:LEU:HD22	1:R:535:MET:CE	2.45	0.47
1:B:182:GLY:O	1:B:185:TRP:HB3	2.14	0.47
1:B:463:VAL:CG1	1:B:533:ILE:HD12	2.45	0.47
1:R:539:ASP:OD1	1:R:540:THR:N	2.47	0.47
1:1:20:ARG:HB3	1:1:198:PRO:HD3	1.97	0.47
1:I:172:GLU:HB2	1:I:173:PRO:HA	1.97	0.47
1:Z:357:MET:O	1:Z:361:ILE:HG23	2.15	0.47
1:Z:469:ASN:HB2	1:Z:473:GLN:HG3	1.97	0.47
1:1:68:VAL:HG21	1:1:428:VAL:O	2.14	0.47
1:J:272:ALA:HB2	1:J:352:LEU:CD1	2.45	0.47
1:Z:275:GLU:OE1	1:Z:348:GLU:HG2	2.15	0.47
1:1:7:ASN:C	1:1:36:LEU:HD13	2.35	0.47
1:A:253:LEU:HD11	1:A:413:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:LEU:CD1	1:J:484:GLU:HG3	2.45	0.47
1:Z:28:ILE:HG12	1:Z:76:ILE:HB	1.97	0.47
1:1:390:ASN:OD1	1:1:413:ARG:HD3	2.14	0.47
1:A:327:ILE:N	1:A:327:ILE:CD1	2.78	0.47
1:A:440:VAL:HG13	6:A:737:HOH:O	2.15	0.47
1:J:327:ILE:CD1	1:J:327:ILE:N	2.78	0.47
1:S:498:GLU:HG3	6:S:756:HOH:O	2.15	0.47
1:Z:340:GLU:O	1:Z:342:ARG:CG	2.62	0.47
1:Z:36:LEU:HD23	1:Z:36:LEU:HA	1.49	0.47
1:1:9:ARG:O	1:1:13:VAL:HG23	2.15	0.46
1:1:8:ARG:NH2	1:1:43:GLU:OE2	2.47	0.46
1:A:87:TYR:CE1	1:A:91:ILE:HD11	2.50	0.46
1:B:290:THR:HG21	1:B:394:VAL:HG22	1.97	0.46
1:B:419:ASP:HB3	3:B:601:TPP:HM23	1.97	0.46
1:B:106:ASP:OD2	1:B:122:GLN:HB2	2.15	0.46
1:I:534:GLU:O	6:I:902:HOH:O	2.21	0.46
1:J:261:PRO:HB3	1:J:402:GLN:HG3	1.98	0.46
1:S:83:VAL:HG22	1:S:104:THR:HB	1.97	0.46
1:A:307:TRP:CD1	1:A:324:ARG:HG3	2.51	0.46
1:A:381:PRO:O	1:A:407:TYR:OH	2.27	0.46
1:A:421:LEU:HD12	1:A:444:SER:HB3	1.98	0.46
1:A:325:ARG:HB3	1:I:202:GLU:HB2	1.96	0.46
1:S:484:GLU:HB2	1:S:488:PHE:HD2	1.80	0.46
1:1:453:ALA:HB2	1:1:504:PHE:CE1	2.50	0.46
1:I:404:PRO:O	1:I:405:ALA:C	2.53	0.46
1:I:83:VAL:HG13	1:I:104:THR:HG21	1.98	0.46
1:J:113:ASP:OD2	1:J:121:ARG:NH2	2.48	0.46
1:Z:136:LEU:HB2	1:Z:167:ASN:O	2.15	0.46
1:Z:248:LEU:HD21	1:Z:256:THR:HG21	1.95	0.46
1:1:252:VAL:CG1	1:1:397:ILE:HG22	2.46	0.46
1:Z:503:MET:SD	1:1:500:ALA:HB2	2.55	0.46
1:A:30:PRO:HD3	1:B:491:MET:SD	2.55	0.46
1:A:87:TYR:HB3	1:A:88:PRO:HD3	1.97	0.46
1:J:341:LYS:HE2	1:J:341:LYS:HB2	1.62	0.46
1:R:390:ASN:O	1:R:391:SER:HB3	2.15	0.46
1:R:435:PRO:HA	1:R:461:PRO:O	2.16	0.46
1:S:351:ARG:HG2	1:S:355:GLN:HE21	1.81	0.46
1:1:287:SER:HB2	1:1:288:SER:H	1.61	0.46
1:1:5:ALA:O	1:1:9:ARG:HG2	2.16	0.46
1:I:363:ARG:NH1	6:I:695:HOH:O	2.48	0.46
1:I:372:LEU:HD22	1:I:535:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:THR:O	1:J:36:LEU:C	2.53	0.46
1:R:276:LEU:HD13	1:R:297:TRP:CZ2	2.51	0.46
1:S:134:ILE:HD12	1:S:166:ILE:HG12	1.96	0.46
1:S:235:LYS:HE2	1:S:406:GLY:HA3	1.98	0.46
1:1:351:ARG:HG2	1:1:355:GLN:HE21	1.80	0.46
1:A:232:GLU:OE1	1:A:235:LYS:HE3	2.16	0.46
1:A:485:ARG:HA	1:A:489:TYR:HD1	1.81	0.46
1:B:442:ASP:HB3	1:B:468:ASN:HA	1.96	0.46
1:S:220:LYS:NZ	1:S:280:GLN:NE2	2.64	0.46
1:Z:376:ILE:HD12	1:Z:376:ILE:HA	1.72	0.46
1:1:422:LEU:HD22	1:1:464:LEU:HD21	1.97	0.46
1:R:363:ARG:HG3	1:R:549:LEU:HD21	1.98	0.46
1:R:9:ARG:HG3	1:R:182:GLY:HA3	1.98	0.46
1:S:462:LEU:O	1:S:530:THR:HA	2.16	0.46
1:S:204:PRO:HB2	1:1:206:LEU:HD11	1.98	0.46
1:A:393:VAL:HG13	1:A:394:VAL:N	2.31	0.46
1:A:473:GLN:NE2	1:A:539:ASP:HB2	2.31	0.46
1:Z:28:ILE:HD13	1:Z:38:THR:HG23	1.97	0.46
1:1:393:VAL:HG13	1:1:394:VAL:N	2.31	0.45
1:1:426:ALA:HB2	1:1:455:LEU:HD23	1.98	0.45
1:B:298:GLN:O	1:B:321:HIS:CE1	2.69	0.45
1:J:251:ASP:OD2	1:J:253:LEU:HB2	2.16	0.45
1:J:426:ALA:HB2	1:J:455:LEU:HD23	1.98	0.45
1:A:356:ALA:O	1:A:360:VAL:HG23	2.16	0.45
1:B:235:LYS:HE3	1:B:406:GLY:HA3	1.98	0.45
1:B:263:ALA:O	1:B:267:LEU:HB2	2.16	0.45
1:B:58:LEU:CD2	1:B:75:VAL:CG1	2.94	0.45
1:I:167:ASN:O	1:I:169:PRO:HD3	2.16	0.45
1:J:132:HIS:HB2	1:J:164:VAL:HG22	1.98	0.45
1:J:473:GLN:O	1:J:476:SER:HB2	2.16	0.45
1:J:86:LEU:HD13	1:J:102:LEU:HD22	1.98	0.45
1:Z:36:LEU:CD1	1:Z:170:PHE:CD1	2.91	0.45
1:Z:228:ARG:HB3	6:Z:884:HOH:O	2.17	0.45
1:Z:228:ARG:NH2	1:Z:288:SER:OG	2.48	0.45
1:S:252:VAL:CG1	6:S:847:HOH:O	2.63	0.45
1:I:389:GLY:O	1:I:394:VAL:HB	2.17	0.45
1:R:240:TRP:CD2	1:R:334:LEU:HD22	2.51	0.45
1:S:462:LEU:HD23	1:S:462:LEU:C	2.36	0.45
1:Z:392:LEU:HB2	3:Z:601:TPP:O1B	2.16	0.45
1:A:276:LEU:HD13	1:A:297:TRP:NE1	2.32	0.45
1:S:463:VAL:HG11	1:S:521:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:1:MET:HB2	1:Z:2:SER:H	1.57	0.45
1:1:67:LYS:HG3	1:1:98:GLU:OE2	2.16	0.45
1:J:245:GLY:O	1:J:344:PRO:HA	2.16	0.45
1:R:255:GLN:HA	6:R:625:HOH:O	2.17	0.45
1:B:310:ASP:OD1	1:B:311:ASP:N	2.47	0.45
1:B:312:ILE:CG1	1:B:313:GLU:N	2.80	0.45
1:J:421:LEU:HD12	1:J:444:SER:HB3	1.98	0.45
1:J:8:ARG:HG2	1:J:8:ARG:NH2	2.31	0.45
1:R:263:ALA:HA	1:R:266:TRP:NE1	2.32	0.45
1:Z:58:LEU:O	1:Z:61:LEU:HB3	2.17	0.45
1:A:30:PRO:HG2	3:B:601:TPP:CM4	2.46	0.45
1:A:68:VAL:HG22	1:A:410:TYR:CE1	2.52	0.45
1:B:58:LEU:HD21	1:B:75:VAL:CG1	2.47	0.45
1:R:447:TYR:OH	1:S:55:GLU:HB2	2.17	0.45
1:Z:5:ALA:O	1:Z:9:ARG:HG3	2.16	0.45
1:A:15:LEU:HD22	1:A:41:ALA:HB2	1.98	0.45
1:A:476:SER:OG	1:A:490:LEU:HD21	2.17	0.45
1:I:407:TYR:HA	1:I:408:PRO:HD3	1.88	0.45
1:I:478:LEU:HD13	1:J:32:SER:OG	2.16	0.45
1:S:487:ARG:CG	1:S:488:PHE:CE2	3.00	0.45
1:1:108:PRO:HD3	1:1:170:PHE:O	2.16	0.45
1:1:224:VAL:CG1	1:1:248:LEU:HD13	2.47	0.45
1:1:234:GLY:O	1:1:256:THR:HG22	2.17	0.45
1:1:357:MET:O	1:1:361:ILE:HG13	2.17	0.45
1:1:99:LYS:HD3	1:1:159:LEU:CD2	2.44	0.45
1:B:269:ASN:OD1	1:B:271:LYS:HB2	2.16	0.45
1:B:461:PRO:HB2	1:B:525:TRP:HE3	1.82	0.45
1:I:84:ALA:HB2	1:I:125:MET:HE3	1.98	0.45
1:I:12:ALA:HA	1:I:40:ALA:HB1	1.99	0.45
1:R:52:HIS:CD2	1:R:454:LEU:HD11	2.51	0.45
1:Z:449:LEU:O	1:Z:452:LEU:HG	2.17	0.45
1:1:87:TYR:HB3	1:1:88:PRO:HD3	1.99	0.44
1:A:373:ALA:O	1:A:401:SER:HB2	2.16	0.44
1:B:24:ARG:CZ	1:B:48:ILE:HD11	2.45	0.44
1:S:179:ASP:OD1	1:S:181:THR:OG1	2.30	0.44
1:1:212:ARG:HH11	1:1:212:ARG:HG2	1.78	0.44
1:A:154:HIS:O	1:A:158:THR:HG23	2.17	0.44
1:I:224:VAL:HG12	1:I:248:LEU:HD13	1.98	0.44
1:J:179:ASP:CG	1:J:181:THR:HG1	2.21	0.44
1:J:307:TRP:CE2	1:J:324:ARG:HD2	2.52	0.44
1:Z:122:GLN:H	1:Z:123:PRO:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:158:THR:CG2	1:Z:202:GLU:HG2	2.47	0.44
1:Z:28:ILE:HG21	1:Z:38:THR:HG23	1.99	0.44
1:R:361:ILE:O	1:R:364:ARG:HD2	2.17	0.44
1:R:415:ALA:O	1:R:416:SER:CB	2.65	0.44
1:Z:272:ALA:HB2	1:Z:352:LEU:HD12	1.99	0.44
1:Z:487:ARG:O	1:Z:491:MET:HG2	2.18	0.44
1:I:72:PRO:HB3	1:I:99:LYS:HB2	1.99	0.44
1:A:221:ARG:HB3	1:A:345:TRP:CE2	2.52	0.44
1:R:15:LEU:HD21	1:R:76:ILE:HD11	1.98	0.44
1:1:134:ILE:O	1:1:166:ILE:HA	2.16	0.44
1:1:36:LEU:N	1:1:36:LEU:HD23	2.31	0.44
1:A:87:TYR:OH	1:B:125:MET:HB2	2.17	0.44
1:I:122:GLN:HA	1:I:125:MET:HG3	2.00	0.44
1:I:224:VAL:HG12	1:I:248:LEU:CD1	2.48	0.44
1:J:498:GLU:HG3	1:J:508:TYR:CD2	2.53	0.44
1:J:477:LEU:HD13	1:J:543:ALA:HB1	1.99	0.44
1:1:23:VAL:HG22	1:1:72:PRO:HB2	2.00	0.44
1:A:298:GLN:O	1:A:321:HIS:HE1	2.00	0.44
1:I:463:VAL:HG13	1:I:533:ILE:HD12	1.99	0.44
1:J:58:LEU:O	1:J:61:LEU:HB3	2.16	0.44
1:Z:6:PHE:CE1	1:Z:141:GLN:HG2	2.53	0.44
1:1:125:MET:O	1:1:125:MET:HG3	2.17	0.44
1:1:191:ASP:C	1:1:191:ASP:OD1	2.55	0.44
1:A:215:PHE:CE2	1:A:218:ARG:NH1	2.86	0.44
1:A:343:GLN:HB2	1:A:343:GLN:HE21	1.43	0.44
1:A:361:ILE:HG13	1:A:362:ALA:N	2.27	0.44
1:A:68:VAL:HB	1:A:431:ALA:HB3	1.99	0.44
1:J:343:GLN:HE21	1:J:344:PRO:HD2	1.83	0.44
1:J:453:ALA:HA	1:J:456:ARG:HD2	2.00	0.44
1:R:310:ASP:O	1:R:325:ARG:NH1	2.50	0.44
1:R:485:ARG:O	1:R:489:TYR:HB2	2.18	0.44
1:R:462:LEU:HD22	1:R:530:THR:HG23	2.00	0.44
1:A:462:LEU:O	1:A:530:THR:HA	2.17	0.44
1:A:54:ASP:O	1:A:57:GLY:N	2.51	0.44
1:I:184:SER:O	1:I:188:ARG:HG2	2.18	0.44
1:J:3:VAL:CB	1:J:173:PRO:HD2	2.42	0.44
1:R:391:SER:OG	1:R:392:LEU:N	2.51	0.44
1:S:15:LEU:HD13	1:S:40:ALA:HB3	1.99	0.44
1:S:60:HIS:HE1	1:S:88:PRO:HB2	1.82	0.44
1:Z:374:HIS:HB2	1:Z:400:LEU:HB3	2.00	0.44
1:Z:87:TYR:OH	1:1:125:MET:O	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:413:ARG:HA	1:1:413:ARG:HD2	1.59	0.43
1:A:87:TYR:N	1:A:88:PRO:CD	2.81	0.43
1:B:439:ILE:HG23	1:B:465:ILE:HB	1.98	0.43
1:B:54:ASP:C	1:B:54:ASP:OD1	2.57	0.43
1:I:90:LEU:HD12	1:I:163:GLY:HA3	2.00	0.43
1:J:217:TRP:CE3	1:J:281:ILE:HD12	2.53	0.43
1:J:306:TYR:O	1:J:323:GLY:HA3	2.18	0.43
1:R:435:PRO:HD3	1:R:460:ALA:HB1	2.00	0.43
1:S:158:THR:HG22	1:S:202:GLU:HG2	2.00	0.43
1:S:312:ILE:HD11	1:S:316:LEU:HD21	2.00	0.43
1:S:463:VAL:HG13	1:S:533:ILE:HD12	1.99	0.43
1:1:108:PRO:HB2	1:1:110:GLU:OE2	2.17	0.43
1:A:465:ILE:HD11	1:A:521:PHE:HZ	1.82	0.43
1:I:269:ASN:O	1:I:272:ALA:HB3	2.18	0.43
1:I:288:SER:O	1:I:289:LEU:C	2.57	0.43
1:A:110:GLU:HG3	1:J:143:ILE:HG12	2.00	0.43
1:R:436:THR:O	1:R:462:LEU:HA	2.18	0.43
1:1:470:ASN:O	1:1:492:PRO:HB3	2.19	0.43
1:1:523:ASP:O	1:1:526:ARG:HB2	2.18	0.43
1:A:86:LEU:HD13	1:A:102:LEU:HD13	2.00	0.43
1:B:131:THR:OG1	1:B:161:ALA:O	2.26	0.43
1:S:521:PHE:O	1:S:524:ALA:N	2.51	0.43
1:Z:222:GLY:HA3	1:Z:246:TRP:CE3	2.53	0.43
1:1:230:SER:O	1:1:255:GLN:NE2	2.51	0.43
1:A:208:SER:HA	1:I:204:PRO:HA	2.00	0.43
1:J:359:ALA:CB	1:J:552:GLN:HE22	2.27	0.43
1:R:26:ILE:HG13	1:R:74:ALA:CB	2.48	0.43
1:S:203:ALA:N	1:S:204:PRO:HD3	2.34	0.43
1:S:327:ILE:HD13	1:1:204:PRO:HG3	2.00	0.43
1:Z:382:GLU:HG2	1:Z:383:GLN:HG2	2.01	0.43
1:Z:262:CYS:HA	1:Z:399:ALA:O	2.18	0.43
1:1:212:ARG:NH1	1:1:212:ARG:HG2	2.32	0.43
1:1:407:TYR:HA	1:1:408:PRO:HD3	1.81	0.43
1:A:54:ASP:HA	1:B:447:TYR:CZ	2.53	0.43
1:A:89:ALA:CB	6:A:755:HOH:O	2.67	0.43
1:B:188:ARG:HA	1:B:188:ARG:HD2	1.53	0.43
1:I:52:HIS:HB3	1:I:58:LEU:HD13	2.00	0.43
1:R:52:HIS:HB2	1:R:454:LEU:HD21	2.00	0.43
1:S:234:GLY:O	1:S:256:THR:HA	2.18	0.43
1:S:263:ALA:HB1	1:S:267:LEU:HD12	1.99	0.43
1:S:367:PHE:CD1	1:S:513:ASN:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:228:ARG:HG2	1:J:229:MET:N	2.33	0.43
1:J:426:ALA:HB2	1:J:455:LEU:CD2	2.48	0.43
1:S:298:GLN:O	1:S:321:HIS:CE1	2.71	0.43
1:S:366:ALA:O	1:S:371:GLN:HG2	2.18	0.43
1:Z:60:HIS:O	1:Z:424:THR:HA	2.18	0.43
1:1:255:GLN:HB2	1:1:255:GLN:HE21	1.69	0.43
1:J:106:ASP:O	1:J:169:PRO:HA	2.19	0.43
1:R:386:LEU:HG	1:R:388:VAL:HG23	2.01	0.43
1:S:360:VAL:HG22	1:S:549:LEU:HD13	1.98	0.43
1:Z:327:ILE:HD12	1:Z:327:ILE:N	2.33	0.43
1:I:386:LEU:HG	1:I:388:VAL:HG23	2.00	0.43
1:J:446:LEU:HD21	1:J:495:VAL:HG11	2.00	0.43
1:Z:511:PRO:HD2	1:Z:534:GLU:O	2.19	0.43
1:1:120:ILE:HG13	1:1:122:GLN:CG	2.49	0.43
1:Z:39:LEU:HD21	1:1:484:GLU:HG3	2.00	0.43
1:A:5:ALA:HB3	1:A:181:THR:HB	2.00	0.43
1:A:393:VAL:HG13	1:A:394:VAL:H	1.83	0.43
1:A:544:GLN:O	1:A:547:GLN:HB2	2.19	0.43
1:B:391:SER:OG	3:B:601:TPP:O3B	2.34	0.43
1:J:36:LEU:N	1:J:36:LEU:HD12	2.32	0.43
1:J:366:ALA:O	1:J:371:GLN:CG	2.66	0.43
1:J:436:THR:HB	1:J:462:LEU:HG	2.00	0.43
1:S:422:LEU:HD21	1:S:445:ALA:HA	2.01	0.43
1:S:511:PRO:HD2	1:S:534:GLU:O	2.19	0.43
1:S:66:ALA:HB1	6:S:865:HOH:O	2.19	0.43
1:R:263:ALA:HA	1:R:266:TRP:CE2	2.54	0.43
1:S:102:LEU:O	1:S:166:ILE:N	2.47	0.43
1:A:276:LEU:HD13	1:A:297:TRP:CE2	2.54	0.42
1:A:456:ARG:HG2	6:A:567:HOH:O	2.19	0.42
1:I:315:ARG:O	1:J:114:CYS:HA	2.19	0.42
1:R:55:GLU:OE1	3:S:601:TPP:N1'	2.52	0.42
1:Z:3:VAL:HB	1:Z:173:PRO:HD2	2.01	0.42
1:B:449:LEU:O	1:B:452:LEU:HG	2.19	0.42
1:R:56:ARG:HA	1:R:85:ASN:O	2.19	0.42
1:A:254:SER:O	1:A:255:GLN:C	2.54	0.42
1:I:87:TYR:N	1:I:88:PRO:CD	2.83	0.42
1:R:284:GLN:NE2	1:R:286:GLY:O	2.33	0.42
1:S:35:THR:HG22	1:S:36:LEU:N	2.34	0.42
1:Z:446:LEU:HD13	1:Z:493:GLN:HG3	1.99	0.42
1:A:285:LEU:CD1	1:A:334:LEU:HD21	2.50	0.42
1:A:285:LEU:N	1:A:285:LEU:HD23	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:HA	1:A:489:TYR:CD1	2.54	0.42
1:I:72:PRO:HB3	1:I:99:LYS:CB	2.48	0.42
1:R:283:VAL:HG12	1:R:285:LEU:CD2	2.49	0.42
1:A:129:HIS:N	1:A:130:PRO:CD	2.79	0.42
1:A:143:ILE:HG12	1:J:110:GLU:CG	2.50	0.42
1:A:254:SER:HB2	1:A:256:THR:HG23	2.02	0.42
1:B:289:LEU:HA	1:B:289:LEU:HD12	1.89	0.42
1:J:60:HIS:CG	1:J:420:GLY:HA3	2.55	0.42
1:R:9:ARG:HH21	1:R:180:ASP:HA	1.84	0.42
1:S:148:LEU:O	1:S:152:ILE:HD12	2.20	0.42
1:Z:415:ALA:O	1:I:118:GLN:HG3	2.20	0.42
1:A:154:HIS:ND1	1:A:202:GLU:OE1	2.44	0.42
1:A:87:TYR:HB3	1:B:84:ALA:HB1	2.01	0.42
1:B:220:LYS:HD3	1:B:280:GLN:HE22	1.84	0.42
1:B:527:THR:HA	1:B:528:PRO:HD3	1.94	0.42
1:B:539:ASP:OD1	1:B:539:ASP:N	2.52	0.42
1:A:205:ARG:N	1:I:207:GLU:O	2.51	0.42
1:I:387:PHE:CD2	1:I:425:ALA:HB2	2.55	0.42
1:J:325:ARG:NH1	1:J:326:LEU:O	2.51	0.42
1:S:3:VAL:HG12	1:S:173:PRO:HD2	2.01	0.42
1:S:361:ILE:O	1:S:364:ARG:HG2	2.19	0.42
1:Z:143:ILE:HA	1:Z:144:PRO:HD3	1.85	0.42
1:B:136:LEU:HB2	1:B:167:ASN:O	2.20	0.42
1:I:2:SER:O	1:I:3:VAL:C	2.58	0.42
1:S:108:PRO:HB2	1:S:110:GLU:OE2	2.20	0.42
1:Z:9:ARG:O	1:Z:12:ALA:HB3	2.19	0.42
1:I:12:ALA:HA	1:I:40:ALA:HB1	2.02	0.42
1:I:152:ILE:HG23	1:I:156:LEU:HD13	2.02	0.42
1:I:436:THR:HB	1:I:462:LEU:CD1	2.44	0.42
1:I:95:LEU:HD11	1:J:120:ILE:HG23	2.01	0.42
1:S:310:ASP:OD1	1:S:311:ASP:N	2.53	0.42
1:I:122:GLN:N	1:I:123:PRO:CD	2.83	0.42
1:I:210:LYS:HB3	1:I:212:ARG:HH12	1.84	0.42
1:I:60:HIS:CG	1:I:420:GLY:HA3	2.55	0.42
1:R:343:GLN:HB2	1:R:343:GLN:HE21	1.29	0.42
1:R:460:ALA:O	1:R:461:PRO:C	2.55	0.42
1:S:237:VAL:HG22	1:S:334:LEU:HD11	2.01	0.42
1:Z:8:ARG:HA	1:Z:36:LEU:CD2	2.50	0.42
1:Z:447:TYR:OH	1:I:55:GLU:OE1	2.30	0.41
1:A:7:ASN:HB3	1:A:36:LEU:CD1	2.34	0.41
1:B:207:GLU:O	1:J:205:ARG:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:36:LEU:HD13	1:J:170:PHE:CG	2.55	0.41
1:J:470:ASN:O	1:J:492:PRO:HB3	2.20	0.41
1:R:325:ARG:NH1	1:R:326:LEU:O	2.53	0.41
1:B:485:ARG:HG3	1:B:490:LEU:HG	2.02	0.41
1:I:146:ARG:HA	1:I:149:VAL:HG12	2.02	0.41
1:I:251:ASP:C	1:I:253:LEU:N	2.70	0.41
1:R:237:VAL:CG2	1:R:334:LEU:HD11	2.49	0.41
1:R:68:VAL:HB	1:R:431:ALA:HB3	2.02	0.41
1:Z:106:ASP:HB2	1:Z:122:GLN:NE2	2.35	0.41
1:1:368:GLY:HA3	1:1:371:GLN:OE1	2.21	0.41
1:1:403:LEU:HA	1:1:404:PRO:HD3	1.86	0.41
1:A:107:ARG:NH2	1:A:118:GLN:HB3	2.35	0.41
1:B:218:ARG:NH1	1:B:340:GLU:HB2	2.35	0.41
1:B:429:GLN:CG	1:B:458:VAL:HG12	2.47	0.41
1:R:138:ARG:HG2	1:R:138:ARG:NH1	2.35	0.41
1:S:453:ALA:HA	1:S:456:ARG:HD2	2.02	0.41
1:S:154:HIS:CE1	1:1:314:GLY:HA2	2.55	0.41
1:I:424:THR:O	1:I:428:VAL:HG23	2.21	0.41
1:I:477:LEU:HD12	1:I:547:GLN:HE21	1.84	0.41
1:B:206:LEU:HD12	1:J:205:ARG:O	2.21	0.41
1:J:521:PHE:O	1:J:525:TRP:CD1	2.74	0.41
1:1:91:ILE:HG12	1:1:129:HIS:ND1	2.35	0.41
1:A:36:LEU:HG	1:A:36:LEU:H	1.59	0.41
1:A:54:ASP:HA	1:B:447:TYR:CE2	2.55	0.41
1:B:312:ILE:HG12	1:B:313:GLU:N	2.35	0.41
1:J:312:ILE:CG1	1:J:313:GLU:N	2.83	0.41
1:S:13:VAL:HB	1:S:148:LEU:HD23	2.02	0.41
1:Z:87:TYR:HB3	1:Z:88:PRO:HD3	2.03	0.41
1:1:527:THR:HG1	1:1:529:THR:HG1	1.59	0.41
1:A:30:PRO:HB2	1:B:475:PHE:CE2	2.55	0.41
1:B:469:ASN:O	1:B:539:ASP:HB3	2.21	0.41
1:J:255:GLN:HG2	1:J:407:TYR:O	2.20	0.41
1:J:389:GLY:HA3	1:J:440:VAL:HG23	2.03	0.41
1:R:503:MET:HG2	1:R:504:PHE:CE2	2.56	0.41
1:S:16:GLU:OE1	1:S:16:GLU:HA	2.21	0.41
1:Z:203:ALA:N	1:Z:204:PRO:HD3	2.36	0.41
1:Z:222:GLY:HA3	1:Z:246:TRP:CZ3	2.56	0.41
1:Z:386:LEU:HG	1:Z:388:VAL:HG23	2.02	0.41
1:Z:407:TYR:HA	1:Z:408:PRO:HD3	1.89	0.41
1:1:377:CYS:HA	1:1:380:LEU:HG	2.01	0.41
1:A:16:GLU:O	1:A:19:THR:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG23	1:A:334:LEU:HD11	2.01	0.41
1:A:297:TRP:O	1:A:301:CYS:HB3	2.21	0.41
1:S:103:LEU:HD23	1:S:166:ILE:HB	2.02	0.41
1:S:81:THR:O	1:S:85:ASN:ND2	2.54	0.41
1:Z:391:SER:HG	3:Z:601:TPP:PB	2.43	0.41
1:Z:67:LYS:HB2	1:Z:67:LYS:HE2	1.93	0.41
1:1:376:ILE:HA	1:1:376:ILE:HD12	1.66	0.41
1:1:262:CYS:HA	1:1:399:ALA:O	2.20	0.41
1:1:527:THR:HG23	6:1:801:HOH:O	2.20	0.41
1:A:487:ARG:HG2	1:A:488:PHE:CE2	2.55	0.41
1:A:87:TYR:CD1	1:A:91:ILE:HD11	2.56	0.41
1:B:285:LEU:HD22	1:B:330:ILE:HG23	2.02	0.41
1:B:244:LEU:HG	1:B:339:ALA:HB1	2.02	0.41
1:I:72:PRO:HA	1:I:99:LYS:HB2	2.02	0.41
1:J:136:LEU:HD23	1:J:136:LEU:HA	1.84	0.41
1:R:369:GLU:HG2	6:R:662:HOH:O	2.20	0.41
1:S:252:VAL:HG12	1:S:403:LEU:HD11	2.02	0.41
1:Z:220:LYS:HD3	1:Z:220:LYS:HA	1.71	0.41
1:Z:393:VAL:HG13	1:Z:394:VAL:N	2.34	0.41
1:Z:96:THR:OG1	1:Z:98:GLU:OE1	2.39	0.41
1:1:145:ALA:HA	1:1:185:TRP:CZ2	2.56	0.41
1:B:9:ARG:HD2	1:B:186:GLN:OE1	2.21	0.41
1:A:56:ARG:NH1	1:B:85:ASN:OD1	2.53	0.41
1:J:312:ILE:HG12	1:J:313:GLU:N	2.34	0.41
1:J:407:TYR:HA	1:J:408:PRO:HD3	1.83	0.41
1:R:34:SER:O	1:R:35:THR:C	2.59	0.41
1:1:18:LEU:HD23	1:1:18:LEU:HA	1.82	0.41
1:1:222:GLY:HA2	1:1:281:ILE:O	2.20	0.41
1:1:257:GLY:O	1:1:258:GLN:C	2.59	0.41
1:A:109:PRO:C	1:A:111:LEU:H	2.25	0.41
1:A:157:GLY:O	1:A:203:ALA:HA	2.21	0.41
1:B:255:GLN:HB2	1:B:255:GLN:HE21	1.70	0.41
1:B:87:TYR:HB3	1:B:88:PRO:HD3	2.03	0.41
1:J:538:ASN:O	1:J:541:ASP:HB2	2.21	0.41
1:Z:460:ALA:O	1:Z:461:PRO:C	2.59	0.41
1:1:120:ILE:HG13	1:1:122:GLN:HG3	2.02	0.41
1:1:248:LEU:HD21	1:1:256:THR:HG21	2.03	0.41
1:A:551:ALA:O	1:A:552:GLN:C	2.59	0.41
1:B:263:ALA:HA	1:B:266:TRP:NE1	2.36	0.41
1:I:144:PRO:O	1:I:147:TRP:N	2.49	0.41
1:I:39:LEU:HA	1:I:39:LEU:HD12	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:204:PRO:HA	1:Z:208:SER:HA	2.03	0.41
1:R:391:SER:HG	1:R:392:LEU:H	1.69	0.41
1:R:390:ASN:OD1	1:R:413:ARG:HD2	2.21	0.41
1:A:19:THR:HG22	1:A:19:THR:O	2.21	0.40
1:A:28:ILE:O	1:A:51:THR:HA	2.21	0.40
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.90	0.40
1:I:473:GLN:HG3	1:I:539:ASP:O	2.21	0.40
1:J:317:ASP:C	1:J:319:ALA:H	2.23	0.40
1:R:3:VAL:O	1:R:4:SER:C	2.59	0.40
1:S:412:ASN:O	1:S:416:SER:HA	2.20	0.40
1:Z:455:LEU:HD13	1:Z:530:THR:HG21	2.03	0.40
1:1:143:ILE:HD13	1:1:143:ILE:HG21	1.80	0.40
1:A:343:GLN:O	1:A:344:PRO:C	2.59	0.40
1:A:366:ALA:O	1:A:371:GLN:CG	2.69	0.40
1:B:391:SER:OG	3:B:601:TPP:PB	2.79	0.40
1:J:160:HIS:O	1:J:161:ALA:HB2	2.21	0.40
1:J:228:ARG:HB2	1:J:253:LEU:HD23	2.02	0.40
1:R:254:SER:HB2	1:R:256:THR:HG23	2.03	0.40
1:R:446:LEU:HD23	1:R:446:LEU:HA	1.92	0.40
1:S:317:ASP:HA	1:S:318:PRO:HD2	1.75	0.40
1:A:68:VAL:HG22	1:A:410:TYR:CZ	2.55	0.40
1:I:211:GLN:OE1	1:I:324:ARG:NH2	2.54	0.40
1:R:182:GLY:O	1:R:185:TRP:HB3	2.22	0.40
1:R:370:ALA:HB3	6:R:727:HOH:O	2.21	0.40
1:Z:122:GLN:N	1:Z:123:PRO:HD2	2.37	0.40
1:1:101:ILE:HG13	1:1:156:LEU:HD21	2.04	0.40
1:1:228:ARG:HA	1:1:253:LEU:HB3	2.04	0.40
1:1:444:SER:OG	3:1:601:TPP:O2A	2.40	0.40
1:A:464:LEU:HA	1:A:464:LEU:HD12	1.86	0.40
1:B:361:ILE:O	1:B:364:ARG:HG2	2.22	0.40
1:B:507:LYS:HE2	1:B:507:LYS:HB2	1.89	0.40
1:I:285:LEU:HD22	1:I:285:LEU:N	2.37	0.40
1:R:211:GLN:OE1	1:R:324:ARG:HD3	2.22	0.40
1:1:61:LEU:HD12	1:1:427:GLY:CA	2.52	0.40
1:B:10:TRP:O	1:B:14:ILE:HG13	2.21	0.40
1:J:474:ILE:HG21	3:J:601:TPP:S1	2.62	0.40
1:J:508:TYR:HA	1:J:532:VAL:O	2.22	0.40
1:R:109:PRO:HG2	1:R:138:ARG:HD2	2.03	0.40
1:S:17:ALA:HB2	1:S:149:VAL:HG23	2.04	0.40
1:Z:108:PRO:CB	1:Z:110:GLU:OE1	2.43	0.40
1:Z:371:GLN:O	1:Z:375:ARG:N	2.53	0.40



There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	554/556 (100%)	511 (92%)	38 (7%)	5 (1%)	19	38
1	A	551/556 (99%)	517 (94%)	32 (6%)	2 (0%)	36	60
1	B	554/556 (100%)	516 (93%)	34 (6%)	4 (1%)	24	46
1	I	550/556 (99%)	494 (90%)	49 (9%)	7 (1%)	13	27
1	J	554/556 (100%)	508 (92%)	44 (8%)	2 (0%)	36	60
1	R	550/556 (99%)	504 (92%)	44 (8%)	2 (0%)	36	60
1	S	554/556 (100%)	506 (91%)	46 (8%)	2 (0%)	36	60
1	Z	550/556 (99%)	509 (92%)	39 (7%)	2 (0%)	36	60
All	All	4417/4448 (99%)	4065 (92%)	326 (7%)	26 (1%)	27	51

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	THR
1	B	179	ASP
1	J	179	ASP
1	1	179	ASP
1	A	181	THR
1	B	376	ILE
1	I	231	ALA
1	I	341	LYS
1	J	539	ASP
1	1	376	ILE
1	B	178	MET
1	I	539	ASP
1	S	367	PHE
1	I	3	VAL

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Mol	Chain	Res	Type
1	R	4	SER
1	R	35	THR
1	Z	539	ASP
1	1	202	GLU
1	A	514	TRP
1	1	212	ARG
1	I	2	SER
1	I	393	VAL
1	Z	2	SER
1	1	23	VAL
1	I	252	VAL
1	S	91	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	452/452 (100%)	421 (93%)	31 (7%)	17	34
1	A	451/452 (100%)	415 (92%)	36 (8%)	13	26
1	B	452/452 (100%)	420 (93%)	32 (7%)	16	32
1	I	451/452 (100%)	415 (92%)	36 (8%)	13	26
1	J	452/452 (100%)	419 (93%)	33 (7%)	15	31
1	R	451/452 (100%)	417 (92%)	34 (8%)	15	29
1	S	452/452 (100%)	415 (92%)	37 (8%)	12	25
1	Z	451/452 (100%)	419 (93%)	32 (7%)	16	32
All	All	3612/3616 (100%)	3341 (92%)	271 (8%)	15	29

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	24	ARG
1	A	35	THR

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Mol	Chain	Res	Type
1	A	39	LEU
1	A	87	TYR
1	A	140	THR
1	A	141	GLN
1	A	156	LEU
1	A	184	SER
1	A	219	GLN
1	A	239	LEU
1	A	252	VAL
1	A	255	GLN
1	A	273	THR
1	A	277	GLN
1	A	288	SER
1	A	289	LEU
1	A	293	ARG
1	A	301	CYS
1	A	325	ARG
1	A	343	GLN
1	A	347	VAL
1	A	351	ARG
1	A	361	ILE
1	A	375	ARG
1	A	422	LEU
1	A	423	SER
1	A	444	SER
1	A	447	TYR
1	A	474	ILE
1	A	483	SER
1	A	485	ARG
1	A	495	VAL
1	A	535	MET
1	A	550	LEU
1	A	556	LEU
1	B	15	LEU
1	B	20	ARG
1	B	24	ARG
1	B	35	THR
1	B	87	TYR
1	B	107	ARG
1	B	133	SER
1	B	178	MET
1	B	179	ASP

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Mol	Chain	Res	Type
1	B	183	LEU
1	B	236	LYS
1	B	253	LEU
1	B	254	SER
1	B	255	GLN
1	B	287	SER
1	B	289	LEU
1	B	325	ARG
1	B	348	GLU
1	B	388	VAL
1	B	422	LEU
1	B	429	GLN
1	B	447	TYR
1	B	458	VAL
1	B	484	GLU
1	B	485	ARG
1	B	487	ARG
1	B	495	VAL
1	B	512	GLN
1	B	515	GLN
1	B	523	ASP
1	B	539	ASP
1	B	550	LEU
1	I	8	ARG
1	I	9	ARG
1	I	15	LEU
1	I	24	ARG
1	I	33	ARG
1	I	36	LEU
1	I	39	LEU
1	I	87	TYR
1	I	107	ARG
1	I	110	GLU
1	I	146	ARG
1	I	156	LEU
1	I	174	LEU
1	I	252	VAL
1	I	255	GLN
1	I	273	THR
1	I	281	ILE
1	I	285	LEU
1	I	289	LEU

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Mol	Chain	Res	Type
1	I	293	ARG
1	I	325	ARG
1	I	341	LYS
1	I	343	GLN
1	I	347	VAL
1	I	358	GLN
1	I	361	ILE
1	I	382	GLU
1	I	422	LEU
1	I	423	SER
1	I	429	GLN
1	I	447	TYR
1	I	495	VAL
1	I	507	LYS
1	I	535	MET
1	I	550	LEU
1	I	556	LEU
1	J	8	ARG
1	J	32	SER
1	J	35	THR
1	J	36	LEU
1	J	87	TYR
1	J	146	ARG
1	J	178	MET
1	J	183	LEU
1	J	184	SER
1	J	197	LYS
1	J	212	ARG
1	J	252	VAL
1	J	253	LEU
1	J	255	GLN
1	J	274	SER
1	J	284	GLN
1	J	287	SER
1	J	289	LEU
1	J	301	CYS
1	J	325	ARG
1	J	343	GLN
1	J	357	MET
1	J	363	ARG
1	J	391	SER
1	J	429	GLN

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Mol	Chain	Res	Type
1	J	439	ILE
1	J	440	VAL
1	J	447	TYR
1	J	484	GLU
1	J	485	ARG
1	J	507	LYS
1	J	539	ASP
1	J	544	GLN
1	R	4	SER
1	R	15	LEU
1	R	24	ARG
1	R	39	LEU
1	R	58	LEU
1	R	87	TYR
1	R	133	SER
1	R	135	SER
1	R	149	VAL
1	R	156	LEU
1	R	166	ILE
1	R	178	MET
1	R	179	ASP
1	R	209	GLU
1	R	252	VAL
1	R	255	GLN
1	R	262	CYS
1	R	273	THR
1	R	285	LEU
1	R	289	LEU
1	R	293	ARG
1	R	325	ARG
1	R	341	LYS
1	R	343	GLN
1	R	375	ARG
1	R	377	CYS
1	R	440	VAL
1	R	447	TYR
1	R	519	THR
1	R	526	ARG
1	R	535	MET
1	R	550	LEU
1	R	554	SER
1	R	556	LEU

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Mol	Chain	Res	Type
1	S	9	ARG
1	S	15	LEU
1	S	20	ARG
1	S	24	ARG
1	S	35	THR
1	S	87	TYR
1	S	178	MET
1	S	179	ASP
1	S	188	ARG
1	S	197	LYS
1	S	252	VAL
1	S	253	LEU
1	S	255	GLN
1	S	273	THR
1	S	274	SER
1	S	285	LEU
1	S	296	GLN
1	S	325	ARG
1	S	336	LEU
1	S	354	GLU
1	S	357	MET
1	S	375	ARG
1	S	377	CYS
1	S	382	GLU
1	S	391	SER
1	S	422	LEU
1	S	429	GLN
1	S	439	ILE
1	S	447	TYR
1	S	484	GLU
1	S	485	ARG
1	S	487	ARG
1	S	495	VAL
1	S	507	LYS
1	S	508	TYR
1	S	546	LEU
1	S	550	LEU
1	Z	1	MET
1	Z	4	SER
1	Z	15	LEU
1	Z	35	THR
1	Z	87	TYR

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Mol	Chain	Res	Type
1	Z	110	GLU
1	Z	140	THR
1	Z	146	ARG
1	Z	156	LEU
1	Z	252	VAL
1	Z	255	GLN
1	Z	284	GLN
1	Z	285	LEU
1	Z	289	LEU
1	Z	293	ARG
1	Z	324	ARG
1	Z	325	ARG
1	Z	343	GLN
1	Z	347	VAL
1	Z	357	MET
1	Z	364	ARG
1	Z	375	ARG
1	Z	377	CYS
1	Z	423	SER
1	Z	440	VAL
1	Z	447	TYR
1	Z	483	SER
1	Z	495	VAL
1	Z	515	GLN
1	Z	519	THR
1	Z	535	MET
1	Z	556	LEU
1	1	15	LEU
1	1	20	ARG
1	1	24	ARG
1	1	35	THR
1	1	87	TYR
1	1	107	ARG
1	1	151	THR
1	1	152	ILE
1	1	183	LEU
1	1	208	SER
1	1	212	ARG
1	1	252	VAL
1	1	255	GLN
1	1	285	LEU
1	1	289	LEU

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Mol	Chain	Res	Type
1	1	302	GLU
1	1	348	GLU
1	1	376	ILE
1	1	377	CYS
1	1	391	SER
1	1	429	GLN
1	1	440	VAL
1	1	447	TYR
1	1	462	LEU
1	1	484	GLU
1	1	485	ARG
1	1	495	VAL
1	1	515	GLN
1	1	518	GLU
1	1	527	THR
1	1	539	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	160	HIS
1	A	296	GLN
1	A	343	GLN
1	A	509	HIS
1	A	547	GLN
1	B	141	GLN
1	B	278	GLN
1	B	280	GLN
1	B	320	HIS
1	I	355	GLN
1	I	547	GLN
1	J	129	HIS
1	J	343	GLN
1	J	355	GLN
1	J	358	GLN
1	J	544	GLN
1	J	552	GLN
1	R	320	HIS
1	R	343	GLN
1	S	280	GLN
1	S	320	HIS

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Mol	Chain	Res	Type
1	Z	141	GLN
1	Z	343	GLN
1	1	355	GLN
1	1	385	GLN
1	1	544	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 carbohydrates in this entry.

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

Of 33 ligands modelled in this entry, 23 are monoatomic - leaving 10 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	$\# Z  > 2$
5	GOL	1	558	-	5,5,5	0.59	0	5,5,5	0.77	0
3	TPP	1	601	4	21,27,27	1.23	3 (14%)	26,40,40	2.03	10 (38%)
3	TPP	A	601	4	21,27,27	1.54	5 (23%)	26,40,40	1.90	7 (26%)
3	TPP	B	601	4	21,27,27	1.74	5 (23%)	26,40,40	2.01	7 (26%)
3	TPP	I	601	4	21,27,27	1.78	7 (33%)	26,40,40	2.06	11 (42%)
5	GOL	J	557	-	5,5,5	0.38	0	5,5,5	0.54	0
3	TPP	J	601	4	21,27,27	1.23	4 (19%)	26,40,40	2.39	9 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TPP	R	601	4	21,27,27	1.43	5 (23%)	26,40,40	2.17	9 (34%)
3	TPP	S	601	4	21,27,27	1.85	3 (14%)	26,40,40	1.68	6 (23%)
3	TPP	Z	601	4	21,27,27	1.43	5 (23%)	26,40,40	2.27	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	1	558	-	-	0/4/4/4	0/0/0/0
3	TPP	1	601	4	-	0/16/17/17	0/2/2/2
3	TPP	A	601	4	-	0/16/17/17	0/2/2/2
3	TPP	B	601	4	-	0/16/17/17	0/2/2/2
3	TPP	I	601	4	-	0/16/17/17	0/2/2/2
5	GOL	J	557	-	-	0/4/4/4	0/0/0/0
3	TPP	J	601	4	-	0/16/17/17	0/2/2/2
3	TPP	R	601	4	-	0/16/17/17	0/2/2/2
3	TPP	S	601	4	-	0/16/17/17	0/2/2/2
3	TPP	Z	601	4	-	0/16/17/17	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	601	TPP	C4-N3	-5.97	1.34	1.39
3	B	601	TPP	C4-N3	-4.47	1.35	1.39
3	A	601	TPP	C4-N3	-3.53	1.36	1.39
3	I	601	TPP	PB-O3B	-3.29	1.41	1.54
3	S	601	TPP	C7'-N3	-3.04	1.43	1.48
3	Z	601	TPP	C4-N3	-2.87	1.37	1.39
3	B	601	TPP	C7'-N3	-2.86	1.43	1.48
3	A	601	TPP	C7'-N3	-2.84	1.43	1.48
3	R	601	TPP	C7'-N3	-2.71	1.43	1.48
3	S	601	TPP	C5'-C4'	-2.69	1.38	1.42
3	I	601	TPP	C4-N3	-2.59	1.37	1.39
3	I	601	TPP	C7'-N3	-2.36	1.44	1.48
3	R	601	TPP	C5'-C4'	-2.24	1.39	1.42
3	1	601	TPP	C4-N3	-2.15	1.37	1.39
3	B	601	TPP	C5'-C4'	-2.08	1.39	1.42
3	Z	601	TPP	C7'-N3	-2.02	1.45	1.48
3	1	601	TPP	C4'-N3'	2.03	1.38	1.35
3	Z	601	TPP	C2'-N1'	2.14	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	601	TPP	C2'-N1'	2.16	1.38	1.34
3	J	601	TPP	C2'-N1'	2.19	1.38	1.34
3	A	601	TPP	C2'-N1'	2.24	1.38	1.34
3	J	601	TPP	C2'-N3'	2.29	1.38	1.34
3	J	601	TPP	C6'-N1'	2.32	1.39	1.34
3	A	601	TPP	C2'-N3'	2.38	1.38	1.34
3	B	601	TPP	C2'-N3'	2.40	1.38	1.34
3	R	601	TPP	C2'-N3'	2.50	1.38	1.34
3	A	601	TPP	C4'-N3'	2.56	1.38	1.35
3	1	601	TPP	C2'-N3'	2.61	1.38	1.34
3	I	601	TPP	C4'-N3'	2.61	1.38	1.35
3	I	601	TPP	C2'-N1'	2.62	1.38	1.34
3	Z	601	TPP	C2'-N3'	2.67	1.38	1.34
3	Z	601	TPP	C4'-N3'	2.77	1.39	1.35
3	I	601	TPP	C2'-N3'	3.01	1.39	1.34
3	J	601	TPP	C4'-N3'	3.17	1.39	1.35
3	R	601	TPP	C4'-N3'	3.23	1.39	1.35
3	I	601	TPP	PB-O3A	3.28	1.65	1.60
3	B	601	TPP	C2'-N1'	3.35	1.39	1.34

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	601	TPP	N1'-C2'-N3'	-4.18	118.18	125.55
3	A	601	TPP	PA-O3A-PB	-3.73	120.08	132.63
3	1	601	TPP	PA-O3A-PB	-3.59	120.57	132.63
3	Z	601	TPP	N1'-C2'-N3'	-3.47	119.44	125.55
3	R	601	TPP	N1'-C2'-N3'	-3.40	119.56	125.55
3	S	601	TPP	PA-O3A-PB	-3.32	121.48	132.63
3	J	601	TPP	CM4-C4-C5	-3.26	120.47	127.60
3	I	601	TPP	O3B-PB-O1B	-3.10	98.49	110.60
3	B	601	TPP	C5'-C6'-N1'	-3.04	118.69	123.83
3	S	601	TPP	N1'-C2'-N3'	-2.90	120.44	125.55
3	B	601	TPP	PA-O3A-PB	-2.83	123.11	132.63
3	J	601	TPP	PA-O3A-PB	-2.77	123.31	132.63
3	I	601	TPP	N1'-C2'-N3'	-2.68	120.82	125.55
3	Z	601	TPP	PA-O3A-PB	-2.67	123.66	132.63
3	A	601	TPP	N1'-C2'-N3'	-2.52	121.11	125.55
3	B	601	TPP	N1'-C2'-N3'	-2.48	121.18	125.55
3	R	601	TPP	CM4-C4-C5	-2.48	122.19	127.60
3	1	601	TPP	CM4-C4-C5	-2.43	122.28	127.60
3	I	601	TPP	C5'-C6'-N1'	-2.42	119.74	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	601	TPP	C5'-C6'-N1'	-2.41	119.75	123.83
3	I	601	TPP	C5'-C4'-N4'	-2.38	118.88	122.23
3	R	601	TPP	PA-O3A-PB	-2.32	124.83	132.63
3	1	601	TPP	N1'-C2'-N3'	-2.30	121.50	125.55
3	I	601	TPP	O2B-PB-O1B	-2.05	102.58	110.60
3	B	601	TPP	C6'-N1'-C2'	2.01	119.44	115.95
3	S	601	TPP	C2'-N3'-C4'	2.02	121.56	118.14
3	J	601	TPP	CM2-C2'-N3'	2.05	120.64	117.20
3	A	601	TPP	N4'-C4'-N3'	2.11	120.04	117.01
3	1	601	TPP	C6'-N1'-C2'	2.11	119.63	115.95
3	Z	601	TPP	CM2-C2'-N3'	2.12	120.76	117.20
3	J	601	TPP	C6'-N1'-C2'	2.22	119.83	115.95
3	J	601	TPP	C2'-N3'-C4'	2.29	122.02	118.14
3	A	601	TPP	CM2-C2'-N1'	2.32	119.65	117.07
3	I	601	TPP	C6'-N1'-C2'	2.36	120.07	115.95
3	S	601	TPP	N4'-C4'-N3'	2.36	120.40	117.01
3	R	601	TPP	C6'-N1'-C2'	2.41	120.16	115.95
3	Z	601	TPP	CM2-C2'-N1'	2.46	119.80	117.07
3	I	601	TPP	N4'-C4'-N3'	2.60	120.74	117.01
3	1	601	TPP	N4'-C4'-N3'	2.63	120.78	117.01
3	S	601	TPP	C6'-C5'-C4'	2.66	119.41	115.72
3	1	601	TPP	CM2-C2'-N3'	2.67	121.67	117.20
3	I	601	TPP	CM4-C4-N3	2.73	126.01	122.53
3	I	601	TPP	CM2-C2'-N3'	2.83	121.94	117.20
3	A	601	TPP	CM4-C4-N3	2.83	126.14	122.53
3	Z	601	TPP	C6'-N1'-C2'	2.87	120.95	115.95
3	R	601	TPP	CM2-C2'-N3'	2.93	122.11	117.20
3	I	601	TPP	C6'-C5'-C4'	3.00	119.88	115.72
3	A	601	TPP	C6'-C5'-C4'	3.25	120.22	115.72
3	1	601	TPP	C6'-C5'-C4'	3.31	120.31	115.72
3	R	601	TPP	C6'-C5'-C4'	3.35	120.37	115.72
3	R	601	TPP	N4'-C4'-N3'	3.47	122.00	117.01
3	S	601	TPP	CM2-C2'-N1'	3.58	121.04	117.07
3	Z	601	TPP	CM4-C4-N3	3.61	127.13	122.53
3	R	601	TPP	C6-C5-C4	3.68	130.38	127.43
3	J	601	TPP	CM2-C2'-N1'	3.70	121.18	117.07
3	B	601	TPP	CM2-C2'-N1'	3.82	121.31	117.07
3	1	601	TPP	CM4-C4-N3	4.08	127.73	122.53
3	B	601	TPP	CM4-C4-N3	4.10	127.75	122.53
3	A	601	TPP	C6-C5-C4	4.41	130.97	127.43
3	1	601	TPP	C6-C5-C4	4.49	131.04	127.43
3	B	601	TPP	C6'-C5'-C4'	4.84	122.42	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	601	TPP	CM4-C4-N3	5.24	129.21	122.53
3	J	601	TPP	CM4-C4-N3	5.47	129.50	122.53
3	I	601	TPP	C6-C5-C4	5.50	131.85	127.43
3	J	601	TPP	C6-C5-C4	6.59	132.73	127.43
3	Z	601	TPP	C6-C5-C4	7.92	133.79	127.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	601	TPP	1	0
3	A	601	TPP	1	0
3	B	601	TPP	7	0
3	I	601	TPP	1	0
3	J	601	TPP	1	0
3	R	601	TPP	3	0
3	S	601	TPP	1	0
3	Z	601	TPP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	556/556 (100%)	-0.39	3 (0%) 90 89	4, 13, 25, 38	10 (1%)
1	A	555/556 (99%)	-0.50	1 (0%) 94 95	2, 11, 24, 39	11 (1%)
1	B	556/556 (100%)	-0.50	1 (0%) 94 95	3, 12, 22, 35	10 (1%)
1	I	554/556 (99%)	-0.42	3 (0%) 90 89	3, 13, 26, 46	11 (1%)
1	J	556/556 (100%)	-0.25	2 (0%) 92 91	5, 17, 30, 38	10 (1%)
1	R	554/556 (99%)	-0.52	1 (0%) 94 95	4, 12, 22, 42	11 (1%)
1	S	556/556 (100%)	-0.47	3 (0%) 90 89	3, 12, 24, 37	10 (1%)
1	Z	554/556 (99%)	-0.42	0 100 100	4, 15, 29, 43	11 (1%)
All	All	4441/4448 (99%)	-0.44	14 (0%) 93 93	2, 13, 26, 46	84 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.7
1	I	522	ALA	3.4
1	S	1	MET	3.3
1	1	1	MET	3.2
1	R	1	MET	3.1
1	1	190	GLY	2.7
1	J	1	MET	2.6
1	I	1	MET	2.6
1	J	178	MET	2.6
1	1	178	MET	2.3
1	S	183	LEU	2.1
1	S	181	THR	2.1
1	I	178	MET	2.0
1	A	194	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	1	557	1/1	0.83	0.16	26,26,26,26	0
2	NA	A	558	1/1	0.87	0.16	23,23,23,23	0
2	NA	Z	558	1/1	0.90	0.11	28,28,28,28	0
5	GOL	J	557	6/6	0.91	0.24	35,37,37,39	0
5	GOL	1	558	6/6	0.91	0.16	29,32,32,33	0
2	NA	R	558	1/1	0.91	0.11	34,34,34,34	0
2	NA	B	557	1/1	0.92	0.11	30,30,30,30	0
4	MG	I	602	1/1	0.93	0.23	2,2,2,2	0
2	NA	S	558	1/1	0.94	0.16	25,25,25,25	0
2	NA	I	559	1/1	0.94	0.10	18,18,18,18	0
2	NA	Z	557	1/1	0.95	0.25	33,33,33,33	0
2	NA	S	559	1/1	0.95	0.19	18,18,18,18	0
4	MG	R	602	1/1	0.95	0.22	2,2,2,2	0
2	NA	A	557	1/1	0.95	0.16	17,17,17,17	0
2	NA	S	557	1/1	0.95	0.12	19,19,19,19	0
2	NA	R	559	1/1	0.95	0.10	26,26,26,26	0
2	NA	R	557	1/1	0.96	0.20	29,29,29,29	0
4	MG	S	602	1/1	0.96	0.13	8,8,8,8	0
4	MG	J	602	1/1	0.96	0.14	2,2,2,2	0
2	NA	I	558	1/1	0.96	0.12	17,17,17,17	0
3	TPP	I	601	26/26	0.97	0.13	2,12,14,14	0
3	TPP	S	601	26/26	0.97	0.11	2,5,7,12	0
3	TPP	B	601	26/26	0.97	0.11	5,8,10,11	0
3	TPP	1	601	26/26	0.97	0.13	3,7,10,11	0
3	TPP	J	601	26/26	0.97	0.12	7,13,19,24	0
3	TPP	R	601	26/26	0.98	0.10	2,7,11,11	0
4	MG	1	602	1/1	0.98	0.23	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TPP	A	601	26/26	0.98	0.11	2,4,11,12	0
4	MG	A	602	1/1	0.98	0.13	2,2,2,2	0
2	NA	I	557	1/1	0.98	0.16	20,20,20,20	0
3	TPP	Z	601	26/26	0.98	0.14	4,10,12,13	0
4	MG	B	602	1/1	0.99	0.18	2,2,2,2	0
4	MG	Z	602	1/1	0.99	0.17	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.