Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:46 AM GMT

PDB ID	:	2SOD
Title	:	DETERMINATION AND ANALYSIS OF THE 2 ANGSTROM STRUCTURE OF COPPER, ZINC SUPEROXIDE DISMUTASE
Authors	:	Tainer, J.A.; Getzoff, E.D.; Richardson, J.S.; Richardson, D.C.
Deposited on	:	1980-03-25
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

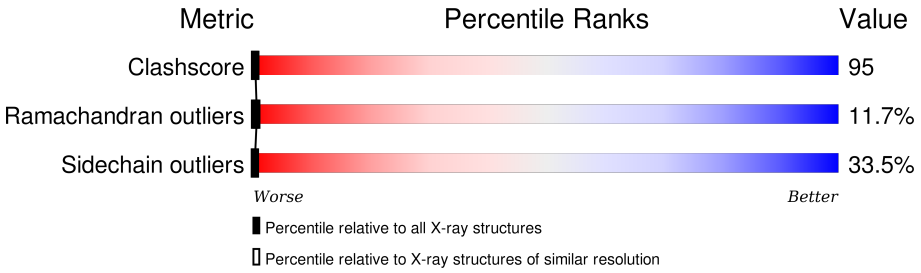
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	152	19% 32% 31% 18%
1	G	152	7% 32% 36% 25%
1	O	152	14% 30% 34% 22%
1	Y	152	7% 34% 38% 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4392 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 COPPER,ZINC SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	152	Total	C	N	O	S	0	0	0
			1095	672	198	221	4			
1	Y	152	Total	C	N	O	S	0	0	0
			1095	672	198	221	4			
1	B	152	Total	C	N	O	S	0	0	0
			1095	672	198	221	4			
1	G	152	Total	C	N	O	S	0	0	0
			1095	672	198	221	4			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	Y	1	Total	Cu	0	0
			1	1		
2	G	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	Y	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	O	1	Total O 1 1	0	0
4	Y	1	Total O 1 1	0	0

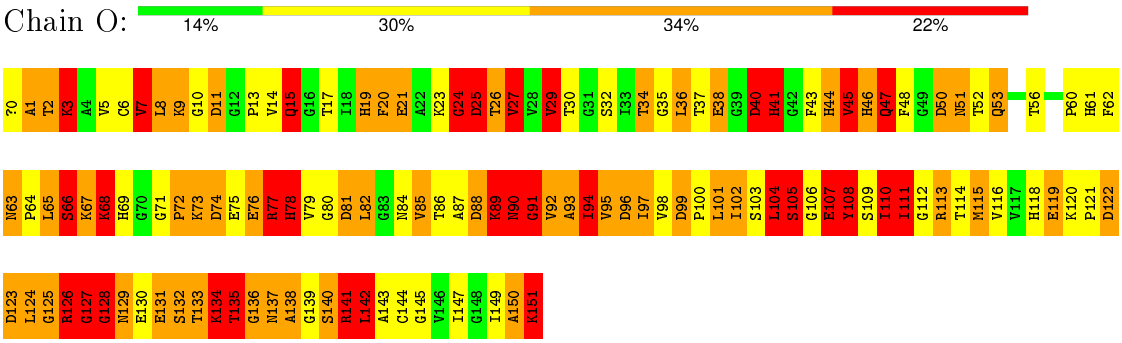
3 Residue-property plots (i)

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

Note EDS was not executed.

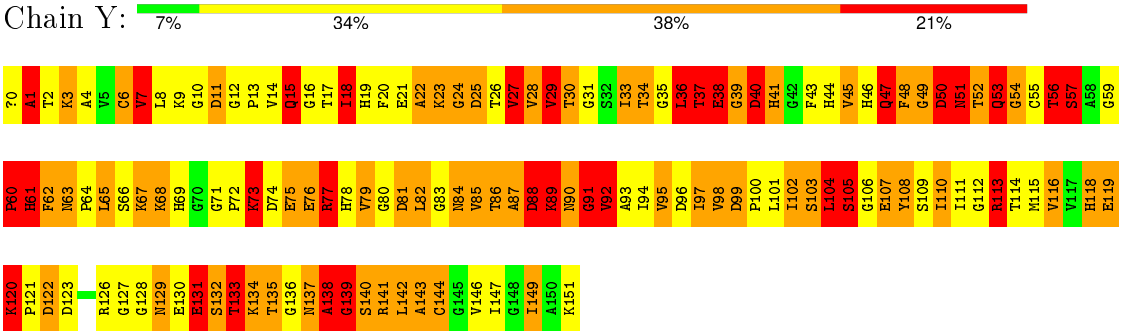
- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain O:



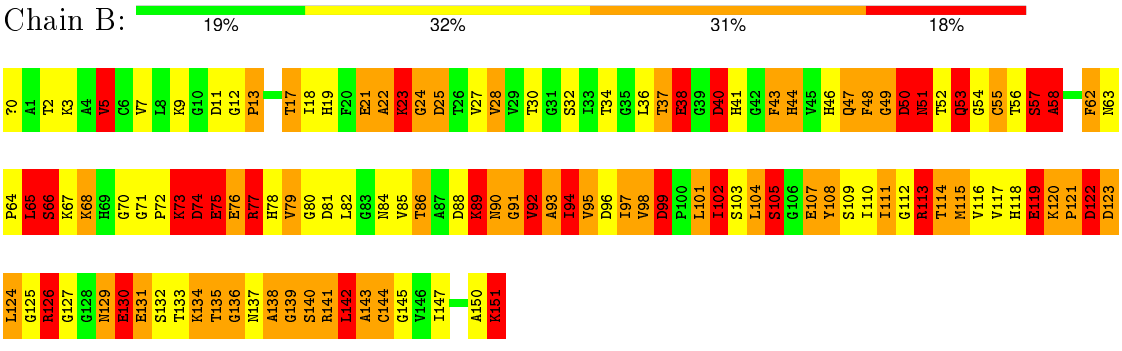
- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain Y:



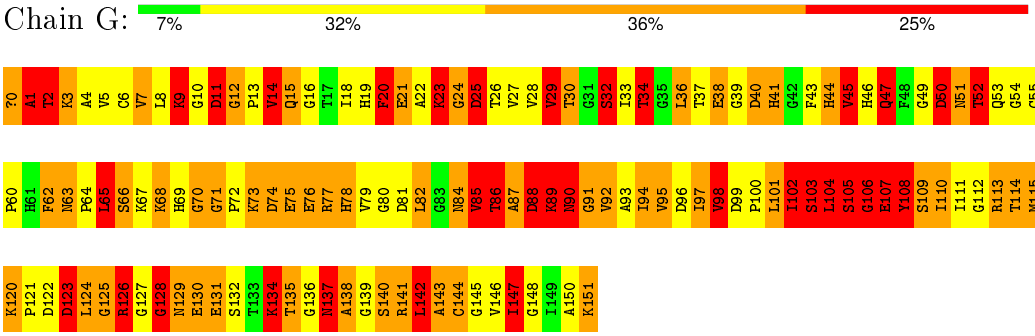
- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain B:



• Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain G:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.65Å 90.33Å 71.65Å 90.00° 95.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.256 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4392	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU, ACE

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	B	1.68	14/1111 (1.3%)	3.38	145/1501 (9.7%)
1	G	1.88	18/1111 (1.6%)	3.59	189/1501 (12.6%)
1	O	1.70	9/1111 (0.8%)	3.34	152/1501 (10.1%)
1	Y	1.88	25/1111 (2.3%)	3.81	179/1501 (11.9%)
All	All	1.79	66/4444 (1.5%)	3.54	665/6004 (11.1%)

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	G	0	2
1	Y	0	2
All	All	0	4

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	139	GLY	N-CA	-11.00	1.29	1.46
1	G	140	SER	CB-OG	10.52	1.55	1.42
1	G	88	ASP	CA-CB	10.23	1.76	1.53
1	G	127	GLY	N-CA	9.80	1.60	1.46
1	O	89	LYS	CA-CB	9.04	1.73	1.53
1	G	144	CYS	CB-SG	-8.93	1.67	1.82
1	G	119	GLU	CG-CD	-8.09	1.39	1.51
1	G	141	ARG	N-CA	-7.79	1.30	1.46
1	Y	54	GLY	N-CA	-7.74	1.34	1.46
1	B	136	GLY	N-CA	7.72	1.57	1.46
1	B	76	GLU	CD-OE1	-7.63	1.17	1.25
1	G	128	GLY	N-CA	-7.35	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	88	ASP	CA-CB	7.24	1.69	1.53
1	Y	60	PRO	C-O	7.18	1.37	1.23
1	Y	39	GLY	N-CA	-7.16	1.35	1.46
1	O	76	GLU	CD-OE1	-7.08	1.17	1.25
1	Y	25	ASP	CB-CG	6.93	1.66	1.51
1	Y	118	HIS	CA-CB	6.87	1.69	1.53
1	G	144	CYS	CA-CB	-6.83	1.39	1.53
1	Y	139	GLY	CA-C	-6.77	1.41	1.51
1	G	66	SER	CB-OG	6.75	1.51	1.42
1	B	95	VAL	N-CA	-6.66	1.33	1.46
1	O	127	GLY	C-O	6.65	1.34	1.23
1	O	94	ILE	N-CA	-6.65	1.33	1.46
1	G	108	TYR	N-CA	6.64	1.59	1.46
1	B	57	SER	C-O	6.63	1.35	1.23
1	Y	24	GLY	N-CA	6.61	1.55	1.46
1	O	151	LYS	N-CA	6.51	1.59	1.46
1	O	127	GLY	N-CA	-6.43	1.36	1.46
1	G	85	VAL	C-O	6.40	1.35	1.23
1	Y	119	GLU	CD-OE1	-6.33	1.18	1.25
1	O	21	GLU	CD-OE2	6.30	1.32	1.25
1	B	139	GLY	N-CA	-6.21	1.36	1.46
1	G	141	ARG	CA-CB	6.19	1.67	1.53
1	B	113	ARG	CD-NE	-6.12	1.36	1.46
1	G	126	ARG	C-O	6.08	1.34	1.23
1	Y	123	ASP	N-CA	6.05	1.58	1.46
1	B	140	SER	CA-CB	-6.04	1.43	1.52
1	G	88	ASP	N-CA	-6.01	1.34	1.46
1	B	95	VAL	CA-CB	5.88	1.67	1.54
1	Y	49	GLY	N-CA	-5.88	1.37	1.46
1	Y	38	GLU	C-N	-5.81	1.22	1.33
1	Y	107	GLU	CD-OE2	5.80	1.32	1.25
1	Y	48	PHE	CB-CG	-5.74	1.41	1.51
1	B	139	GLY	CA-C	-5.71	1.42	1.51
1	Y	133	THR	CA-CB	5.65	1.68	1.53
1	G	12	GLY	N-CA	5.53	1.54	1.46
1	Y	89	LYS	N-CA	-5.45	1.35	1.46
1	O	104	LEU	N-CA	5.43	1.57	1.46
1	Y	131	GLU	CB-CG	-5.42	1.41	1.52
1	B	76	GLU	CD-OE2	5.40	1.31	1.25
1	B	138	ALA	CA-CB	5.30	1.63	1.52
1	Y	126	ARG	C-N	-5.29	1.23	1.33
1	O	136	GLY	N-CA	5.28	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	131	GLU	CG-CD	-5.26	1.44	1.51
1	G	91	GLY	N-CA	-5.23	1.38	1.46
1	G	41	HIS	CA-CB	5.23	1.65	1.53
1	B	49	GLY	N-CA	-5.20	1.38	1.46
1	G	32	SER	CB-OG	5.15	1.49	1.42
1	B	77	ARG	CD-NE	-5.15	1.37	1.46
1	Y	56	THR	CB-OG1	5.07	1.53	1.43
1	Y	52	THR	CB-OG1	5.07	1.53	1.43
1	B	142	LEU	CA-CB	5.06	1.65	1.53
1	Y	83	GLY	N-CA	-5.04	1.38	1.46
1	Y	57	SER	CA-CB	5.03	1.60	1.52
1	Y	103	SER	CB-OG	5.02	1.48	1.42

All (665) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	141	ARG	NE-CZ-NH1	40.80	140.70	120.30
1	B	77	ARG	CD-NE-CZ	36.32	174.45	123.60
1	B	113	ARG	NE-CZ-NH1	34.65	137.62	120.30
1	O	113	ARG	NE-CZ-NH1	29.42	135.01	120.30
1	Y	96	ASP	CA-CB-CG	29.36	178.00	113.40
1	G	77	ARG	NE-CZ-NH2	25.11	132.85	120.30
1	G	85	VAL	CA-C-N	23.41	168.71	117.20
1	O	89	LYS	C-N-CA	23.17	179.62	121.70
1	B	113	ARG	CD-NE-CZ	21.38	153.54	123.60
1	Y	25	ASP	CB-CA-C	20.23	150.86	110.40
1	G	126	ARG	NE-CZ-NH1	19.97	130.28	120.30
1	Y	38	GLU	C-N-CA	19.80	163.88	122.30
1	Y	139	GLY	N-CA-C	19.66	162.25	113.10
1	O	89	LYS	N-CA-C	19.46	163.54	111.00
1	Y	77	ARG	NE-CZ-NH1	19.29	129.94	120.30
1	G	102	ILE	C-N-CA	18.50	167.96	121.70
1	B	40	ASP	CB-CG-OD2	-18.21	101.91	118.30
1	Y	88	ASP	C-N-CA	18.16	167.09	121.70
1	B	50	ASP	C-N-CA	17.79	166.18	121.70
1	Y	126	ARG	NE-CZ-NH2	-17.16	111.72	120.30
1	Y	141	ARG	CD-NE-CZ	16.93	147.30	123.60
1	G	87	ALA	C-N-CA	16.80	163.71	121.70
1	G	89	LYS	N-CA-CB	16.63	140.53	110.60
1	G	108	TYR	CB-CA-C	16.62	143.65	110.40
1	O	93	ALA	C-N-CA	16.39	162.67	121.70
1	G	119	GLU	CB-CG-CD	15.88	157.06	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	89	LYS	CA-C-O	15.79	153.25	120.10
1	O	81	ASP	CB-CG-OD1	-14.43	105.31	118.30
1	B	99	ASP	CB-CG-OD2	-14.32	105.42	118.30
1	O	99	ASP	CB-CG-OD1	-14.25	105.47	118.30
1	G	85	VAL	O-C-N	-14.24	99.92	122.70
1	O	113	ARG	NH1-CZ-NH2	-14.12	103.87	119.40
1	G	85	VAL	CA-C-O	-13.98	90.73	120.10
1	G	75	GLU	OE1-CD-OE2	13.88	139.96	123.30
1	O	134	LYS	C-N-CA	13.81	156.22	121.70
1	Y	141	ARG	NE-CZ-NH2	-13.74	113.43	120.30
1	Y	143	ALA	N-CA-CB	13.72	129.30	110.10
1	Y	25	ASP	CB-CG-OD1	-13.28	106.35	118.30
1	O	23	LYS	N-CA-CB	13.26	134.47	110.60
1	B	77	ARG	CG-CD-NE	13.23	139.59	111.80
1	Y	60	PRO	CA-C-N	12.99	145.78	117.20
1	B	126	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	G	123	ASP	CA-CB-CG	12.59	141.09	113.40
1	Y	113	ARG	CD-NE-CZ	-12.55	106.03	123.60
1	G	119	GLU	OE1-CD-OE2	-12.54	108.25	123.30
1	Y	123	ASP	CB-CA-C	12.52	135.44	110.40
1	Y	60	PRO	O-C-N	-12.43	102.81	122.70
1	B	113	ARG	NE-CZ-NH2	-12.43	114.09	120.30
1	Y	25	ASP	CA-CB-CG	-12.37	86.19	113.40
1	Y	141	ARG	NH1-CZ-NH2	-12.30	105.86	119.40
1	Y	126	ARG	CD-NE-CZ	12.28	140.79	123.60
1	B	139	GLY	N-CA-C	12.28	143.79	113.10
1	Y	113	ARG	NE-CZ-NH1	-12.27	114.16	120.30
1	O	131	GLU	OE1-CD-OE2	12.27	138.02	123.30
1	O	96	ASP	CB-CG-OD1	12.13	129.22	118.30
1	B	17	THR	N-CA-CB	11.99	133.08	110.30
1	O	102	ILE	CB-CG1-CD1	11.96	147.39	113.90
1	G	130	GLU	CA-CB-CG	11.79	139.35	113.40
1	O	77	ARG	NE-CZ-NH1	-11.73	114.43	120.30
1	Y	131	GLU	CB-CG-CD	11.72	145.86	114.20
1	Y	149	ILE	C-N-CA	11.63	150.78	121.70
1	O	89	LYS	O-C-N	-11.55	104.22	122.70
1	Y	75	GLU	CA-CB-CG	11.52	138.74	113.40
1	Y	74	ASP	CB-CG-OD2	-11.52	107.94	118.30
1	Y	24	GLY	O-C-N	11.48	141.07	122.70
1	G	106	GLY	C-N-CA	11.47	150.37	121.70
1	G	57	SER	C-N-CA	11.45	150.33	121.70
1	G	144	CYS	CA-CB-SG	11.43	134.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	126	ARG	C-N-CA	11.28	145.99	122.30
1	Y	87	ALA	CB-CA-C	11.22	126.93	110.10
1	O	127	GLY	N-CA-C	11.21	141.13	113.10
1	O	108	TYR	CB-CG-CD1	11.20	127.72	121.00
1	G	0	ACE	O-C-N	-11.07	104.99	122.70
1	O	73	LYS	CB-CG-CD	11.06	140.36	111.60
1	O	131	GLU	CB-CA-C	-11.01	88.39	110.40
1	G	141	ARG	NE-CZ-NH2	10.95	125.77	120.30
1	G	81	ASP	CB-CG-OD2	10.89	128.11	118.30
1	G	113	ARG	NE-CZ-NH1	-10.80	114.90	120.30
1	O	78	HIS	N-CA-CB	-10.78	91.20	110.60
1	G	86	THR	C-N-CA	10.68	148.40	121.70
1	O	74	ASP	CB-CG-OD2	10.66	127.89	118.30
1	B	123	ASP	CB-CG-OD1	10.65	127.88	118.30
1	Y	89	LYS	N-CA-CB	10.62	129.71	110.60
1	Y	88	ASP	N-CA-C	10.54	139.46	111.00
1	Y	127	GLY	N-CA-C	-10.54	86.76	113.10
1	Y	50	ASP	C-N-CA	10.37	147.63	121.70
1	Y	51	ASN	N-CA-CB	10.33	129.19	110.60
1	Y	25	ASP	CB-CG-OD2	10.29	127.56	118.30
1	O	113	ARG	CD-NE-CZ	10.20	137.89	123.60
1	B	113	ARG	NH1-CZ-NH2	-10.13	108.26	119.40
1	G	77	ARG	NH1-CZ-NH2	-10.12	108.27	119.40
1	Y	87	ALA	C-N-CA	10.11	146.98	121.70
1	G	66	SER	CB-CA-C	10.10	129.29	110.10
1	B	40	ASP	CB-CG-OD1	10.09	127.38	118.30
1	O	89	LYS	N-CA-CB	-10.04	92.52	110.60
1	Y	131	GLU	CB-CA-C	-10.01	90.39	110.40
1	G	108	TYR	CA-C-O	9.94	140.97	120.10
1	O	128	GLY	C-N-CA	9.92	146.51	121.70
1	O	125	GLY	C-N-CA	9.90	146.46	121.70
1	G	74	ASP	CB-CG-OD2	-9.81	109.47	118.30
1	Y	40	ASP	CB-CG-OD2	-9.80	109.48	118.30
1	Y	126	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	O	123	ASP	CA-CB-CG	9.76	134.87	113.40
1	Y	108	TYR	CA-CB-CG	9.73	131.89	113.40
1	G	141	ARG	CD-NE-CZ	9.71	137.20	123.60
1	O	25	ASP	CB-CG-OD2	9.71	127.04	118.30
1	Y	88	ASP	N-CA-CB	-9.70	93.13	110.60
1	G	7	VAL	CB-CA-C	9.61	129.66	111.40
1	B	130	GLU	OE1-CD-OE2	9.60	134.82	123.30
1	B	122	ASP	CB-CG-OD1	9.55	126.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	88	ASP	N-CA-CB	9.55	127.79	110.60
1	G	144	CYS	N-CA-CB	9.55	127.78	110.60
1	G	108	TYR	C-N-CA	9.50	145.46	121.70
1	B	144	CYS	CB-CA-C	-9.41	91.57	110.40
1	B	77	ARG	NE-CZ-NH2	9.41	125.01	120.30
1	Y	36	LEU	N-CA-C	9.40	136.39	111.00
1	B	94	ILE	C-N-CA	9.40	145.21	121.70
1	G	141	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	Y	47	GLN	CA-CB-CG	9.37	134.01	113.40
1	Y	33	ILE	N-CA-CB	9.37	132.34	110.80
1	G	141	ARG	NH1-CZ-NH2	-9.34	109.13	119.40
1	Y	106	GLY	O-C-N	9.33	137.62	122.70
1	G	109	SER	O-C-N	9.32	137.61	122.70
1	Y	110	ILE	CB-CG1-CD1	9.31	139.97	113.90
1	B	107	GLU	OE1-CD-OE2	9.29	134.44	123.30
1	O	123	ASP	CB-CG-OD1	9.24	126.62	118.30
1	G	130	GLU	C-N-CA	9.21	144.72	121.70
1	G	140	SER	CA-C-O	9.20	139.43	120.10
1	Y	51	ASN	O-C-N	9.18	137.39	122.70
1	G	88	ASP	N-CA-C	9.15	135.72	111.00
1	Y	48	PHE	C-N-CA	9.15	141.51	122.30
1	Y	55	CYS	CA-CB-SG	9.14	130.45	114.00
1	Y	104	LEU	C-N-CA	9.11	144.47	121.70
1	G	77	ARG	CD-NE-CZ	-9.10	110.86	123.60
1	O	85	VAL	CB-CA-C	9.08	128.65	111.40
1	G	41	HIS	CA-CB-CG	-9.06	98.20	113.60
1	G	2	THR	CA-CB-CG2	9.05	125.08	112.40
1	G	140	SER	C-N-CA	9.06	144.34	121.70
1	Y	61	HIS	N-CA-CB	8.93	126.67	110.60
1	G	66	SER	N-CA-CB	-8.93	97.11	110.50
1	G	51	ASN	N-CA-CB	8.88	126.58	110.60
1	B	23	LYS	N-CA-CB	8.84	126.51	110.60
1	G	25	ASP	CB-CG-OD1	8.83	126.25	118.30
1	B	22	ALA	CB-CA-C	8.80	123.29	110.10
1	Y	88	ASP	CA-CB-CG	-8.79	94.06	113.40
1	G	123	ASP	CB-CG-OD1	8.75	126.18	118.30
1	Y	106	GLY	CA-C-O	-8.74	104.87	120.60
1	B	126	ARG	NH1-CZ-NH2	-8.73	109.79	119.40
1	G	11	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	Y	113	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	G	76	GLU	N-CA-CB	8.69	126.24	110.60
1	Y	53	GLN	C-N-CA	8.66	140.50	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	129	ASN	CB-CA-C	8.61	127.62	110.40
1	B	57	SER	N-CA-CB	-8.60	97.61	110.50
1	Y	25	ASP	CA-C-O	8.56	138.08	120.10
1	G	74	ASP	CB-CG-OD1	8.54	125.99	118.30
1	Y	40	ASP	O-C-N	8.53	136.35	122.70
1	Y	134	LYS	CB-CA-C	-8.48	93.44	110.40
1	O	77	ARG	NH1-CZ-NH2	8.47	128.72	119.40
1	B	65	LEU	CB-CA-C	8.46	126.28	110.20
1	G	85	VAL	CB-CA-C	8.40	127.36	111.40
1	Y	133	THR	N-CA-CB	-8.35	94.44	110.30
1	Y	50	ASP	CB-CG-OD1	8.29	125.76	118.30
1	Y	77	ARG	NH1-CZ-NH2	-8.26	110.31	119.40
1	O	126	ARG	NE-CZ-NH1	-8.25	116.17	120.30
1	B	94	ILE	CA-CB-CG1	-8.25	95.32	111.00
1	B	76	GLU	OE1-CD-OE2	8.23	133.17	123.30
1	G	130	GLU	CA-C-N	8.21	135.27	117.20
1	Y	48	PHE	CA-CB-CG	8.21	133.60	113.90
1	Y	138	ALA	C-N-CA	8.21	139.53	122.30
1	O	36	LEU	CA-CB-CG	8.20	134.17	115.30
1	Y	60	PRO	N-CA-C	8.20	133.43	112.10
1	O	32	SER	N-CA-CB	8.17	122.76	110.50
1	G	62	PHE	CB-CA-C	8.17	126.73	110.40
1	Y	22	ALA	CB-CA-C	8.16	122.34	110.10
1	Y	41	HIS	CA-CB-CG	-8.14	99.76	113.60
1	O	44	HIS	CB-CA-C	-8.13	94.14	110.40
1	B	77	ARG	CB-CG-CD	8.13	132.75	111.60
1	G	105	SER	CB-CA-C	8.13	125.54	110.10
1	Y	48	PHE	CA-C-O	8.12	137.15	120.10
1	B	107	GLU	CG-CD-OE2	-8.09	102.12	118.30
1	Y	74	ASP	N-CA-C	8.09	132.83	111.00
1	Y	98	VAL	CB-CA-C	8.04	126.68	111.40
1	Y	25	ASP	CA-C-N	-8.04	99.51	117.20
1	Y	96	ASP	CB-CG-OD2	8.03	125.53	118.30
1	G	62	PHE	CB-CG-CD1	-8.03	115.18	120.80
1	G	105	SER	N-CA-CB	-8.03	98.46	110.50
1	B	89	LYS	CB-CA-C	8.01	126.42	110.40
1	G	88	ASP	CB-CG-OD2	7.99	125.50	118.30
1	Y	17	THR	CA-CB-CG2	7.99	123.58	112.40
1	O	19	HIS	N-CA-CB	7.97	124.95	110.60
1	Y	127	GLY	CA-C-O	-7.95	106.29	120.60
1	O	122	ASP	CB-CG-OD1	7.91	125.42	118.30
1	O	24	GLY	N-CA-C	7.90	132.86	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	105	SER	N-CA-CB	7.90	122.35	110.50
1	O	89	LYS	CB-CA-C	-7.90	94.60	110.40
1	O	15	GLN	CB-CG-CD	7.89	132.12	111.60
1	B	90	ASN	N-CA-CB	7.89	124.80	110.60
1	B	131	GLU	CG-CD-OE1	7.86	134.02	118.30
1	B	126	ARG	CB-CA-C	7.84	126.08	110.40
1	G	125	GLY	C-N-CA	7.83	141.28	121.70
1	O	110	ILE	N-CA-CB	-7.82	92.81	110.80
1	B	73	LYS	CA-CB-CG	-7.82	96.19	113.40
1	O	105	SER	N-CA-CB	-7.82	98.77	110.50
1	O	25	ASP	CA-CB-CG	7.82	130.60	113.40
1	G	96	ASP	N-CA-CB	-7.80	96.56	110.60
1	G	123	ASP	OD1-CG-OD2	-7.80	108.48	123.30
1	O	45	VAL	CB-CA-C	7.79	126.21	111.40
1	G	50	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	Y	116	VAL	CG1-CB-CG2	-7.78	98.45	110.90
1	B	38	GLU	N-CA-CB	-7.77	96.62	110.60
1	G	23	LYS	N-CA-CB	7.77	124.58	110.60
1	O	96	ASP	CB-CA-C	7.76	125.93	110.40
1	Y	56	THR	CA-CB-CG2	7.74	123.24	112.40
1	G	119	GLU	CG-CD-OE1	7.74	133.78	118.30
1	G	88	ASP	N-CA-CB	-7.74	96.67	110.60
1	G	123	ASP	CB-CG-OD2	7.73	125.26	118.30
1	G	88	ASP	CB-CA-C	-7.73	94.94	110.40
1	B	57	SER	CA-C-N	7.73	134.20	117.20
1	G	126	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	O	7	VAL	CA-CB-CG2	7.68	122.42	110.90
1	O	124	LEU	CB-CA-C	7.67	124.78	110.20
1	Y	128	GLY	C-N-CA	7.67	140.87	121.70
1	O	94	ILE	C-N-CA	-7.66	102.54	121.70
1	G	1	ALA	N-CA-CB	7.66	120.82	110.10
1	B	124	LEU	CB-CA-C	7.64	124.72	110.20
1	G	86	THR	N-CA-CB	7.64	124.82	110.30
1	Y	36	LEU	CB-CG-CD1	-7.63	98.03	111.00
1	Y	34	THR	N-CA-CB	7.62	124.78	110.30
1	G	14	VAL	CA-C-N	-7.62	100.44	117.20
1	B	73	LYS	N-CA-C	7.62	131.57	111.00
1	O	25	ASP	OD1-CG-OD2	-7.61	108.84	123.30
1	G	140	SER	CA-C-N	-7.59	100.51	117.20
1	O	41	HIS	N-CA-CB	7.58	124.25	110.60
1	O	113	ARG	CB-CG-CD	7.58	131.30	111.60
1	O	81	ASP	CB-CA-C	7.56	125.52	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	89	LYS	N-CA-C	-7.56	90.59	111.00
1	O	25	ASP	CB-CA-C	7.55	125.51	110.40
1	G	131	GLU	OE1-CD-OE2	-7.54	114.25	123.30
1	G	52	THR	CB-CA-C	7.53	131.93	111.60
1	G	124	LEU	CB-CA-C	7.53	124.50	110.20
1	Y	87	ALA	CA-C-N	7.52	133.75	117.20
1	G	43	PHE	CA-CB-CG	7.52	131.95	113.90
1	O	29	VAL	CB-CA-C	7.50	125.65	111.40
1	G	45	VAL	CA-CB-CG1	7.50	122.15	110.90
1	G	14	VAL	CA-C-O	7.49	135.82	120.10
1	G	73	LYS	C-N-CA	7.47	140.38	121.70
1	O	150	ALA	C-N-CA	-7.47	103.02	121.70
1	B	40	ASP	CA-CB-CG	-7.46	96.99	113.40
1	G	127	GLY	C-N-CA	7.46	137.97	122.30
1	Y	122	ASP	CB-CG-OD1	-7.45	111.60	118.30
1	G	84	ASN	O-C-N	7.45	134.61	122.70
1	O	151	LYS	CB-CA-C	7.44	125.27	110.40
1	B	135	THR	CA-CB-OG1	-7.43	93.41	109.00
1	G	40	ASP	CA-CB-CG	-7.41	97.10	113.40
1	B	75	GLU	CB-CA-C	-7.40	95.60	110.40
1	Y	134	LYS	N-CA-C	7.39	130.95	111.00
1	B	38	GLU	CG-CD-OE2	-7.39	103.53	118.30
1	G	57	SER	CA-C-N	7.38	133.44	117.20
1	G	119	GLU	N-CA-CB	-7.38	97.33	110.60
1	G	143	ALA	CB-CA-C	7.35	121.13	110.10
1	O	135	THR	CA-CB-CG2	7.30	122.62	112.40
1	O	81	ASP	C-N-CA	7.29	139.93	121.70
1	Y	2	THR	N-CA-CB	7.29	124.15	110.30
1	Y	118	HIS	CB-CA-C	-7.29	95.83	110.40
1	Y	39	GLY	O-C-N	7.28	134.35	122.70
1	G	122	ASP	CB-CA-C	7.27	124.95	110.40
1	O	126	ARG	CB-CA-C	-7.27	95.86	110.40
1	O	23	LYS	CA-CB-CG	7.25	129.35	113.40
1	Y	3	LYS	O-C-N	7.25	134.29	122.70
1	Y	14	VAL	CB-CA-C	7.24	125.15	111.40
1	O	11	ASP	N-CA-CB	7.22	123.59	110.60
1	Y	123	ASP	C-N-CA	7.20	139.70	121.70
1	O	129	ASN	N-CA-CB	-7.19	97.65	110.60
1	G	107	GLU	N-CA-CB	7.19	123.55	110.60
1	O	123	ASP	CB-CA-C	-7.17	96.05	110.40
1	G	51	ASN	O-C-N	7.17	134.17	122.70
1	Y	24	GLY	N-CA-C	-7.15	95.23	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	111	ILE	CB-CA-C	7.15	125.90	111.60
1	O	36	LEU	N-CA-CB	-7.14	96.13	110.40
1	B	139	GLY	CA-C-O	-7.12	107.78	120.60
1	B	79	VAL	CA-CB-CG1	7.12	121.58	110.90
1	B	46	HIS	CA-CB-CG	-7.10	101.53	113.60
1	G	131	GLU	CB-CA-C	-7.10	96.20	110.40
1	B	38	GLU	CG-CD-OE1	7.10	132.49	118.30
1	O	119	GLU	CB-CG-CD	7.09	133.35	114.20
1	B	139	GLY	CA-C-N	7.09	132.80	117.20
1	Y	135	THR	N-CA-CB	-7.08	96.84	110.30
1	O	91	GLY	CA-C-N	-7.08	101.63	117.20
1	B	52	THR	CA-CB-OG1	-7.06	94.17	109.00
1	G	87	ALA	O-C-N	-7.04	111.43	122.70
1	B	50	ASP	CB-CG-OD1	7.04	124.63	118.30
1	G	70	GLY	O-C-N	7.03	135.15	123.20
1	G	128	GLY	C-N-CA	7.03	139.27	121.70
1	B	53	GLN	CA-CB-CG	-7.03	97.94	113.40
1	Y	141	ARG	CG-CD-NE	7.02	126.54	111.80
1	Y	135	THR	CA-CB-OG1	-7.00	94.31	109.00
1	B	24	GLY	CA-C-O	-6.99	108.01	120.60
1	O	91	GLY	N-CA-C	-6.99	95.62	113.10
1	Y	12	GLY	N-CA-C	-6.98	95.64	113.10
1	Y	134	LYS	C-N-CA	6.98	139.15	121.70
1	O	66	SER	CA-C-N	6.97	132.54	117.20
1	O	143	ALA	N-CA-CB	6.95	119.83	110.10
1	Y	126	ARG	CG-CD-NE	-6.95	97.21	111.80
1	O	29	VAL	CA-CB-CG1	6.95	121.32	110.90
1	G	62	PHE	CA-C-O	6.94	134.67	120.10
1	O	91	GLY	O-C-N	6.94	133.80	122.70
1	Y	74	ASP	CA-CB-CG	-6.93	98.14	113.40
1	O	77	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	Y	151	LYS	CA-C-O	-6.92	105.58	120.10
1	G	7	VAL	CA-CB-CG1	6.91	121.26	110.90
1	B	138	ALA	CA-C-O	6.90	134.59	120.10
1	O	141	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	Y	92	VAL	N-CA-C	6.89	129.62	111.00
1	B	135	THR	CA-CB-CG2	6.88	122.03	112.40
1	Y	63	ASN	CB-CG-OD1	-6.88	107.85	121.60
1	Y	11	ASP	C-N-CA	6.87	136.72	122.30
1	O	104	LEU	CA-CB-CG	6.86	131.08	115.30
1	Y	106	GLY	N-CA-C	-6.86	95.95	113.10
1	O	104	LEU	N-CA-C	-6.86	92.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	126	ARG	N-CA-CB	6.85	122.92	110.60
1	G	103	SER	N-CA-CB	6.80	120.70	110.50
1	B	115	MET	N-CA-CB	6.80	122.83	110.60
1	G	115	MET	CA-CB-CG	6.79	124.85	113.30
1	B	94	ILE	CB-CA-C	-6.78	98.03	111.60
1	Y	143	ALA	N-CA-C	-6.77	92.72	111.00
1	O	94	ILE	CB-CA-C	-6.76	98.07	111.60
1	O	112	GLY	N-CA-C	-6.76	96.19	113.10
1	G	0	ACE	C-N-CA	6.76	138.59	121.70
1	O	104	LEU	N-CA-CB	-6.73	96.94	110.40
1	B	126	ARG	CA-C-O	6.73	134.23	120.10
1	B	93	ALA	N-CA-CB	6.72	119.51	110.10
1	Y	29	VAL	CB-CA-C	6.72	124.17	111.40
1	B	135	THR	CA-C-O	-6.71	106.00	120.10
1	B	143	ALA	C-N-CA	6.70	138.46	121.70
1	O	89	LYS	CA-C-N	-6.70	102.46	117.20
1	Y	134	LYS	N-CA-CB	-6.69	98.56	110.60
1	Y	18	ILE	CB-CA-C	6.66	124.93	111.60
1	G	29	VAL	CB-CA-C	6.66	124.06	111.40
1	O	53	GLN	CG-CD-OE1	-6.64	108.31	121.60
1	B	81	ASP	CB-CG-OD1	6.64	124.28	118.30
1	G	130	GLU	CB-CA-C	-6.64	97.13	110.40
1	Y	21	GLU	O-C-N	6.63	133.31	122.70
1	Y	51	ASN	CB-CA-C	-6.63	97.13	110.40
1	Y	107	GLU	OE1-CD-OE2	-6.63	115.34	123.30
1	G	70	GLY	N-CA-C	-6.63	96.52	113.10
1	B	38	GLU	CA-CB-CG	-6.62	98.84	113.40
1	G	141	ARG	CG-CD-NE	6.61	125.67	111.80
1	O	50	ASP	CB-CG-OD1	6.60	124.24	118.30
1	O	108	TYR	N-CA-CB	6.60	122.48	110.60
1	G	107	GLU	C-N-CA	-6.60	105.20	121.70
1	B	136	GLY	N-CA-C	-6.58	96.66	113.10
1	O	68	LYS	CA-CB-CG	6.58	127.86	113.40
1	B	141	ARG	O-C-N	6.58	133.22	122.70
1	O	90	ASN	N-CA-CB	6.55	122.39	110.60
1	O	73	LYS	CD-CE-NZ	6.55	126.75	111.70
1	O	43	PHE	CB-CA-C	6.54	123.49	110.40
1	B	96	ASP	CA-C-O	-6.54	106.36	120.10
1	B	126	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	O	46	HIS	CA-CB-CG	-6.54	102.48	113.60
1	O	121	PRO	C-N-CA	6.54	138.04	121.70
1	G	140	SER	N-CA-CB	6.53	120.30	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	63	ASN	CB-CA-C	-6.53	97.35	110.40
1	Y	92	VAL	CA-C-O	6.53	133.81	120.10
1	B	43	PHE	CB-CG-CD1	-6.52	116.24	120.80
1	Y	123	ASP	CB-CG-OD1	6.51	124.16	118.30
1	G	91	GLY	N-CA-C	6.50	129.36	113.10
1	Y	25	ASP	N-CA-C	-6.46	93.54	111.00
1	Y	123	ASP	CA-C-O	6.45	133.65	120.10
1	B	142	LEU	CA-CB-CG	-6.45	100.47	115.30
1	B	74	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	Y	40	ASP	CA-C-N	-6.42	103.06	117.20
1	B	5	VAL	CA-CB-CG1	6.42	120.54	110.90
1	G	109	SER	N-CA-CB	6.42	120.14	110.50
1	O	76	GLU	CA-C-N	-6.42	103.07	117.20
1	Y	37	THR	C-N-CA	-6.42	105.65	121.70
1	O	36	LEU	CB-CA-C	6.41	122.38	110.20
1	O	128	GLY	O-C-N	-6.39	112.47	122.70
1	Y	15	GLN	CA-CB-CG	-6.38	99.37	113.40
1	B	89	LYS	CG-CD-CE	6.37	131.02	111.90
1	B	131	GLU	CB-CA-C	-6.37	97.66	110.40
1	Y	151	LYS	CA-CB-CG	6.36	127.40	113.40
1	B	134	LYS	C-N-CA	6.36	137.60	121.70
1	Y	27	VAL	CB-CA-C	6.36	123.48	111.40
1	G	47	GLN	CG-CD-NE2	-6.36	101.44	116.70
1	Y	135	THR	OG1-CB-CG2	6.36	124.62	110.00
1	O	63	ASN	N-CA-CB	-6.34	99.18	110.60
1	B	92	VAL	CA-CB-CG1	6.33	120.40	110.90
1	O	25	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	131	GLU	CG-CD-OE2	-6.33	105.65	118.30
1	B	50	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	96	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	G	102	ILE	CB-CA-C	-6.31	98.98	111.60
1	G	77	ARG	CG-CD-NE	6.31	125.04	111.80
1	G	143	ALA	N-CA-C	-6.30	93.98	111.00
1	B	108	TYR	CB-CG-CD2	6.29	124.77	121.00
1	B	95	VAL	N-CA-C	6.28	127.96	111.00
1	O	23	LYS	N-CA-C	-6.27	94.07	111.00
1	Y	52	THR	CA-CB-CG2	6.26	121.17	112.40
1	O	72	PRO	CA-C-O	6.26	135.22	120.20
1	O	131	GLU	CG-CD-OE2	-6.25	105.79	118.30
1	Y	132	SER	C-N-CA	6.25	137.33	121.70
1	O	135	THR	N-CA-CB	6.25	122.17	110.30
1	G	98	VAL	CB-CA-C	6.24	123.25	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	74	ASP	CB-CG-OD1	6.23	123.91	118.30
1	O	27	VAL	CB-CA-C	6.22	123.23	111.40
1	G	21	GLU	N-CA-CB	6.21	121.78	110.60
1	O	51	ASN	CB-CG-OD1	6.21	134.02	121.60
1	Y	52	THR	N-CA-C	-6.21	94.23	111.00
1	B	25	ASP	CB-CA-C	6.20	122.80	110.40
1	O	77	ARG	CD-NE-CZ	-6.20	114.93	123.60
1	Y	60	PRO	N-CA-CB	-6.20	95.78	102.60
1	G	147	ILE	CA-C-O	6.20	133.11	120.10
1	Y	73	LYS	C-N-CA	6.18	137.16	121.70
1	G	132	SER	C-N-CA	6.18	137.15	121.70
1	Y	48	PHE	N-CA-C	6.17	127.65	111.00
1	G	116	VAL	C-N-CA	6.16	137.11	121.70
1	G	47	GLN	N-CA-CB	-6.16	99.51	110.60
1	B	66	SER	N-CA-CB	6.16	119.74	110.50
1	B	120	LYS	CD-CE-NZ	6.16	125.87	111.70
1	G	118	HIS	C-N-CA	6.15	137.08	121.70
1	B	96	ASP	CB-CG-OD1	-6.14	112.78	118.30
1	Y	96	ASP	OD1-CG-OD2	-6.13	111.65	123.30
1	O	74	ASP	OD1-CG-OD2	-6.12	111.66	123.30
1	B	53	GLN	CG-CD-OE1	6.12	133.84	121.60
1	B	53	GLN	CG-CD-NE2	-6.11	102.04	116.70
1	B	47	GLN	CB-CG-CD	6.11	127.47	111.60
1	Y	144	CYS	O-C-N	6.10	133.57	123.20
1	O	137	ASN	CB-CA-C	6.10	122.59	110.40
1	G	101	LEU	C-N-CA	6.09	136.93	121.70
1	G	71	GLY	N-CA-C	6.09	128.32	113.10
1	G	10	GLY	N-CA-C	-6.08	97.91	113.10
1	Y	48	PHE	CA-C-N	-6.07	104.06	116.20
1	B	143	ALA	N-CA-C	-6.07	94.61	111.00
1	G	92	VAL	C-N-CA	6.07	136.87	121.70
1	Y	91	GLY	N-CA-C	6.07	128.27	113.10
1	B	86	THR	N-CA-CB	-6.06	98.79	110.30
1	Y	60	PRO	C-N-CA	6.05	136.82	121.70
1	O	3	LYS	CD-CE-NZ	-6.04	97.81	111.70
1	Y	67	LYS	N-CA-CB	6.04	121.46	110.60
1	B	140	SER	CA-CB-OG	6.03	127.47	111.20
1	B	138	ALA	CA-C-N	-6.02	104.16	116.20
1	G	115	MET	CB-CA-C	6.02	122.44	110.40
1	B	57	SER	CB-CA-C	6.01	121.51	110.10
1	O	132	SER	C-N-CA	6.00	136.71	121.70
1	B	50	ASP	CA-C-O	6.00	132.71	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	76	GLU	CA-C-N	-6.00	104.00	117.20
1	B	75	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	G	90	ASN	N-CA-C	-5.99	94.82	111.00
1	B	140	SER	N-CA-CB	5.99	119.48	110.50
1	O	134	LYS	CG-CD-CE	5.98	129.84	111.90
1	G	94	ILE	C-N-CA	5.98	136.65	121.70
1	O	122	ASP	C-N-CA	5.97	136.62	121.70
1	B	9	LYS	CB-CG-CD	5.97	127.12	111.60
1	Y	96	ASP	O-C-N	-5.97	113.15	122.70
1	G	126	ARG	C-N-CA	-5.97	109.77	122.30
1	B	143	ALA	N-CA-CB	5.96	118.45	110.10
1	B	104	LEU	CA-CB-CG	5.96	129.00	115.30
1	O	40	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	96	ASP	OD1-CG-OD2	5.95	134.60	123.30
1	Y	49	GLY	CA-C-O	-5.95	109.90	120.60
1	Y	143	ALA	CB-CA-C	5.95	119.02	110.10
1	G	126	ARG	N-CA-C	5.94	127.04	111.00
1	B	93	ALA	C-N-CA	5.93	136.53	121.70
1	G	38	GLU	CA-CB-CG	5.92	126.43	113.40
1	O	143	ALA	CB-CA-C	5.92	118.98	110.10
1	Y	99	ASP	CB-CG-OD2	5.91	123.62	118.30
1	O	126	ARG	CD-NE-CZ	-5.90	115.33	123.60
1	B	151	LYS	CA-CB-CG	-5.90	100.41	113.40
1	G	14	VAL	CA-CB-CG1	5.90	119.75	110.90
1	Y	116	VAL	CA-CB-CG2	5.90	119.75	110.90
1	Y	126	ARG	CB-CG-CD	-5.89	96.28	111.60
1	O	85	VAL	CA-CB-CG1	5.88	119.72	110.90
1	O	138	ALA	CB-CA-C	5.87	118.91	110.10
1	B	28	VAL	CB-CA-C	5.86	122.53	111.40
1	Y	88	ASP	O-C-N	-5.85	113.34	122.70
1	B	138	ALA	N-CA-CB	-5.85	101.91	110.10
1	G	126	ARG	NH1-CZ-NH2	-5.84	112.97	119.40
1	G	51	ASN	N-CA-C	-5.84	95.23	111.00
1	G	25	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	O	2	THR	CA-CB-CG2	5.82	120.55	112.40
1	Y	56	THR	C-N-CA	5.82	136.25	121.70
1	O	126	ARG	C-N-CA	5.82	134.51	122.30
1	Y	107	GLU	CG-CD-OE1	5.81	129.92	118.30
1	Y	122	ASP	C-N-CA	-5.81	107.18	121.70
1	G	50	ASP	OD1-CG-OD2	5.79	134.30	123.30
1	O	96	ASP	CA-CB-CG	5.79	126.14	113.40
1	O	127	GLY	CA-C-N	5.79	127.77	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	141	ARG	CD-NE-CZ	5.79	131.70	123.60
1	Y	81	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	G	57	SER	CA-C-O	-5.78	107.97	120.10
1	G	40	ASP	N-CA-C	5.77	126.59	111.00
1	Y	1	ALA	N-CA-C	5.77	126.58	111.00
1	Y	120	LYS	CB-CA-C	-5.77	98.86	110.40
1	O	94	ILE	N-CA-CB	5.76	124.06	110.80
1	B	11	ASP	N-CA-CB	5.76	120.96	110.60
1	B	40	ASP	N-CA-CB	-5.75	100.25	110.60
1	Y	129	ASN	CA-C-O	5.75	132.18	120.10
1	Y	63	ASN	OD1-CG-ND2	5.75	135.12	121.90
1	Y	122	ASP	OD1-CG-OD2	5.75	134.22	123.30
1	G	107	GLU	CB-CA-C	-5.74	98.93	110.40
1	B	48	PHE	CA-C-O	5.72	132.11	120.10
1	G	106	GLY	O-C-N	-5.71	113.56	122.70
1	O	38	GLU	CG-CD-OE1	5.71	129.71	118.30
1	Y	131	GLU	O-C-N	5.71	131.83	122.70
1	O	128	GLY	CA-C-O	5.70	130.87	120.60
1	O	151	LYS	N-CA-CB	-5.69	100.36	110.60
1	Y	96	ASP	N-CA-CB	-5.69	100.36	110.60
1	G	87	ALA	CA-C-N	5.68	129.70	117.20
1	Y	75	GLU	CB-CA-C	5.68	121.76	110.40
1	B	74	ASP	CA-CB-CG	-5.68	100.91	113.40
1	G	123	ASP	N-CA-CB	5.68	120.82	110.60
1	O	129	ASN	CA-CB-CG	-5.68	100.91	113.40
1	G	20	PHE	CB-CG-CD2	5.67	124.77	120.80
1	G	108	TYR	CA-C-N	-5.67	104.72	117.20
1	B	134	LYS	CD-CE-NZ	5.67	124.74	111.70
1	G	128	GLY	N-CA-C	5.66	127.25	113.10
1	G	137	ASN	C-N-CA	5.65	135.82	121.70
1	B	23	LYS	CB-CA-C	-5.64	99.11	110.40
1	G	34	THR	CA-C-N	-5.64	104.91	116.20
1	Y	113	ARG	CG-CD-NE	-5.64	99.95	111.80
1	G	50	ASP	CA-C-O	5.64	131.94	120.10
1	Y	4	ALA	CB-CA-C	5.63	118.55	110.10
1	G	135	THR	CA-CB-CG2	-5.63	104.52	112.40
1	G	116	VAL	CA-C-O	5.63	131.92	120.10
1	G	134	LYS	CB-CA-C	5.63	121.66	110.40
1	B	104	LEU	C-N-CA	5.63	135.76	121.70
1	B	51	ASN	CB-CG-ND2	5.62	130.20	116.70
1	Y	104	LEU	CA-CB-CG	5.62	128.23	115.30
1	G	20	PHE	CA-CB-CG	5.62	127.39	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	108	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	B	12	GLY	N-CA-C	-5.62	99.06	113.10
1	B	0	ACE	O-C-N	-5.61	113.72	122.70
1	B	98	VAL	O-C-N	5.61	131.67	122.70
1	G	96	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	O	44	HIS	N-CA-C	5.60	126.12	111.00
1	G	147	ILE	CA-C-N	-5.60	105.00	116.20
1	G	66	SER	CA-CB-OG	-5.59	96.11	111.20
1	G	129	ASN	N-CA-C	-5.59	95.91	111.00
1	O	40	ASP	CA-CB-CG	-5.58	101.12	113.40
1	B	55	CYS	CA-CB-SG	5.58	124.05	114.00
1	B	23	LYS	CA-C-N	-5.58	105.04	116.20
1	G	108	TYR	N-CA-CB	-5.58	100.56	110.60
1	O	44	HIS	N-CA-CB	-5.57	100.57	110.60
1	Y	88	ASP	CB-CA-C	-5.57	99.26	110.40
1	Y	62	PHE	CB-CA-C	5.56	121.53	110.40
1	O	19	HIS	O-C-N	5.56	131.60	122.70
1	O	65	LEU	N-CA-CB	-5.55	99.31	110.40
1	Y	3	LYS	N-CA-CB	5.54	120.57	110.60
1	Y	102	ILE	CB-CA-C	5.54	122.67	111.60
1	O	34	THR	CA-CB-OG1	-5.51	97.42	109.00
1	G	78	HIS	N-CA-CB	5.51	120.52	110.60
1	Y	132	SER	CA-C-N	-5.51	105.08	117.20
1	G	130	GLU	CA-C-O	-5.50	108.54	120.10
1	G	142	LEU	N-CA-CB	5.50	121.39	110.40
1	B	75	GLU	CA-C-N	-5.49	105.11	117.20
1	B	123	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	G	40	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	O	11	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	108	TYR	O-C-N	-5.46	113.96	122.70
1	O	108	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	O	81	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	108	TYR	C-N-CA	5.44	135.30	121.70
1	G	9	LYS	CA-CB-CG	5.44	125.36	113.40
1	O	94	ILE	CA-C-O	-5.42	108.72	120.10
1	B	32	SER	N-CA-CB	5.42	118.63	110.50
1	Y	118	HIS	CA-CB-CG	-5.42	104.39	113.60
1	B	102	ILE	CB-CA-C	5.41	122.42	111.60
1	Y	85	VAL	CA-CB-CG1	5.41	119.02	110.90
1	Y	37	THR	N-CA-CB	5.41	120.57	110.30
1	O	80	GLY	C-N-CA	-5.40	108.19	121.70
1	O	111	ILE	CB-CA-C	5.40	122.41	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	VAL	CA-CB-CG2	5.40	119.00	110.90
1	B	48	PHE	C-N-CA	5.40	133.63	122.30
1	Y	23	LYS	C-N-CA	-5.39	110.97	122.30
1	Y	143	ALA	O-C-N	5.39	131.33	122.70
1	G	38	GLU	CB-CG-CD	5.38	128.74	114.20
1	B	73	LYS	CB-CA-C	-5.38	99.64	110.40
1	B	95	VAL	N-CA-CB	-5.38	99.67	111.50
1	Y	38	GLU	CB-CG-CD	5.38	128.72	114.20
1	G	65	LEU	CA-CB-CG	-5.38	102.94	115.30
1	B	62	PHE	CB-CA-C	5.38	121.15	110.40
1	O	37	THR	N-CA-CB	-5.37	100.10	110.30
1	O	142	LEU	CB-CA-C	5.37	120.40	110.20
1	Y	128	GLY	CA-C-O	5.37	130.26	120.60
1	G	144	CYS	O-C-N	5.36	132.32	123.20
1	O	81	ASP	CA-C-N	-5.35	105.42	117.20
1	B	122	ASP	OD1-CG-OD2	-5.35	113.13	123.30
1	B	119	GLU	CG-CD-OE1	5.35	129.00	118.30
1	B	121	PRO	CB-CA-C	5.35	125.38	112.00
1	G	89	LYS	CA-C-N	-5.35	105.43	117.20
1	G	58	ALA	CB-CA-C	-5.34	102.09	110.10
1	Y	84	ASN	CA-CB-CG	5.34	125.14	113.40
1	B	141	ARG	N-CA-CB	5.33	120.20	110.60
1	Y	2	THR	CA-CB-CG2	5.31	119.83	112.40
1	Y	50	ASP	CB-CA-C	5.31	121.02	110.40
1	G	143	ALA	N-CA-CB	5.31	117.53	110.10
1	O	93	ALA	CA-C-N	-5.28	105.58	117.20
1	Y	30	THR	CB-CA-C	-5.28	97.34	111.60
1	O	45	VAL	CA-CB-CG1	5.28	118.82	110.90
1	G	22	ALA	N-CA-CB	5.27	117.48	110.10
1	G	75	GLU	CG-CD-OE2	-5.27	107.76	118.30
1	G	44	HIS	CA-C-O	5.26	131.15	120.10
1	G	108	TYR	O-C-N	-5.26	114.28	122.70
1	O	66	SER	CA-C-O	-5.25	109.06	120.10
1	Y	35	GLY	C-N-CA	5.25	134.82	121.70
1	Y	24	GLY	CA-C-O	-5.24	111.16	120.60
1	O	104	LEU	CB-CA-C	5.24	120.15	110.20
1	Y	123	ASP	N-CA-CB	-5.24	101.17	110.60
1	G	95	VAL	O-C-N	5.24	131.08	122.70
1	O	34	THR	O-C-N	5.23	132.10	123.20
1	B	57	SER	CA-CB-OG	-5.23	97.08	111.20
1	B	95	VAL	CB-CA-C	-5.23	101.47	111.40
1	G	76	GLU	O-C-N	5.22	131.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	5	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	G	63	ASN	N-CA-CB	-5.21	101.22	110.60
1	Y	78	HIS	CB-CA-C	-5.20	100.00	110.40
1	G	84	ASN	CB-CG-OD1	-5.19	111.21	121.60
1	G	126	ARG	CB-CA-C	-5.19	100.01	110.40
1	B	96	ASP	CA-C-N	5.19	128.62	117.20
1	O	76	GLU	CA-C-O	5.19	131.00	120.10
1	G	24	GLY	CA-C-N	5.19	128.61	117.20
1	G	142	LEU	C-N-CA	-5.19	108.73	121.70
1	G	21	GLU	CA-CB-CG	5.18	124.80	113.40
1	G	130	GLU	OE1-CD-OE2	5.18	129.51	123.30
1	B	101	LEU	CB-CA-C	5.16	120.01	110.20
1	G	90	ASN	O-C-N	5.15	131.96	123.20
1	O	111	ILE	O-C-N	5.15	131.96	123.20
1	Y	105	SER	CB-CA-C	-5.15	100.32	110.10
1	O	67	LYS	CB-CA-C	-5.14	100.12	110.40
1	B	58	ALA	N-CA-CB	5.14	117.30	110.10
1	Y	51	ASN	CA-C-N	-5.14	105.90	117.20
1	G	132	SER	N-CA-CB	-5.14	102.79	110.50
1	O	112	GLY	O-C-N	5.13	130.91	122.70
1	O	140	SER	O-C-N	-5.13	114.49	122.70
1	O	95	VAL	CA-CB-CG2	5.13	118.59	110.90
1	Y	98	VAL	CA-CB-CG2	5.12	118.59	110.90
1	Y	79	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	G	131	GLU	CA-C-N	-5.12	105.94	117.20
1	Y	6	CYS	CB-CA-C	5.11	120.63	110.40
1	B	56	THR	CA-CB-CG2	-5.11	105.25	112.40
1	G	128	GLY	CA-C-O	5.10	129.78	120.60
1	G	20	PHE	CB-CG-CD1	-5.09	117.24	120.80
1	O	34	THR	CA-C-N	-5.09	106.02	116.20
1	G	131	GLU	C-N-CA	5.08	134.41	121.70
1	Y	29	VAL	C-N-CA	5.08	134.40	121.70
1	G	81	ASP	C-N-CA	5.07	134.38	121.70
1	G	129	ASN	CA-C-O	-5.07	109.45	120.10
1	G	139	GLY	O-C-N	5.07	130.82	122.70
1	B	51	ASN	OD1-CG-ND2	-5.07	110.24	121.90
1	G	21	GLU	CG-CD-OE1	5.07	128.44	118.30
1	G	129	ASN	C-N-CA	5.07	134.36	121.70
1	O	68	LYS	N-CA-CB	5.06	119.71	110.60
1	G	3	LYS	N-CA-CB	-5.06	101.50	110.60
1	G	74	ASP	CA-C-O	-5.05	109.50	120.10
1	O	113	ARG	CB-CA-C	5.05	120.49	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	90	ASN	CA-CB-CG	-5.04	102.32	113.40
1	Y	78	HIS	O-C-N	5.03	130.75	122.70
1	B	13	PRO	N-CA-CB	-5.03	97.07	102.60
1	O	74	ASP	CA-CB-CG	5.03	124.46	113.40
1	Y	7	VAL	CA-CB-CG2	5.01	118.42	110.90
1	O	21	GLU	CG-CD-OE1	5.01	128.33	118.30
1	B	40	ASP	CB-CA-C	5.01	120.42	110.40
1	G	94	ILE	CB-CA-C	5.01	121.62	111.60
1	B	119	GLU	CB-CG-CD	5.00	127.71	114.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	126	ARG	Sidechain
1	G	85	VAL	Mainchain
1	Y	113	ARG	Sidechain
1	Y	60	PRO	Mainchain

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	B	1095	0	1062	162	26
1	G	1095	0	1053	242	7
1	O	1095	0	1061	208	22
1	Y	1095	0	1053	225	4
2	B	1	0	0	0	0
2	G	1	0	0	0	0
2	O	1	0	0	0	0
2	Y	1	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
3	O	1	0	0	0	0
3	Y	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	1	0	0	1	0
4	Y	1	0	0	0	0
All	All	4392	0	4229	820	30

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 95.

All (820) 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:G:88:ASP:CB	1:G:88:ASP:CA	1.76	1.60
1:B:119:GLU:HG2	1:B:142:LEU:CD2	1.48	1.43
1:G:65:LEU:HD13	1:G:66:SER:N	1.28	1.41
1:G:151:LYS:HA	1:G:151:LYS:CE	1.42	1.40
1:B:126:ARG:HB3	1:B:126:ARG:NH1	1.39	1.35
1:B:126:ARG:CB	1:B:126:ARG:HH11	1.39	1.33
1:O:74:ASP:OD1	1:O:125:GLY:HA3	1.30	1.29
1:Y:121:PRO:O	1:Y:138:ALA:HA	1.30	1.29
1:G:120:LYS:HB3	1:G:138:ALA:O	1.33	1.23
1:O:88:ASP:OD2	1:O:89:LYS:HG3	1.39	1.21
1:B:68:LYS:NZ	1:B:76:GLU:OE1	1.75	1.18
1:Y:109:SER:O	1:Y:113:ARG:NH2	1.75	1.18
1:B:151:LYS:HA	1:B:151:LYS:CE	1.69	1.14
1:Y:29:VAL:HG13	1:Y:97:ILE:HG12	1.30	1.14
1:B:94:ILE:HD12	1:B:94:ILE:N	1.41	1.14
1:Y:122:ASP:HA	1:Y:138:ALA:HB2	1.15	1.11
1:G:27:VAL:HG23	1:G:102:ILE:HG21	1.21	1.11
1:O:1:ALA:HA	1:O:104:LEU:HD21	1.13	1.11
1:O:150:ALA:O	1:O:151:LYS:HB2	1.35	1.10
1:G:151:LYS:HE3	1:G:151:LYS:HA	1.34	1.10
1:B:119:GLU:HG2	1:B:142:LEU:HD23	1.27	1.09
1:O:78:HIS:HE2	1:O:134:LYS:HD2	1.08	1.09
1:O:82:LEU:HG	1:O:97:ILE:HD11	1.25	1.09
1:G:151:LYS:HA	1:G:151:LYS:HE2	1.20	1.09
1:G:51:ASN:O	1:G:53:GLN:N	1.85	1.09
1:Y:53:GLN:O	1:Y:53:GLN:HG3	1.43	1.08
1:O:123:ASP:OD2	1:O:132:SER:OG	1.70	1.08
1:B:135:THR:HG22	1:B:137:ASN:H	1.12	1.08
1:Y:23:LYS:CD	1:Y:28:VAL:HG21	1.84	1.07
1:Y:23:LYS:HD3	1:Y:28:VAL:HG21	1.23	1.07
1:B:94:ILE:CD1	1:B:94:ILE:N	2.12	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:104:LEU:HD22	1:O:104:LEU:O	1.52	1.07
1:B:123:ASP:OD1	1:B:137:ASN:HB2	1.55	1.07
1:G:65:LEU:CD1	1:G:66:SER:N	2.18	1.07
1:B:99:ASP:HB3	1:B:102:ILE:CD1	1.83	1.07
1:G:89:LYS:C	1:G:90:ASN:HD22	1.56	1.06
1:B:99:ASP:HB3	1:B:102:ILE:HD11	1.07	1.06
1:G:47:GLN:HG3	1:G:60:PRO:CD	1.86	1.06
1:Y:122:ASP:CA	1:Y:138:ALA:HB2	1.85	1.06
1:B:38:GLU:HB3	1:B:89:LYS:HG3	1.05	1.04
1:B:38:GLU:HB3	1:B:89:LYS:CG	1.87	1.04
1:G:27:VAL:HB	1:G:102:ILE:HG23	1.40	1.04
1:O:106:GLY:H	1:O:109:SER:HB2	1.19	1.03
1:G:27:VAL:CG2	1:G:102:ILE:CG2	2.36	1.03
1:O:105:SER:H	1:O:109:SER:HB2	1.23	1.03
1:Y:84:ASN:HD21	1:Y:122:ASP:N	1.57	1.02
1:G:47:GLN:HG3	1:G:60:PRO:HD2	1.06	1.02
1:G:151:LYS:CA	1:G:151:LYS:CE	2.38	1.02
1:G:117:VAL:CG1	1:G:143:ALA:HB3	1.90	1.02
1:Y:79:VAL:HG22	1:Y:101:LEU:HD12	1.40	1.01
1:B:119:GLU:HG2	1:B:142:LEU:CG	1.90	1.00
1:G:105:SER:O	1:G:109:SER:HB2	1.59	1.00
1:O:51:ASN:HB3	1:Y:7:VAL:HG11	1.41	1.00
1:O:125:GLY:O	1:O:126:ARG:HG2	1.62	1.00
1:O:120:LYS:HB2	1:O:138:ALA:O	1.61	0.99
1:G:64:PRO:HB3	1:G:108:TYR:CD2	1.99	0.98
1:G:23:LYS:O	1:G:26:THR:HG22	1.63	0.98
1:O:1:ALA:CA	1:O:104:LEU:HD21	1.94	0.97
1:G:77:ARG:NH2	1:G:99:ASP:OD2	1.96	0.97
1:O:1:ALA:HA	1:O:104:LEU:CD2	1.94	0.97
1:Y:118:HIS:HA	1:Y:140:SER:O	1.63	0.97
1:B:119:GLU:CG	1:B:142:LEU:CD2	2.41	0.97
1:G:123:ASP:HB2	1:G:136:GLY:O	1.65	0.97
1:O:46:HIS:CD2	1:O:116:VAL:CG1	2.47	0.97
1:Y:0:ACE:O	1:Y:1:ALA:HB2	1.64	0.96
1:B:99:ASP:CB	1:B:102:ILE:HD11	1.96	0.96
1:G:27:VAL:CG2	1:G:102:ILE:HG21	1.93	0.96
1:B:102:ILE:HD13	1:B:102:ILE:H	1.31	0.95
1:B:151:LYS:HA	1:B:151:LYS:HE2	1.45	0.95
1:G:27:VAL:HB	1:G:102:ILE:CG2	1.96	0.95
1:G:27:VAL:HG23	1:G:102:ILE:CG2	1.96	0.94
1:O:119:GLU:HG2	1:O:119:GLU:O	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:HA	1:B:151:LYS:HE3	1.50	0.94
1:Y:131:GLU:H	1:Y:133:THR:HG22	1.33	0.94
1:O:9:LYS:HD3	1:O:10:GLY:N	1.82	0.94
1:G:20:PHE:HD1	1:G:29:VAL:HB	1.33	0.93
1:O:62:PHE:HE2	1:O:113:ARG:NH1	1.66	0.93
1:O:150:ALA:O	1:O:151:LYS:CB	2.16	0.93
1:B:38:GLU:CB	1:B:89:LYS:HG3	1.96	0.93
1:B:119:GLU:CG	1:B:142:LEU:HD23	1.97	0.93
1:G:120:LYS:HG3	1:G:121:PRO:HD2	1.48	0.92
1:G:142:LEU:O	1:G:142:LEU:HD12	1.69	0.92
1:Y:65:LEU:N	1:Y:65:LEU:HD22	1.83	0.92
1:B:151:LYS:CA	1:B:151:LYS:HE3	2.00	0.92
1:Y:121:PRO:O	1:Y:138:ALA:CA	2.17	0.91
1:Y:119:GLU:O	1:Y:120:LYS:HG3	1.70	0.91
1:Y:84:ASN:ND2	1:Y:122:ASP:H	1.69	0.91
1:G:88:ASP:N	1:G:88:ASP:CB	2.33	0.91
1:O:115:MET:HG2	1:O:147:ILE:HD11	1.52	0.91
1:G:68:LYS:O	1:G:78:HIS:NE2	2.04	0.90
1:O:24:GLY:O	1:O:25:ASP:HB2	1.69	0.90
1:O:78:HIS:NE2	1:O:134:LYS:HD2	1.85	0.90
1:G:8:LEU:O	1:G:15:GLN:HB2	1.70	0.90
1:Y:84:ASN:HD21	1:Y:122:ASP:H	0.92	0.90
1:O:5:VAL:HG13	1:Y:50:ASP:CB	2.01	0.90
1:B:51:ASN:HA	1:B:54:GLY:O	1.72	0.90
1:G:151:LYS:HE2	1:G:151:LYS:CA	1.99	0.90
1:G:129:ASN:CG	1:G:129:ASN:O	2.10	0.90
1:B:135:THR:HG22	1:B:137:ASN:N	1.87	0.89
1:O:45:VAL:HG11	1:O:110:ILE:CD1	2.01	0.89
1:B:151:LYS:CA	1:B:151:LYS:CE	2.47	0.89
1:G:51:ASN:O	1:G:54:GLY:N	2.05	0.89
1:G:89:LYS:HE3	1:G:89:LYS:HA	1.55	0.89
1:G:12:GLY:H	1:G:142:LEU:HD13	1.38	0.89
1:G:1:ALA:HB3	1:G:105:SER:OG	1.72	0.89
1:O:78:HIS:HE1	1:O:134:LYS:NZ	1.70	0.89
1:Y:38:GLU:HG3	1:Y:39:GLY:HA3	1.55	0.88
1:O:88:ASP:OD2	1:O:89:LYS:CG	2.20	0.88
1:O:29:VAL:HG13	1:O:97:ILE:HG12	1.54	0.88
1:B:7:VAL:HG11	1:G:51:ASN:CB	2.03	0.88
1:Y:137:ASN:O	1:Y:139:GLY:N	2.06	0.88
1:Y:47:GLN:O	1:Y:113:ARG:HD3	1.74	0.88
1:G:27:VAL:CB	1:G:102:ILE:CG2	2.51	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:ASP:C	1:G:88:ASP:CB	2.42	0.87
1:Y:0:ACE:O	1:Y:1:ALA:CB	2.22	0.87
1:O:86:THR:O	1:O:93:ALA:HB3	1.75	0.87
1:G:47:GLN:CG	1:G:60:PRO:HD2	1.99	0.87
1:B:71:GLY:N	1:B:74:ASP:OD1	2.08	0.86
1:B:67:LYS:HD3	1:B:76:GLU:HA	1.57	0.86
1:Y:38:GLU:HG3	1:Y:39:GLY:CA	2.05	0.86
1:Y:18:ILE:HD11	1:Y:20:PHE:CZ	2.11	0.86
1:O:135:THR:HG23	1:O:136:GLY:H	1.41	0.86
1:G:64:PRO:HB3	1:G:108:TYR:CE2	2.11	0.85
1:O:82:LEU:HG	1:O:97:ILE:CD1	2.07	0.85
1:O:46:HIS:CE1	1:O:141:ARG:HH21	1.94	0.85
1:B:85:VAL:HG12	1:B:93:ALA:HB1	1.57	0.85
1:G:70:GLY:HA2	1:G:124:LEU:O	1.75	0.85
1:O:104:LEU:HA	1:O:109:SER:OG	1.76	0.84
1:B:119:GLU:HG2	1:B:142:LEU:HD21	1.56	0.84
1:O:5:VAL:CG1	1:Y:50:ASP:CB	2.55	0.84
1:Y:44:HIS:NE2	1:Y:122:ASP:OD1	2.10	0.83
1:O:131:GLU:O	1:O:135:THR:HG22	1.77	0.83
1:O:133:THR:O	1:O:134:LYS:HB2	1.79	0.83
1:Y:53:GLN:CG	1:Y:53:GLN:O	2.25	0.83
1:G:65:LEU:HD13	1:G:66:SER:H	0.98	0.82
1:O:62:PHE:CE2	1:O:113:ARG:NH1	2.47	0.82
1:G:3:LYS:HD3	1:G:151:LYS:HD2	1.61	0.82
1:G:119:GLU:OE2	1:G:142:LEU:HG	1.79	0.82
1:G:51:ASN:O	1:G:52:THR:C	2.17	0.82
1:Y:38:GLU:CG	1:Y:39:GLY:N	2.34	0.82
1:Y:23:LYS:HG2	1:Y:28:VAL:CG2	2.09	0.82
1:O:45:VAL:HG11	1:O:110:ILE:HD13	1.59	0.82
1:G:72:PRO:O	1:G:77:ARG:NH1	2.13	0.81
1:Y:119:GLU:HG2	1:Y:140:SER:HB3	1.62	0.81
1:B:70:GLY:HA2	1:B:124:LEU:O	1.80	0.81
1:G:6:CYS:HB2	1:G:147:ILE:HG22	1.61	0.81
1:B:68:LYS:N	1:B:68:LYS:HD3	1.94	0.81
1:Y:38:GLU:CG	1:Y:39:GLY:HA3	2.10	0.81
1:G:65:LEU:HD13	1:G:65:LEU:C	1.96	0.81
1:O:88:ASP:CG	1:O:89:LYS:H	1.85	0.81
1:G:90:ASN:HD22	1:G:90:ASN:N	1.72	0.80
1:B:38:GLU:O	1:B:89:LYS:HE3	1.79	0.80
1:O:103:SER:OG	1:O:104:LEU:N	2.13	0.80
1:O:5:VAL:CG1	1:Y:50:ASP:HB2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:131:GLU:N	1:Y:133:THR:HG22	1.97	0.80
1:B:3:LYS:HE3	1:B:21:GLU:HG3	1.63	0.79
1:G:14:VAL:HG22	1:G:143:ALA:HB2	1.64	0.79
1:G:20:PHE:CD1	1:G:29:VAL:HB	2.17	0.79
1:O:106:GLY:O	1:O:109:SER:N	2.15	0.79
1:Y:104:LEU:N	1:Y:104:LEU:HD22	1.98	0.79
1:Y:23:LYS:CG	1:Y:28:VAL:HG21	2.12	0.79
1:G:46:HIS:CD2	1:G:116:VAL:HG13	2.18	0.79
1:G:12:GLY:N	1:G:142:LEU:HD13	1.97	0.79
1:O:107:GLU:O	1:O:108:TYR:CD2	2.36	0.78
1:G:89:LYS:CE	1:G:89:LYS:HA	2.10	0.78
1:B:119:GLU:HG2	1:B:142:LEU:HG	1.65	0.78
1:Y:37:THR:HG22	1:Y:38:GLU:CG	2.12	0.78
1:O:65:LEU:O	1:O:67:LYS:N	2.16	0.78
1:G:117:VAL:HG13	1:G:143:ALA:HB3	1.65	0.78
1:G:27:VAL:CB	1:G:102:ILE:HG23	2.14	0.78
1:B:77:ARG:NH1	1:B:99:ASP:OD2	2.16	0.78
1:Y:29:VAL:CG1	1:Y:97:ILE:HG12	2.14	0.78
1:G:107:GLU:C	1:G:109:SER:H	1.88	0.77
1:B:90:ASN:O	1:B:92:VAL:N	2.16	0.77
1:O:104:LEU:CD2	1:O:104:LEU:O	2.32	0.77
1:B:7:VAL:HG11	1:G:51:ASN:HB2	1.66	0.77
1:Y:118:HIS:CA	1:Y:140:SER:O	2.32	0.77
1:O:5:VAL:CG1	1:Y:50:ASP:HB3	2.14	0.77
1:O:40:ASP:N	1:O:40:ASP:OD2	2.16	0.76
1:O:47:GLN:OE1	1:O:48:PHE:CZ	2.37	0.76
1:G:117:VAL:HG12	1:G:143:ALA:HB3	1.67	0.76
1:O:78:HIS:HE1	1:O:134:LYS:HZ2	1.32	0.76
1:Y:37:THR:HG22	1:Y:38:GLU:CD	2.05	0.76
1:G:113:ARG:O	1:G:147:ILE:HD13	1.85	0.76
1:G:72:PRO:HA	1:G:77:ARG:NH1	2.01	0.76
1:B:34:THR:HG22	1:B:92:VAL:HB	1.65	0.76
1:O:5:VAL:HG13	1:Y:50:ASP:HB3	1.66	0.76
1:G:53:GLN:HG2	1:G:56:THR:HB	1.68	0.75
1:B:130:GLU:OE1	1:B:130:GLU:N	2.14	0.75
1:O:119:GLU:O	1:O:120:LYS:HG3	1.86	0.75
1:Y:38:GLU:CG	1:Y:39:GLY:CA	2.63	0.75
1:Y:103:SER:HB2	1:Y:105:SER:HB2	1.68	0.75
1:G:67:LYS:HB3	1:G:76:GLU:HG3	1.68	0.75
1:B:151:LYS:N	1:B:151:LYS:HE3	2.01	0.75
1:Y:82:LEU:CD1	1:Y:97:ILE:HD11	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:PHE:HZ	1:G:108:TYR:CG	2.04	0.75
1:O:125:GLY:O	1:O:126:ARG:CG	2.33	0.74
1:O:105:SER:N	1:O:109:SER:HB2	2.02	0.74
1:Y:53:GLN:HE22	1:G:13:PRO:HB3	1.52	0.74
1:G:118:HIS:HA	1:G:140:SER:O	1.87	0.74
1:O:15:GLN:HG3	1:O:15:GLN:O	1.79	0.74
1:O:30:THR:HA	1:O:95:VAL:O	1.88	0.74
1:Y:137:ASN:O	1:Y:139:GLY:HA2	1.88	0.73
1:O:129:ASN:OD1	1:O:130:GLU:N	2.20	0.73
1:Y:82:LEU:HD12	1:Y:97:ILE:HD11	1.69	0.73
1:O:88:ASP:OD2	1:O:89:LYS:N	2.22	0.73
1:O:36:LEU:HG	1:O:41:HIS:CE1	2.24	0.73
1:Y:135:THR:HG22	1:Y:137:ASN:H	1.54	0.73
1:G:120:LYS:CB	1:G:138:ALA:O	2.26	0.73
1:G:63:ASN:CG	1:G:78:HIS:HD2	1.92	0.73
1:G:25:ASP:O	1:G:102:ILE:HD11	1.89	0.73
1:G:123:ASP:CB	1:G:136:GLY:O	2.37	0.73
1:Y:22:ALA:HB2	1:Y:104:LEU:CD2	2.19	0.73
1:G:88:ASP:CG	1:G:88:ASP:CA	2.56	0.72
1:O:5:VAL:HG13	1:Y:50:ASP:HB2	1.69	0.72
1:G:53:GLN:O	1:G:53:GLN:HG2	1.89	0.72
1:O:92:VAL:O	1:O:93:ALA:HB2	1.88	0.72
1:O:68:LYS:HD2	1:O:133:THR:CG2	2.20	0.72
1:G:85:VAL:O	1:G:86:THR:OG1	2.07	0.72
1:O:103:SER:OG	1:O:105:SER:HB3	1.89	0.72
1:O:123:ASP:OD2	1:O:132:SER:CB	2.36	0.72
1:O:106:GLY:N	1:O:109:SER:HB2	2.00	0.72
1:O:78:HIS:CE1	1:O:134:LYS:NZ	2.58	0.72
1:Y:40:ASP:HB3	1:Y:84:ASN:HB3	1.70	0.72
1:B:34:THR:HA	1:B:91:GLY:O	1.87	0.72
1:B:64:PRO:O	1:B:65:LEU:O	2.08	0.72
1:O:69:HIS:CG	1:O:135:THR:O	2.42	0.72
1:Y:131:GLU:H	1:Y:133:THR:CG2	2.03	0.71
1:O:64:PRO:HG3	1:O:108:TYR:CD1	2.25	0.71
1:G:103:SER:O	1:G:109:SER:HA	1.89	0.71
1:B:102:ILE:H	1:B:102:ILE:CD1	2.03	0.71
1:G:5:VAL:HG23	1:G:150:ALA:HB2	1.72	0.71
1:O:86:THR:O	1:O:93:ALA:CB	2.39	0.71
1:Y:104:LEU:HD13	1:Y:110:ILE:HD11	1.72	0.71
1:Y:139:GLY:O	1:Y:140:SER:HB3	1.89	0.71
1:B:49:GLY:O	1:B:50:ASP:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:HB3	1:B:126:ARG:HH11	0.57	0.71
1:O:46:HIS:CD2	1:O:116:VAL:HG11	2.24	0.71
1:Y:38:GLU:HG2	1:Y:39:GLY:N	2.04	0.71
1:G:103:SER:HB3	1:G:108:TYR:C	2.11	0.70
1:B:7:VAL:HG11	1:G:51:ASN:HB3	1.70	0.70
1:B:71:GLY:HA2	1:B:124:LEU:HD23	1.72	0.70
1:G:24:GLY:O	1:G:25:ASP:HB2	1.91	0.70
1:B:119:GLU:CB	1:B:142:LEU:HD23	2.21	0.70
1:Y:15:GLN:O	1:Y:15:GLN:HG3	1.90	0.70
1:Y:116:VAL:HG21	1:Y:141:ARG:HG2	1.73	0.70
1:Y:131:GLU:O	1:Y:135:THR:HB	1.91	0.70
1:G:89:LYS:C	1:G:90:ASN:ND2	2.39	0.70
1:G:89:LYS:HD3	1:G:90:ASN:H	1.55	0.70
1:Y:38:GLU:HG3	1:Y:39:GLY:N	2.07	0.70
1:B:43:PHE:HB2	1:B:85:VAL:HG23	1.74	0.70
1:O:93:ALA:HB1	1:O:94:ILE:CG1	2.22	0.69
1:O:46:HIS:CD2	1:O:116:VAL:HG12	2.26	0.69
1:Y:88:ASP:HB2	1:Y:89:LYS:C	2.12	0.69
1:G:5:VAL:HG13	1:G:19:HIS:CD2	2.28	0.69
1:B:30:THR:HA	1:B:95:VAL:O	1.93	0.69
1:Y:119:GLU:HG3	1:Y:120:LYS:HE2	1.74	0.69
1:Y:141:ARG:O	1:Y:142:LEU:HB2	1.92	0.69
1:B:67:LYS:NZ	1:B:75:GLU:O	2.21	0.69
1:Y:27:VAL:CG1	1:Y:102:ILE:HG13	2.21	0.69
1:B:5:VAL:HG13	1:B:150:ALA:HB2	1.75	0.69
1:G:89:LYS:O	1:G:90:ASN:HB2	1.91	0.69
1:G:105:SER:O	1:G:109:SER:CB	2.38	0.69
1:G:90:ASN:ND2	1:G:90:ASN:N	2.41	0.69
1:G:27:VAL:CG2	1:G:102:ILE:HG22	2.23	0.69
1:G:46:HIS:CD2	1:G:116:VAL:CG1	2.75	0.68
1:B:130:GLU:H	1:B:130:GLU:CD	1.96	0.68
1:G:64:PRO:CB	1:G:108:TYR:CD2	2.74	0.68
1:G:65:LEU:CD1	1:G:66:SER:H	1.92	0.68
1:Y:65:LEU:H	1:Y:65:LEU:HD22	1.55	0.68
1:G:63:ASN:CG	1:G:78:HIS:CD2	2.66	0.68
1:O:78:HIS:HE2	1:O:134:LYS:CD	1.97	0.68
1:B:48:PHE:O	1:B:114:THR:OG1	2.11	0.68
1:B:53:GLN:HG3	1:B:57:SER:OG	1.94	0.68
1:G:65:LEU:CD1	1:G:65:LEU:C	2.60	0.67
1:Y:1:ALA:HB1	1:Y:104:LEU:O	1.94	0.67
1:G:46:HIS:HD2	1:G:116:VAL:HG13	1.56	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:106:GLY:H	1:O:109:SER:CB	2.04	0.67
1:G:123:ASP:C	1:G:125:GLY:H	1.95	0.67
1:G:68:LYS:O	1:G:78:HIS:CE1	2.47	0.67
1:B:123:ASP:OD1	1:B:137:ASN:CB	2.38	0.67
1:G:1:ALA:CB	1:G:105:SER:OG	2.42	0.67
1:O:45:VAL:HG21	1:O:110:ILE:CD1	2.25	0.67
1:Y:131:GLU:HA	1:Y:134:LYS:HG3	1.77	0.67
1:O:62:PHE:HE1	1:O:79:VAL:HG11	1.60	0.67
1:Y:1:ALA:CB	1:Y:104:LEU:O	2.43	0.66
1:G:136:GLY:O	1:G:137:ASN:HB2	1.94	0.66
1:Y:27:VAL:HG13	1:Y:102:ILE:HG13	1.78	0.66
1:Y:65:LEU:N	1:Y:65:LEU:CD2	2.58	0.66
1:G:140:SER:OG	1:G:141:ARG:N	2.27	0.66
1:Y:111:ILE:HG21	1:Y:149:ILE:HG13	1.76	0.66
1:B:98:VAL:HG13	1:B:98:VAL:O	1.95	0.66
1:O:5:VAL:HG23	1:O:19:HIS:CD2	2.31	0.66
1:G:89:LYS:C	1:G:91:GLY:H	1.99	0.66
1:B:136:GLY:O	1:B:137:ASN:HB2	1.95	0.66
1:Y:52:THR:O	1:Y:53:GLN:HB3	1.94	0.66
1:B:73:LYS:N	1:B:73:LYS:HD2	2.12	0.65
1:O:93:ALA:HB1	1:O:94:ILE:HG12	1.78	0.65
1:G:25:ASP:O	1:G:102:ILE:CD1	2.44	0.65
1:B:49:GLY:HA3	1:B:112:GLY:O	1.95	0.65
1:O:88:ASP:CG	1:O:89:LYS:N	2.50	0.65
1:O:45:VAL:HG11	1:O:110:ILE:HD11	1.78	0.65
1:G:134:LYS:HD3	1:G:135:THR:HG23	1.78	0.65
1:Y:1:ALA:HB1	1:Y:104:LEU:C	2.17	0.65
1:B:82:LEU:HG	1:B:97:ILE:CD1	2.27	0.65
1:G:8:LEU:O	1:G:15:GLN:HA	1.97	0.65
1:Y:77:ARG:HH21	1:Y:101:LEU:CB	2.10	0.65
1:G:6:CYS:CB	1:G:147:ILE:HG22	2.27	0.65
1:O:111:ILE:HD11	1:O:149:ILE:HG12	1.79	0.64
1:O:9:LYS:HD3	1:O:9:LYS:C	2.16	0.64
1:G:85:VAL:O	1:G:86:THR:CB	2.44	0.64
1:B:131:GLU:HG3	1:B:131:GLU:O	1.96	0.64
1:G:110:ILE:HD13	1:G:147:ILE:HG13	1.78	0.64
1:Y:139:GLY:O	1:Y:140:SER:CB	2.45	0.64
1:B:82:LEU:HG	1:B:97:ILE:HD12	1.77	0.64
1:O:14:VAL:HG21	1:O:142:LEU:HG	1.79	0.64
1:B:110:ILE:HA	1:B:113:ARG:HD2	1.79	0.64
1:G:131:GLU:HG2	1:G:137:ASN:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:11:ASP:HB3	1:Y:142:LEU:HD11	1.80	0.64
1:O:0:ACE:H2	1:O:149:ILE:CD1	2.29	0.63
1:Y:36:LEU:HD13	1:Y:41:HIS:CD2	2.33	0.63
1:Y:103:SER:O	1:Y:110:ILE:HG12	1.98	0.63
1:G:47:GLN:O	1:G:113:ARG:NH1	2.30	0.63
1:B:103:SER:O	1:B:109:SER:HA	1.99	0.63
1:O:15:GLN:HG2	1:O:34:THR:OG1	1.98	0.63
1:O:76:GLU:HA	1:O:76:GLU:OE2	1.98	0.63
1:Y:92:VAL:HG23	1:Y:94:ILE:CD1	2.28	0.63
1:O:118:HIS:ND1	1:O:139:GLY:O	2.25	0.63
1:B:119:GLU:CG	1:B:142:LEU:HG	2.28	0.63
1:O:84:ASN:HD21	1:O:122:ASP:HB3	1.63	0.63
1:G:20:PHE:HA	1:G:28:VAL:O	1.97	0.63
1:Y:24:GLY:HA3	1:Y:26:THR:HG22	1.81	0.63
1:Y:10:GLY:HA3	1:Y:142:LEU:O	1.98	0.63
1:G:87:ALA:HA	1:G:92:VAL:O	1.98	0.63
1:Y:53:GLN:O	1:Y:56:THR:OG1	2.15	0.62
1:Y:23:LYS:CG	1:Y:28:VAL:CG2	2.74	0.62
1:G:129:ASN:ND2	1:G:129:ASN:O	2.32	0.62
1:Y:77:ARG:HH21	1:Y:101:LEU:HG	1.64	0.62
1:G:102:ILE:HB	1:G:103:SER:HA	1.82	0.62
1:G:110:ILE:O	1:G:147:ILE:CG1	2.47	0.62
1:B:85:VAL:HG13	1:B:95:VAL:HG22	1.81	0.62
1:Y:77:ARG:NH2	1:Y:101:LEU:HB2	2.15	0.62
1:G:8:LEU:O	1:G:15:GLN:CB	2.46	0.61
1:Y:37:THR:O	1:Y:38:GLU:HB3	2.00	0.61
1:G:126:ARG:C	1:G:128:GLY:H	2.00	0.61
1:G:67:LYS:HB3	1:G:76:GLU:CG	2.30	0.61
1:O:91:GLY:H	1:O:92:VAL:HG12	1.64	0.61
1:G:50:ASP:HB3	1:G:52:THR:OG1	2.00	0.61
1:O:6:CYS:SG	1:O:115:MET:HB2	2.40	0.61
1:O:111:ILE:HD11	1:O:149:ILE:CG1	2.31	0.61
1:G:53:GLN:HB3	1:G:57:SER:OG	2.01	0.61
1:Y:46:HIS:CD2	1:Y:116:VAL:CG1	2.83	0.61
1:O:45:VAL:CG1	1:O:110:ILE:HD11	2.31	0.61
1:Y:37:THR:CG2	1:Y:38:GLU:CD	2.69	0.61
1:Y:46:HIS:CE1	1:Y:116:VAL:HG11	2.36	0.61
1:Y:22:ALA:HB2	1:Y:104:LEU:HD21	1.83	0.61
1:Y:18:ILE:HD12	1:Y:29:VAL:HG23	1.82	0.61
1:O:0:ACE:H2	1:O:149:ILE:HD11	1.82	0.61
1:B:67:LYS:C	1:B:68:LYS:HD3	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:SER:HB3	1:G:108:TYR:O	2.00	0.60
1:O:106:GLY:O	1:O:108:TYR:N	2.34	0.60
1:O:47:GLN:O	1:O:113:ARG:HG2	2.01	0.60
1:Y:77:ARG:HH21	1:Y:101:LEU:CG	2.14	0.60
1:B:51:ASN:CA	1:B:54:GLY:O	2.48	0.60
1:G:39:GLY:O	1:G:86:THR:HA	2.01	0.60
1:Y:115:MET:O	1:Y:144:CYS:HA	2.00	0.60
1:Y:24:GLY:O	1:Y:25:ASP:CG	2.39	0.60
1:O:40:ASP:HA	1:O:85:VAL:O	2.01	0.60
1:B:118:HIS:HA	1:B:140:SER:O	2.02	0.60
1:B:40:ASP:O	1:B:121:PRO:HG3	2.01	0.60
1:B:77:ARG:NE	1:B:101:LEU:HD13	2.16	0.60
1:O:135:THR:HG23	1:O:136:GLY:N	2.13	0.60
1:Y:41:HIS:O	1:Y:84:ASN:HA	2.02	0.60
1:O:47:GLN:OE1	1:O:48:PHE:CE2	2.54	0.60
1:B:50:ASP:OD2	1:G:7:VAL:HG12	2.02	0.59
1:G:4:ALA:HB1	1:G:148:GLY:O	2.02	0.59
1:Y:47:GLN:C	1:Y:113:ARG:HD3	2.22	0.59
1:O:29:VAL:CG1	1:O:97:ILE:HG12	2.29	0.59
1:B:3:LYS:CE	1:B:21:GLU:HG3	2.33	0.59
1:Y:34:THR:HA	1:Y:91:GLY:O	2.02	0.59
1:Y:122:ASP:HA	1:Y:138:ALA:CB	2.11	0.59
1:O:64:PRO:HG3	1:O:108:TYR:HD1	1.65	0.59
1:Y:51:ASN:HB3	1:Y:54:GLY:O	2.02	0.59
1:G:120:LYS:HG3	1:G:121:PRO:CD	2.29	0.59
1:O:133:THR:O	1:O:134:LYS:CB	2.50	0.59
1:G:105:SER:C	1:G:109:SER:HB2	2.23	0.59
1:B:98:VAL:CG1	1:B:98:VAL:O	2.51	0.58
1:B:63:ASN:ND2	1:B:78:HIS:HD2	2.01	0.58
1:G:5:VAL:HG13	1:G:19:HIS:HD2	1.67	0.58
1:Y:22:ALA:HB2	1:Y:104:LEU:HD23	1.85	0.58
1:Y:18:ILE:HD11	1:Y:20:PHE:CE2	2.38	0.58
1:Y:47:GLN:HG3	1:Y:48:PHE:HD2	1.67	0.58
1:Y:88:ASP:N	1:Y:88:ASP:OD1	2.25	0.58
1:G:14:VAL:HB	1:G:34:THR:O	2.03	0.58
1:G:123:ASP:C	1:G:125:GLY:N	2.55	0.58
1:Y:119:GLU:HG3	1:Y:120:LYS:CG	2.34	0.58
1:Y:137:ASN:O	1:Y:139:GLY:CA	2.51	0.58
1:O:92:VAL:O	1:O:93:ALA:CB	2.51	0.58
1:Y:46:HIS:CD2	1:Y:61:HIS:HD2	2.22	0.58
1:O:68:LYS:HD2	1:O:133:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:HIS:NE2	1:O:134:LYS:CD	2.63	0.58
1:O:14:VAL:CG1	1:O:36:LEU:HD13	2.34	0.58
1:O:89:LYS:HB3	1:O:90:ASN:O	2.03	0.57
1:B:49:GLY:O	1:B:50:ASP:CB	2.51	0.57
1:Y:84:ASN:ND2	1:Y:121:PRO:HA	2.18	0.57
1:Y:72:PRO:HA	1:Y:77:ARG:HH11	1.69	0.57
1:O:46:HIS:CE1	1:O:141:ARG:NH2	2.69	0.57
1:G:89:LYS:O	1:G:90:ASN:CB	2.53	0.57
1:G:5:VAL:HG12	1:G:6:CYS:H	1.68	0.57
1:B:53:GLN:CG	1:B:57:SER:OG	2.53	0.57
1:G:1:ALA:CB	1:G:105:SER:HG	2.17	0.57
1:G:62:PHE:CZ	1:G:108:TYR:CG	2.92	0.57
1:Y:52:THR:O	1:Y:53:GLN:CB	2.52	0.57
1:O:88:ASP:OD2	1:O:89:LYS:CD	2.52	0.57
1:G:53:GLN:HB3	1:G:57:SER:CB	2.33	0.57
1:Y:46:HIS:CD2	1:Y:116:VAL:HG12	2.39	0.57
1:G:6:CYS:SG	1:G:147:ILE:HG22	2.44	0.57
1:G:114:THR:HA	1:G:145:GLY:O	2.04	0.57
1:Y:103:SER:O	1:Y:109:SER:HA	2.05	0.57
1:O:104:LEU:HA	1:O:109:SER:CB	2.35	0.56
1:G:26:THR:OG1	1:G:98:VAL:HG23	2.05	0.56
1:B:38:GLU:HA	1:B:88:ASP:O	2.05	0.56
1:Y:84:ASN:ND2	1:Y:122:ASP:N	2.40	0.56
1:G:135:THR:C	1:G:137:ASN:H	2.09	0.56
1:Y:129:ASN:O	1:Y:132:SER:HB3	2.05	0.56
1:G:27:VAL:HG22	1:G:104:LEU:HD22	1.86	0.56
1:Y:71:GLY:O	1:Y:77:ARG:HD2	2.05	0.56
1:Y:119:GLU:O	1:Y:120:LYS:CG	2.48	0.56
1:G:20:PHE:HD1	1:G:29:VAL:CB	2.11	0.56
1:B:22:ALA:HB2	1:B:27:VAL:HG22	1.88	0.56
1:G:9:LYS:HA	1:G:14:VAL:O	2.06	0.56
1:Y:38:GLU:H	1:Y:87:ALA:HB3	1.69	0.55
1:G:68:LYS:O	1:G:78:HIS:CD2	2.58	0.55
1:O:50:ASP:OD1	1:O:52:THR:HG23	2.06	0.55
1:G:45:VAL:HG13	1:G:80:GLY:HA2	1.89	0.55
1:Y:119:GLU:C	1:Y:120:LYS:CG	2.75	0.55
1:Y:11:ASP:H	1:Y:142:LEU:CD1	2.19	0.55
1:O:119:GLU:CG	1:O:119:GLU:O	2.40	0.55
1:B:3:LYS:HE3	1:B:21:GLU:CG	2.36	0.55
1:Y:53:GLN:NE2	1:G:13:PRO:HB3	2.19	0.55
1:B:18:ILE:HG22	1:B:19:HIS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:104:LEU:N	1:Y:104:LEU:CD2	2.64	0.55
1:G:14:VAL:CG2	1:G:143:ALA:HB2	2.36	0.55
1:G:30:THR:HA	1:G:95:VAL:O	2.07	0.55
1:Y:122:ASP:CA	1:Y:138:ALA:CB	2.73	0.55
1:G:12:GLY:CA	1:G:142:LEU:HD13	2.37	0.55
1:G:142:LEU:CD1	1:G:142:LEU:O	2.50	0.55
1:G:134:LYS:HE2	1:G:135:THR:HG23	1.89	0.55
1:B:126:ARG:NH1	1:B:126:ARG:CB	2.24	0.55
1:O:5:VAL:HG12	1:Y:50:ASP:HB2	1.88	0.55
1:G:53:GLN:HB3	1:G:57:SER:HB3	1.89	0.54
1:G:15:GLN:O	1:G:33:ILE:HG23	2.07	0.54
1:O:119:GLU:HB2	1:O:140:SER:O	2.07	0.54
1:B:129:ASN:HB2	1:B:130:GLU:OE1	2.07	0.54
1:Y:29:VAL:HG13	1:Y:97:ILE:CG1	2.21	0.54
1:O:78:HIS:CE1	1:O:134:LYS:HZ2	2.18	0.54
1:G:100:PRO:O	1:G:102:ILE:HG13	2.08	0.54
1:G:103:SER:O	1:G:104:LEU:C	2.44	0.54
1:O:133:THR:HG22	1:O:133:THR:O	2.07	0.54
1:G:39:GLY:H	1:G:87:ALA:HB3	1.72	0.54
1:O:68:LYS:HD2	1:O:133:THR:HG23	1.89	0.54
1:G:77:ARG:NH2	1:G:99:ASP:CG	2.60	0.54
1:O:65:LEU:HG	1:O:108:TYR:HE1	1.72	0.54
1:Y:85:VAL:HG13	1:Y:93:ALA:HB1	1.89	0.54
1:Y:102:ILE:HD12	1:Y:110:ILE:HD13	1.90	0.54
1:G:74:ASP:OD1	1:G:126:ARG:NH1	2.38	0.54
1:B:5:VAL:HG13	1:B:150:ALA:CB	2.37	0.54
1:Y:68:LYS:HE2	1:Y:76:GLU:OE1	2.08	0.54
1:Y:122:ASP:CB	1:Y:138:ALA:HB2	2.38	0.54
1:Y:46:HIS:CD2	1:Y:61:HIS:CD2	2.96	0.54
1:Y:103:SER:HA	1:Y:104:LEU:HD22	1.89	0.54
1:Y:18:ILE:CD1	1:Y:29:VAL:HG23	2.38	0.54
1:O:45:VAL:CG1	1:O:110:ILE:CD1	2.81	0.54
1:Y:119:GLU:C	1:Y:120:LYS:HG3	2.27	0.53
1:O:69:HIS:HB3	1:O:134:LYS:N	2.23	0.53
1:O:65:LEU:O	1:O:67:LYS:HG3	2.08	0.53
1:G:47:GLN:N	1:G:60:PRO:O	2.30	0.53
1:B:43:PHE:CZ	1:B:115:MET:HE2	2.43	0.53
1:O:14:VAL:HG13	1:O:36:LEU:HD13	1.90	0.53
1:Y:119:GLU:CG	1:Y:120:LYS:HE2	2.38	0.53
1:O:78:HIS:HE1	1:O:134:LYS:HZ3	1.53	0.53
1:Y:50:ASP:O	1:Y:57:SER:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:38:GLU:O	1:Y:87:ALA:C	2.46	0.53
1:B:37:THR:HA	1:B:38:GLU:HG2	1.89	0.53
1:Y:38:GLU:HG2	1:Y:39:GLY:CA	2.36	0.53
1:B:85:VAL:HG13	1:B:95:VAL:CG2	2.38	0.53
1:B:57:SER:O	1:B:58:ALA:HB3	2.09	0.53
1:G:38:GLU:HB2	1:G:89:LYS:HZ2	1.74	0.53
1:G:3:LYS:HD3	1:G:151:LYS:CD	2.35	0.53
1:Y:99:ASP:OD2	1:Y:101:LEU:HB2	2.09	0.53
1:G:69:HIS:HB2	1:G:78:HIS:CE1	2.43	0.53
1:B:71:GLY:HA2	1:B:124:LEU:CD2	2.38	0.53
1:O:7:VAL:CG1	1:Y:50:ASP:OD2	2.56	0.53
1:Y:11:ASP:HB3	1:Y:142:LEU:CD1	2.38	0.53
1:Y:49:GLY:HA2	1:Y:112:GLY:O	2.08	0.53
1:G:2:THR:HG23	1:G:3:LYS:HG3	1.91	0.53
1:Y:46:HIS:NE2	1:Y:116:VAL:HG11	2.24	0.53
1:Y:50:ASP:C	1:Y:52:THR:H	2.11	0.53
1:O:103:SER:OG	1:O:105:SER:CB	2.57	0.52
1:O:9:LYS:HD3	1:O:10:GLY:CA	2.38	0.52
1:B:119:GLU:CD	1:B:142:LEU:HG	2.29	0.52
1:G:41:HIS:O	1:G:85:VAL:N	2.42	0.52
1:G:38:GLU:HB2	1:G:89:LYS:NZ	2.24	0.52
1:G:121:PRO:O	1:G:138:ALA:HA	2.10	0.52
1:G:103:SER:O	1:G:104:LEU:O	2.27	0.52
1:O:111:ILE:CD1	1:O:149:ILE:HG12	2.39	0.52
1:O:142:LEU:H	1:O:142:LEU:HD22	1.73	0.52
1:G:8:LEU:O	1:G:15:GLN:CA	2.56	0.52
1:Y:65:LEU:H	1:Y:65:LEU:CD2	2.22	0.52
1:O:36:LEU:HG	1:O:41:HIS:HE1	1.74	0.52
1:Y:23:LYS:O	1:Y:23:LYS:HG3	2.09	0.52
1:O:45:VAL:HG12	1:O:115:MET:CE	2.38	0.52
1:O:27:VAL:HG22	1:O:102:ILE:HD11	1.90	0.52
1:O:125:GLY:O	1:O:126:ARG:CD	2.58	0.52
1:Y:40:ASP:N	1:Y:40:ASP:OD1	2.43	0.52
1:Y:88:ASP:HB2	1:Y:90:ASN:N	2.24	0.52
1:O:116:VAL:CG2	1:O:141:ARG:HB3	2.39	0.52
1:Y:103:SER:C	1:Y:104:LEU:HD22	2.30	0.52
1:O:9:LYS:CD	1:O:9:LYS:C	2.78	0.51
1:O:26:THR:CG2	1:O:98:VAL:HG13	2.40	0.51
1:Y:103:SER:CA	1:Y:104:LEU:HD22	2.41	0.51
1:O:116:VAL:HG21	1:O:141:ARG:HB3	1.93	0.51
1:Y:82:LEU:HD13	1:Y:97:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:HB2	1:B:142:LEU:HD23	1.91	0.51
1:Y:120:LYS:CB	1:Y:121:PRO:CD	2.87	0.51
1:Y:82:LEU:HD13	1:Y:97:ILE:CD1	2.40	0.51
1:B:88:ASP:C	1:B:90:ASN:H	2.12	0.51
1:B:85:VAL:HG12	1:B:93:ALA:CB	2.33	0.51
1:Y:38:GLU:N	1:Y:87:ALA:HB3	2.26	0.51
1:B:107:GLU:HG3	1:B:108:TYR:CD1	2.46	0.51
1:G:64:PRO:CB	1:G:108:TYR:HD2	2.22	0.51
1:B:135:THR:HG22	1:B:137:ASN:CA	2.41	0.51
1:Y:16:GLY:HA3	1:Y:33:ILE:HG22	1.93	0.51
1:Y:40:ASP:N	1:Y:86:THR:HG23	2.26	0.51
1:O:69:HIS:NE2	1:O:122:ASP:OD1	2.36	0.51
1:O:69:HIS:CD2	1:O:135:THR:O	2.63	0.51
1:G:110:ILE:O	1:G:147:ILE:HD11	2.11	0.51
1:G:71:GLY:O	1:G:77:ARG:HD2	2.11	0.50
1:G:89:LYS:CD	1:G:90:ASN:H	2.22	0.50
1:B:38:GLU:O	1:B:89:LYS:CE	2.57	0.50
1:Y:141:ARG:O	1:Y:142:LEU:CB	2.59	0.50
1:O:77:ARG:NE	1:O:101:LEU:HD23	2.26	0.50
1:Y:27:VAL:HG11	1:Y:102:ILE:HG13	1.93	0.50
1:G:27:VAL:HG21	1:G:102:ILE:HG22	1.93	0.50
1:O:24:GLY:O	1:O:25:ASP:CB	2.48	0.50
1:O:45:VAL:HG21	1:O:110:ILE:HG12	1.93	0.50
1:B:71:GLY:C	1:B:73:LYS:N	2.62	0.50
1:O:14:VAL:HG22	1:O:35:GLY:O	2.12	0.50
1:G:107:GLU:CG	1:G:108:TYR:H	2.25	0.50
1:O:62:PHE:CE1	1:O:79:VAL:HG11	2.45	0.50
1:G:134:LYS:HE2	1:G:135:THR:CG2	2.42	0.50
1:G:64:PRO:CB	1:G:108:TYR:CE2	2.91	0.50
1:Y:37:THR:HG22	1:Y:38:GLU:CB	2.41	0.49
1:Y:114:THR:CG2	1:Y:144:CYS:HB2	2.42	0.49
1:B:21:GLU:OE2	1:B:23:LYS:HD3	2.13	0.49
1:G:131:GLU:O	1:G:134:LYS:HD3	2.12	0.49
1:O:15:GLN:HG2	1:O:34:THR:HG1	1.77	0.49
1:G:41:HIS:O	1:G:84:ASN:HA	2.12	0.49
1:O:84:ASN:ND2	1:O:122:ASP:HB3	2.26	0.49
1:G:105:SER:HA	1:G:109:SER:HB2	1.95	0.49
1:Y:132:SER:C	1:Y:134:LYS:H	2.15	0.49
1:G:134:LYS:CE	1:G:135:THR:HG23	2.42	0.49
1:B:57:SER:O	1:B:58:ALA:CB	2.60	0.49
1:B:122:ASP:OD2	1:B:124:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:LYS:CD	1:G:135:THR:HG23	2.41	0.49
1:B:122:ASP:OD2	1:B:124:LEU:N	2.44	0.49
1:B:41:HIS:O	1:B:84:ASN:HA	2.12	0.49
1:Y:11:ASP:C	1:Y:142:LEU:HD12	2.34	0.49
1:G:67:LYS:HD3	1:G:76:GLU:HG3	1.93	0.49
1:G:36:LEU:C	1:G:36:LEU:HD23	2.33	0.49
1:B:90:ASN:O	1:B:92:VAL:CG1	2.60	0.49
1:Y:88:ASP:CB	1:Y:90:ASN:O	2.61	0.49
1:G:151:LYS:HE3	1:G:151:LYS:CA	2.24	0.48
1:Y:119:GLU:HG3	1:Y:120:LYS:HG3	1.94	0.48
1:Y:131:GLU:N	1:Y:133:THR:CG2	2.70	0.48
1:O:103:SER:HG	1:O:104:LEU:H	1.57	0.48
1:O:135:THR:HG23	1:O:137:ASN:H	1.78	0.48
1:O:46:HIS:HE1	4:O:154:HOH:O	1.95	0.48
1:Y:131:GLU:O	1:Y:134:LYS:HB2	2.13	0.48
1:Y:92:VAL:HG23	1:Y:94:ILE:HD12	1.93	0.48
1:G:5:VAL:HG23	1:G:150:ALA:CB	2.42	0.48
1:Y:24:GLY:O	1:Y:25:ASP:OD2	2.31	0.48
1:Y:131:GLU:C	1:Y:134:LYS:HB2	2.34	0.48
1:G:107:GLU:CG	1:G:108:TYR:N	2.75	0.48
1:G:45:VAL:HB	1:G:115:MET:HE2	1.95	0.48
1:O:89:LYS:HD2	1:O:89:LYS:H	1.78	0.48
1:G:47:GLN:HG3	1:G:60:PRO:CG	2.42	0.48
1:B:65:LEU:O	1:B:66:SER:HB2	2.13	0.48
1:G:89:LYS:O	1:G:90:ASN:ND2	2.44	0.48
1:Y:118:HIS:ND1	1:Y:140:SER:O	2.44	0.48
1:G:32:SER:HA	1:G:93:ALA:O	2.14	0.48
1:Y:47:GLN:HG3	1:Y:48:PHE:CD2	2.48	0.48
1:B:135:THR:HG22	1:B:136:GLY:N	2.28	0.48
1:Y:133:THR:HG23	1:Y:134:LYS:HG2	1.95	0.48
1:Y:84:ASN:HD21	1:Y:121:PRO:HA	1.77	0.48
1:G:29:VAL:HG22	1:G:97:ILE:HD13	1.95	0.48
1:O:88:ASP:OD2	1:O:89:LYS:HD2	2.13	0.48
1:O:62:PHE:CE2	1:O:113:ARG:CZ	2.97	0.48
1:O:129:ASN:ND2	1:O:129:ASN:N	2.61	0.48
1:G:51:ASN:O	1:G:53:GLN:C	2.52	0.48
1:G:5:VAL:HG12	1:G:6:CYS:N	2.28	0.48
1:G:70:GLY:HA2	1:G:124:LEU:C	2.33	0.48
1:B:62:PHE:CE1	1:B:64:PRO:HD3	2.48	0.48
1:G:1:ALA:HB3	1:G:105:SER:CB	2.43	0.47
1:Y:64:PRO:HG2	1:Y:65:LEU:CD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:106:GLY:O	1:O:107:GLU:C	2.51	0.47
1:O:107:GLU:O	1:O:108:TYR:CG	2.67	0.47
1:G:51:ASN:O	1:G:53:GLN:CA	2.62	0.47
1:G:117:VAL:CG1	1:G:143:ALA:CB	2.80	0.47
1:Y:72:PRO:HA	1:Y:77:ARG:NH1	2.29	0.47
1:Y:47:GLN:HA	1:Y:62:PHE:HB2	1.96	0.47
1:B:123:ASP:OD1	1:B:136:GLY:O	2.32	0.47
1:G:123:ASP:O	1:G:125:GLY:N	2.47	0.47
1:B:62:PHE:CD1	1:B:64:PRO:HD3	2.49	0.47
1:O:101:LEU:HD12	1:O:101:LEU:O	2.14	0.47
1:O:135:THR:CG2	1:O:136:GLY:N	2.77	0.47
1:O:86:THR:O	1:O:94:ILE:HG13	2.15	0.47
1:Y:46:HIS:NE2	1:Y:116:VAL:CG1	2.78	0.47
1:O:92:VAL:CG2	1:O:93:ALA:N	2.78	0.47
1:Y:19:HIS:O	1:Y:29:VAL:HA	2.15	0.47
1:G:25:ASP:O	1:G:102:ILE:HG12	2.15	0.47
1:O:45:VAL:HG21	1:O:110:ILE:CG1	2.44	0.47
1:B:71:GLY:CA	1:B:124:LEU:HD23	2.43	0.47
1:O:36:LEU:HD23	1:O:87:ALA:HB2	1.97	0.47
1:Y:26:THR:OG1	1:Y:98:VAL:HG23	2.14	0.47
1:G:45:VAL:HB	1:G:115:MET:CE	2.44	0.47
1:G:131:GLU:HG3	1:G:135:THR:OG1	2.15	0.47
1:O:45:VAL:HG12	1:O:115:MET:HE1	1.95	0.47
1:B:114:THR:HG22	1:B:145:GLY:O	2.15	0.47
1:Y:49:GLY:CA	1:Y:112:GLY:O	2.63	0.47
1:Y:3:LYS:HB2	1:Y:3:LYS:HE3	1.76	0.47
1:G:64:PRO:HG3	1:G:79:VAL:HG21	1.96	0.47
1:G:15:GLN:HG2	1:G:16:GLY:N	2.30	0.46
1:B:95:VAL:O	1:B:95:VAL:HG12	2.13	0.46
1:O:114:THR:HG23	1:O:145:GLY:C	2.36	0.46
1:B:3:LYS:HD3	1:B:151:LYS:HD2	1.97	0.46
1:G:74:ASP:O	1:G:75:GLU:CB	2.64	0.46
1:O:115:MET:O	1:O:144:CYS:HA	2.16	0.46
1:Y:77:ARG:O	1:Y:77:ARG:HG3	2.16	0.46
1:G:49:GLY:HA2	1:G:114:THR:OG1	2.15	0.46
1:Y:33:ILE:HG12	1:Y:93:ALA:HB3	1.97	0.46
1:G:65:LEU:HA	1:G:65:LEU:HD22	1.64	0.46
1:Y:69:HIS:NE2	1:Y:136:GLY:HA3	2.31	0.46
1:O:69:HIS:HB2	1:O:134:LYS:HA	1.97	0.46
1:O:64:PRO:CG	1:O:108:TYR:CD1	2.96	0.46
1:O:79:VAL:O	1:O:102:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:SER:H	1:B:109:SER:HB2	1.81	0.46
1:G:107:GLU:C	1:G:109:SER:N	2.63	0.46
1:B:118:HIS:HB3	1:B:138:ALA:O	2.15	0.46
1:O:93:ALA:HB1	1:O:94:ILE:HG13	1.98	0.46
1:G:50:ASP:N	1:G:50:ASP:OD1	2.49	0.46
1:Y:9:LYS:O	1:Y:143:ALA:HA	2.16	0.46
1:B:142:LEU:HA	1:B:142:LEU:HD13	1.17	0.45
1:G:99:ASP:HA	1:G:100:PRO:HD3	1.83	0.45
1:B:64:PRO:O	1:B:65:LEU:C	2.55	0.45
1:B:114:THR:HG22	1:B:145:GLY:H	1.81	0.45
1:Y:62:PHE:HZ	1:Y:108:TYR:HA	1.80	0.45
1:Y:43:PHE:O	1:Y:82:LEU:HB2	2.16	0.45
1:O:69:HIS:HB3	1:O:134:LYS:H	1.80	0.45
1:O:51:ASN:HB3	1:Y:7:VAL:CG1	2.29	0.45
1:O:15:GLN:CG	1:O:34:THR:OG1	2.62	0.45
1:Y:119:GLU:HG3	1:Y:120:LYS:HG2	1.98	0.45
1:Y:103:SER:O	1:Y:110:ILE:CG1	2.64	0.45
1:O:45:VAL:HG21	1:O:110:ILE:HD13	1.98	0.45
1:B:94:ILE:CD1	1:B:94:ILE:C	2.83	0.45
1:O:8:LEU:HD12	1:O:144:CYS:CA	2.47	0.45
1:Y:24:GLY:CA	1:Y:26:THR:HG22	2.44	0.45
1:G:103:SER:O	1:G:109:SER:CA	2.62	0.45
1:O:0:ACE:CH3	1:O:149:ILE:HD13	2.46	0.45
1:B:114:THR:HA	1:B:145:GLY:O	2.17	0.45
1:G:63:ASN:HA	1:G:63:ASN:HD22	1.23	0.45
1:B:135:THR:CG2	1:B:136:GLY:N	2.80	0.45
1:B:115:MET:HG2	1:B:147:ILE:HD11	1.99	0.45
1:O:101:LEU:HD12	1:O:101:LEU:HA	1.58	0.45
1:Y:18:ILE:CD1	1:Y:20:PHE:CZ	2.94	0.45
1:B:64:PRO:HG2	1:B:79:VAL:HG21	1.99	0.45
1:Y:47:GLN:O	1:Y:48:PHE:HB3	2.17	0.45
1:B:27:VAL:HB	1:B:102:ILE:HG12	1.98	0.45
1:Y:77:ARG:NH1	1:Y:81:ASP:O	2.50	0.45
1:Y:44:HIS:CE1	1:Y:61:HIS:CE1	3.06	0.44
1:O:46:HIS:ND1	1:O:141:ARG:NH2	2.66	0.44
1:O:26:THR:HG21	1:O:98:VAL:HG13	1.99	0.44
1:Y:59:GLY:O	1:Y:141:ARG:NH2	2.49	0.44
1:Y:45:VAL:HG13	1:Y:80:GLY:HA2	1.99	0.44
1:G:106:GLY:O	1:G:107:GLU:HG2	2.18	0.44
1:B:36:LEU:O	1:B:91:GLY:HA2	2.17	0.44
1:B:18:ILE:CG2	1:B:19:HIS:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:46:HIS:CE1	1:Y:141:ARG:HH21	2.36	0.44
1:Y:23:LYS:HG2	1:Y:28:VAL:HG22	1.97	0.44
1:G:131:GLU:O	1:G:131:GLU:HG3	2.11	0.44
1:G:140:SER:OG	1:G:141:ARG:CB	2.66	0.44
1:Y:51:ASN:HA	1:Y:54:GLY:O	2.18	0.44
1:O:68:LYS:HA	1:O:134:LYS:HG3	2.00	0.44
1:G:67:LYS:HD3	1:G:76:GLU:HA	1.99	0.44
1:G:44:HIS:CE1	1:G:118:HIS:CD2	3.06	0.44
1:B:38:GLU:HG2	1:B:38:GLU:H	0.69	0.44
1:G:88:ASP:HB3	1:G:89:LYS:O	2.17	0.44
1:Y:132:SER:O	1:Y:136:GLY:HA2	2.17	0.44
1:O:130:GLU:C	1:O:132:SER:H	2.21	0.44
1:B:23:LYS:HE3	1:B:28:VAL:HG11	1.99	0.44
1:B:23:LYS:CE	1:B:28:VAL:HG11	2.47	0.44
1:G:27:VAL:CG2	1:G:104:LEU:HD22	2.47	0.44
1:O:8:LEU:O	1:O:15:GLN:HA	2.17	0.44
1:B:68:LYS:CD	1:B:68:LYS:N	2.71	0.43
1:B:63:ASN:CG	1:B:78:HIS:HD2	2.22	0.43
1:G:2:THR:CG2	1:G:3:LYS:HG3	2.48	0.43
1:Y:79:VAL:CG2	1:Y:101:LEU:HD12	2.29	0.43
1:B:120:LYS:HB3	1:B:121:PRO:CD	2.48	0.43
1:G:114:THR:HG22	1:G:144:CYS:HB2	1.99	0.43
1:Y:31:GLY:O	1:Y:95:VAL:HG13	2.17	0.43
1:Y:18:ILE:CD1	1:Y:29:VAL:CG2	2.97	0.43
1:O:21:GLU:O	1:O:21:GLU:HG2	2.18	0.43
1:Y:135:THR:HG22	1:Y:137:ASN:N	2.28	0.43
1:Y:38:GLU:HG2	1:Y:39:GLY:HA3	1.93	0.43
1:G:71:GLY:H	1:G:74:ASP:HB2	1.82	0.43
1:G:82:LEU:HG	1:G:97:ILE:CD1	2.48	0.43
1:B:125:GLY:HA2	1:B:132:SER:O	2.19	0.43
1:Y:141:ARG:O	1:Y:142:LEU:HD23	2.17	0.43
1:Y:84:ASN:HD21	1:Y:121:PRO:CA	2.31	0.43
1:G:27:VAL:CB	1:G:102:ILE:HG22	2.45	0.43
1:B:123:ASP:HB2	1:B:136:GLY:O	2.18	0.43
1:B:47:GLN:O	1:B:113:ARG:HG2	2.18	0.43
1:O:90:ASN:HB3	1:O:91:GLY:H	1.63	0.43
1:G:89:LYS:CG	1:G:90:ASN:H	2.31	0.43
1:G:105:SER:HA	1:G:109:SER:CB	2.49	0.43
1:G:126:ARG:C	1:G:128:GLY:N	2.68	0.43
1:O:78:HIS:O	1:O:79:VAL:C	2.55	0.43
1:O:0:ACE:H2	1:O:149:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:24:GLY:C	1:Y:25:ASP:CG	2.77	0.43
1:B:116:VAL:HG12	1:B:118:HIS:CD2	2.54	0.43
1:B:23:LYS:HE3	1:B:28:VAL:CG1	2.48	0.43
1:Y:97:ILE:HD12	1:Y:97:ILE:HG21	1.58	0.43
1:O:63:ASN:ND2	1:O:78:HIS:CD2	2.87	0.43
1:Y:104:LEU:HD22	1:Y:104:LEU:H	1.79	0.43
1:B:62:PHE:CZ	1:B:64:PRO:HG3	2.54	0.43
1:Y:49:GLY:O	1:Y:146:VAL:HG22	2.19	0.43
1:O:71:GLY:O	1:O:77:ARG:HG3	2.19	0.43
1:O:99:ASP:HA	1:O:100:PRO:HD3	1.95	0.43
1:B:23:LYS:HE3	1:B:23:LYS:HB2	1.43	0.42
1:G:5:VAL:HG13	1:G:18:ILE:O	2.18	0.42
1:B:71:GLY:C	1:B:73:LYS:H	2.22	0.42
1:G:44:HIS:ND1	1:G:118:HIS:CD2	2.87	0.42
1:Y:36:LEU:CD1	1:Y:87:ALA:HB2	2.49	0.42
1:Y:101:LEU:N	1:Y:101:LEU:CD2	2.82	0.42
1:G:55:CYS:HB3	1:G:141:ARG:HB3	2.00	0.42
1:O:90:ASN:CB	1:O:92:VAL:HG12	2.49	0.42
1:G:25:ASP:O	1:G:102:ILE:CG1	2.67	0.42
1:O:104:LEU:C	1:O:104:LEU:CD2	2.83	0.42
1:O:46:HIS:HD2	1:O:116:VAL:CG1	2.23	0.42
1:Y:73:LYS:H	1:Y:73:LYS:HG2	1.60	0.42
1:B:117:VAL:HG12	1:B:143:ALA:HB3	2.01	0.42
1:B:77:ARG:CZ	1:B:101:LEU:HD13	2.48	0.42
1:Y:36:LEU:CD1	1:Y:41:HIS:CD2	3.01	0.42
1:O:47:GLN:HB2	1:O:60:PRO:O	2.20	0.42
1:O:62:PHE:HZ	1:O:108:TYR:HA	1.85	0.42
1:O:64:PRO:HG2	1:O:108:TYR:CE1	2.54	0.42
1:G:114:THR:CG2	1:G:144:CYS:HB2	2.50	0.42
1:B:55:CYS:O	1:B:141:ARG:HD2	2.19	0.42
1:O:149:ILE:HG22	1:O:150:ALA:N	2.34	0.42
1:G:53:GLN:O	1:G:56:THR:HB	2.20	0.42
1:G:63:ASN:ND2	1:G:78:HIS:HD2	2.18	0.42
1:O:14:VAL:HG21	1:O:142:LEU:CG	2.48	0.42
1:B:72:PRO:HA	1:B:77:ARG:NH1	2.34	0.42
1:B:90:ASN:O	1:B:92:VAL:HG12	2.20	0.42
1:Y:99:ASP:HA	1:Y:100:PRO:HD3	1.66	0.42
1:G:113:ARG:O	1:G:146:VAL:HA	2.19	0.42
1:Y:88:ASP:HB3	1:Y:90:ASN:O	2.19	0.42
1:G:36:LEU:HD23	1:G:36:LEU:O	2.18	0.42
1:B:51:ASN:HA	1:B:57:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:GLY:O	1:G:86:THR:CA	2.67	0.42
1:B:131:GLU:HG3	1:B:135:THR:HB	2.02	0.41
1:Y:79:VAL:HG22	1:Y:101:LEU:CD1	2.30	0.41
1:B:71:GLY:CA	1:B:124:LEU:CD2	2.98	0.41
1:B:43:PHE:CZ	1:B:115:MET:CE	3.03	0.41
1:O:44:HIS:CE1	1:O:61:HIS:CE1	3.08	0.41
1:B:119:GLU:CG	1:B:142:LEU:CG	2.77	0.41
1:B:126:ARG:NH1	1:B:126:ARG:CG	2.83	0.41
1:Y:120:LYS:HG3	1:Y:139:GLY:HA3	2.02	0.41
1:G:88:ASP:C	1:G:88:ASP:HB3	2.38	0.41
1:Y:137:ASN:O	1:Y:138:ALA:C	2.57	0.41
1:G:110:ILE:O	1:G:147:ILE:CD1	2.69	0.41
1:Y:77:ARG:NH2	1:Y:101:LEU:CB	2.73	0.41
1:G:23:LYS:HB3	1:G:23:LYS:HE2	1.30	0.41
1:B:44:HIS:HB3	1:B:80:GLY:O	2.20	0.41
1:O:65:LEU:O	1:O:66:SER:C	2.59	0.41
1:G:88:ASP:C	1:G:89:LYS:O	2.56	0.41
1:Y:45:VAL:HG21	1:Y:110:ILE:HG22	2.02	0.41
1:O:78:HIS:CE1	1:O:134:LYS:CD	3.04	0.41
1:O:62:PHE:CZ	1:O:108:TYR:HA	2.56	0.41
1:G:82:LEU:HG	1:G:97:ILE:HD11	2.03	0.41
1:G:70:GLY:CA	1:G:124:LEU:O	2.57	0.41
1:Y:68:LYS:HD3	1:Y:68:LYS:N	2.36	0.41
1:Y:37:THR:HG22	1:Y:38:GLU:HB3	2.03	0.41
1:B:77:ARG:HD3	1:B:101:LEU:HD13	2.01	0.41
1:B:135:THR:CG2	1:B:136:GLY:H	2.34	0.41
1:G:8:LEU:HD13	1:G:143:ALA:HB1	2.01	0.41
1:O:119:GLU:N	1:O:140:SER:O	2.54	0.41
1:O:72:PRO:O	1:O:77:ARG:NH1	2.54	0.41
1:B:127:GLY:HA3	1:B:132:SER:CB	2.51	0.41
1:O:78:HIS:O	1:O:81:ASP:N	2.50	0.41
1:O:3:LYS:HG2	1:O:150:ALA:HB3	2.03	0.41
1:G:53:GLN:O	1:G:53:GLN:CG	2.62	0.41
1:B:65:LEU:O	1:B:66:SER:CB	2.69	0.41
1:Y:6:CYS:HB2	1:Y:147:ILE:HA	2.03	0.41
1:G:105:SER:O	1:G:109:SER:CA	2.69	0.40
1:O:125:GLY:C	1:O:126:ARG:HG2	2.32	0.40
1:G:0:ACE:H2	1:G:1:ALA:O	2.21	0.40
1:O:78:HIS:NE2	1:O:134:LYS:HG2	2.37	0.40
1:O:5:VAL:CG2	1:O:19:HIS:CD2	3.03	0.40
1:B:88:ASP:C	1:B:90:ASN:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:VAL:HG11	1:Y:50:ASP:OD2	2.19	0.40
1:B:82:LEU:HG	1:B:97:ILE:HD11	2.02	0.40
1:G:112:GLY:N	1:G:147:ILE:O	2.46	0.40
1:O:3:LYS:HA	1:O:20:PHE:O	2.22	0.40
1:B:72:PRO:HG3	1:B:82:LEU:C	2.41	0.40
1:B:120:LYS:HA	1:B:121:PRO:HD3	1.82	0.40
1:O:26:THR:HG23	1:O:98:VAL:HG13	2.02	0.40
1:O:78:HIS:CE1	1:O:134:LYS:HD2	2.54	0.40
1:G:51:ASN:C	1:G:53:GLN:N	2.61	0.40
1:O:127:GLY:O	1:O:128:GLY:O	2.39	0.40

All (30) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:NH2	1:G:75:GLU:OE2[3_445]	0.67	1.53
1:O:107:GLU:CD	1:B:24:GLY:O[1_554]	0.95	1.25
1:O:151:LYS:CE	1:B:130:GLU:OE2[4_455]	1.08	1.12
1:O:151:LYS:CE	1:B:130:GLU:CD[4_455]	1.15	1.05
1:O:107:GLU:OE1	1:B:24:GLY:O[1_554]	1.20	1.00
1:O:107:GLU:OE2	1:B:24:GLY:O[1_554]	1.35	0.85
1:B:126:ARG:NH2	1:G:75:GLU:CD[3_445]	1.42	0.78
1:Y:34:THR:CG2	1:B:90:ASN:OD1[2_455]	1.45	0.75
1:O:107:GLU:OE2	1:B:25:ASP:CA[1_554]	1.55	0.65
1:O:107:GLU:OE1	1:B:24:GLY:C[1_554]	1.61	0.59
1:O:107:GLU:OE2	1:B:24:GLY:C[1_554]	1.62	0.58
1:O:151:LYS:CD	1:B:130:GLU:OE1[4_455]	1.62	0.58
1:O:151:LYS:CE	1:B:130:GLU:OE1[4_455]	1.63	0.57
1:O:151:LYS:NZ	1:B:130:GLU:OE2[4_455]	1.75	0.45
1:O:151:LYS:CD	1:B:130:GLU:CD[4_455]	1.76	0.44
1:O:151:LYS:CG	1:B:130:GLU:OE1[4_455]	1.81	0.39
1:O:107:GLU:CD	1:B:24:GLY:C[1_554]	1.83	0.37
1:O:53:GLN:CD	1:G:129:ASN:ND2[4_445]	1.83	0.37
1:O:107:GLU:OE2	1:B:25:ASP:N[1_554]	1.84	0.36
1:Y:13:PRO:CG	1:Y:90:ASN:OD1[2_455]	1.84	0.36
1:O:53:GLN:NE2	1:G:129:ASN:ND2[4_445]	1.90	0.30
1:O:151:LYS:CD	1:B:130:GLU:OE2[4_455]	1.93	0.27
1:B:126:ARG:CZ	1:G:75:GLU:OE2[3_445]	2.01	0.19
1:O:107:GLU:OE1	1:B:24:GLY:N[1_554]	2.02	0.18
1:Y:34:THR:CG2	1:B:90:ASN:CG[2_455]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:107:GLU:OE1	1:B:24:GLY:CA[1_554]	2.11	0.09
1:Y:68:LYS:CE	1:B:47:GLN:NE2[4_455]	2.13	0.07
1:O:53:GLN:OE1	1:G:129:ASN:ND2[4_445]	2.17	0.03
1:B:126:ARG:NH2	1:G:75:GLU:OE1[3_445]	2.18	0.02
1:O:151:LYS:CG	1:B:130:GLU:CD[4_455]	2.19	0.01

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	B	150/152 (99%)	123 (82%)	18 (12%)	9 (6%)	2	0
1	G	150/152 (99%)	109 (73%)	20 (13%)	21 (14%)	0	0
1	O	150/152 (99%)	111 (74%)	18 (12%)	21 (14%)	0	0
1	Y	150/152 (99%)	114 (76%)	17 (11%)	19 (13%)	0	0
All	All	600/608 (99%)	457 (76%)	73 (12%)	70 (12%)	0	0

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	1	ALA
1	O	2	THR
1	O	3	LYS
1	O	66	SER
1	O	94	ILE
1	O	107	GLU
1	O	108	TYR
1	O	126	ARG
1	O	128	GLY
1	O	133	THR
1	O	134	LYS
1	O	135	THR

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Mol	Chain	Res	Type
1	Y	1	ALA
1	Y	36	LEU
1	Y	53	GLN
1	Y	91	GLY
1	Y	130	GLU
1	Y	131	GLU
1	Y	138	ALA
1	Y	139	GLY
1	Y	140	SER
1	Y	142	LEU
1	B	38	GLU
1	B	65	LEU
1	B	66	SER
1	B	74	ASP
1	B	91	GLY
1	B	139	GLY
1	G	1	ALA
1	G	25	ASP
1	G	47	GLN
1	G	52	THR
1	G	86	THR
1	G	102	ILE
1	G	106	GLY
1	G	107	GLU
1	G	128	GLY
1	G	130	GLU
1	O	25	ASP
1	O	90	ASN
1	O	124	LEU
1	O	127	GLY
1	Y	37	THR
1	Y	38	GLU
1	Y	47	GLN
1	Y	66	SER
1	Y	89	LYS
1	Y	137	ASN
1	B	105	SER
1	G	68	LYS
1	G	90	ASN
1	O	105	SER
1	Y	107	GLU
1	B	75	GLU

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Mol	Chain	Res	Type
1	G	9	LYS
1	G	104	LEU
1	B	58	ALA
1	G	119	GLU
1	G	137	ASN
1	O	47	GLN
1	O	91	GLY
1	O	104	LEU
1	Y	61	HIS
1	Y	133	THR
1	G	11	ASP
1	G	103	SER
1	G	138	ALA
1	G	123	ASP
1	O	24	GLY
1	G	85	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	117/117 (100%)	79 (68%)	38 (32%)	0 0
1	G	117/117 (100%)	77 (66%)	40 (34%)	0 0
1	O	117/117 (100%)	76 (65%)	41 (35%)	0 0
1	Y	117/117 (100%)	79 (68%)	38 (32%)	0 0
All	All	468/468 (100%)	311 (66%)	157 (34%)	0 0

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	7	VAL
1	O	8	LEU
1	O	9	LYS
1	O	11	ASP
1	O	13	PRO

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Mol	Chain	Res	Type
1	O	15	GLN
1	O	17	THR
1	O	20	PHE
1	O	26	THR
1	O	27	VAL
1	O	29	VAL
1	O	38	GLU
1	O	40	ASP
1	O	41	HIS
1	O	45	VAL
1	O	47	GLN
1	O	56	THR
1	O	66	SER
1	O	68	LYS
1	O	73	LYS
1	O	75	GLU
1	O	77	ARG
1	O	78	HIS
1	O	82	LEU
1	O	89	LYS
1	O	90	ASN
1	O	92	VAL
1	O	94	ILE
1	O	96	ASP
1	O	97	ILE
1	O	101	LEU
1	O	104	LEU
1	O	107	GLU
1	O	110	ILE
1	O	111	ILE
1	O	115	MET
1	O	134	LYS
1	O	135	THR
1	O	141	ARG
1	O	142	LEU
1	O	151	LYS
1	Y	7	VAL
1	Y	8	LEU
1	Y	15	GLN
1	Y	18	ILE
1	Y	27	VAL
1	Y	28	VAL

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Mol	Chain	Res	Type
1	Y	29	VAL
1	Y	30	THR
1	Y	36	LEU
1	Y	40	ASP
1	Y	45	VAL
1	Y	50	ASP
1	Y	51	ASN
1	Y	53	GLN
1	Y	56	THR
1	Y	57	SER
1	Y	60	PRO
1	Y	63	ASN
1	Y	65	LEU
1	Y	67	LYS
1	Y	68	LYS
1	Y	73	LYS
1	Y	75	GLU
1	Y	76	GLU
1	Y	77	ARG
1	Y	82	LEU
1	Y	86	THR
1	Y	88	ASP
1	Y	89	LYS
1	Y	90	ASN
1	Y	92	VAL
1	Y	95	VAL
1	Y	97	ILE
1	Y	104	LEU
1	Y	105	SER
1	Y	120	LYS
1	Y	131	GLU
1	Y	133	THR
1	B	2	THR
1	B	5	VAL
1	B	13	PRO
1	B	17	THR
1	B	21	GLU
1	B	23	LYS
1	B	37	THR
1	B	38	GLU
1	B	40	ASP
1	B	44	HIS

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Mol	Chain	Res	Type
1	B	50	ASP
1	B	51	ASN
1	B	53	GLN
1	B	57	SER
1	B	66	SER
1	B	68	LYS
1	B	73	LYS
1	B	77	ARG
1	B	86	THR
1	B	89	LYS
1	B	92	VAL
1	B	94	ILE
1	B	97	ILE
1	B	99	ASP
1	B	102	ILE
1	B	104	LEU
1	B	111	ILE
1	B	113	ARG
1	B	114	THR
1	B	119	GLU
1	B	122	ASP
1	B	126	ARG
1	B	130	GLU
1	B	133	THR
1	B	134	LYS
1	B	142	LEU
1	B	144	CYS
1	B	151	LYS
1	G	2	THR
1	G	11	ASP
1	G	14	VAL
1	G	15	GLN
1	G	20	PHE
1	G	21	GLU
1	G	23	LYS
1	G	29	VAL
1	G	30	THR
1	G	32	SER
1	G	34	THR
1	G	36	LEU
1	G	37	THR
1	G	40	ASP

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Mol	Chain	Res	Type
1	G	45	VAL
1	G	50	ASP
1	G	65	LEU
1	G	73	LYS
1	G	82	LEU
1	G	86	THR
1	G	88	ASP
1	G	89	LYS
1	G	94	ILE
1	G	97	ILE
1	G	98	VAL
1	G	101	LEU
1	G	102	ILE
1	G	104	LEU
1	G	105	SER
1	G	108	TYR
1	G	110	ILE
1	G	111	ILE
1	G	114	THR
1	G	116	VAL
1	G	119	GLU
1	G	120	LYS
1	G	134	LYS
1	G	142	LEU
1	G	147	ILE
1	G	151	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	19	HIS
1	O	41	HIS
1	O	90	ASN
1	Y	15	GLN
1	Y	41	HIS
1	Y	53	GLN
1	Y	63	ASN
1	Y	84	ASN
1	Y	90	ASN
1	B	63	ASN
1	B	137	ASN
1	G	19	HIS

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Mol	Chain	Res	Type
1	G	41	HIS
1	G	63	ASN
1	G	90	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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