Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:06 PM GMT

PDB ID	:	1E0U
Title	:	STRUCTURE R271L MUTANT OF E. COLI PYRUVATE KINASE
Authors	:	Fortin, R.; Mattevi, A.
Deposited on	:	2000-04-10
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

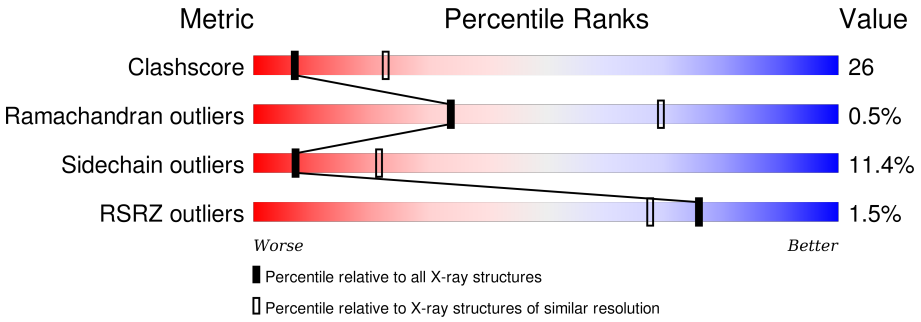
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	470	44% 40% 12%
1	B	470	46% 37% 14%
1	C	470	5% 45% 35% 15%
1	D	470	46% 33% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14000 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.

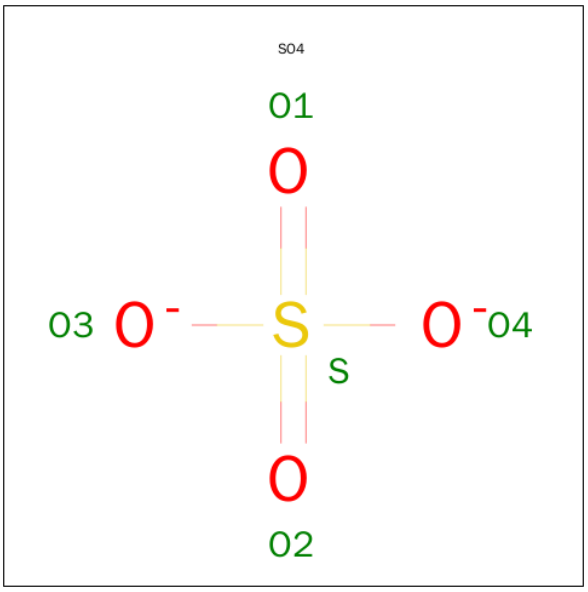
- Molecule 1 is a protein called PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			
1	B	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			
1	C	461	Total	C	N	O	S	11	0	0
			3445	2150	594	676	25			
1	D	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	LEU	ARG	ENGINEERED MUTATION	UNP P14178
B	271	LEU	ARG	ENGINEERED MUTATION	UNP P14178
C	271	LEU	ARG	ENGINEERED MUTATION	UNP P14178
D	271	LEU	ARG	ENGINEERED MUTATION	UNP P14178
A	279	MET	GLN	CONFLICT	UNP P14178
B	279	MET	GLN	CONFLICT	UNP P14178
C	279	MET	GLN	CONFLICT	UNP P14178
D	279	MET	GLN	CONFLICT	UNP P14178

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

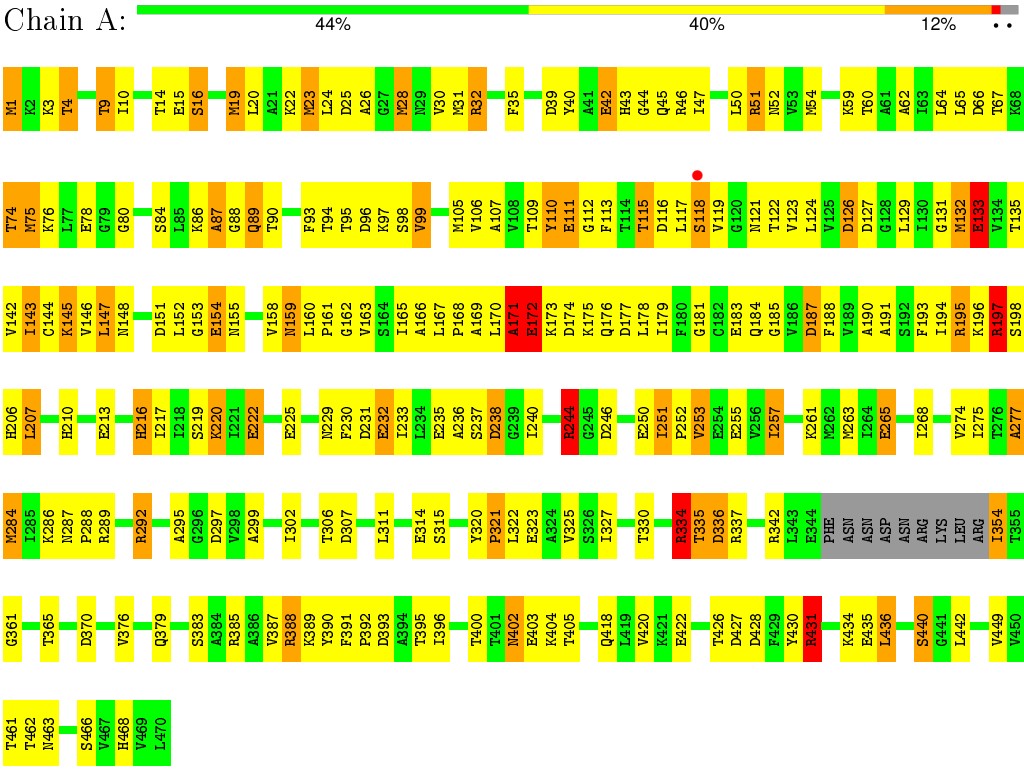
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	55	Total O 55 55	0	0
3	C	48	Total O 48 48	0	0
3	D	59	Total O 59 59	0	0

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.

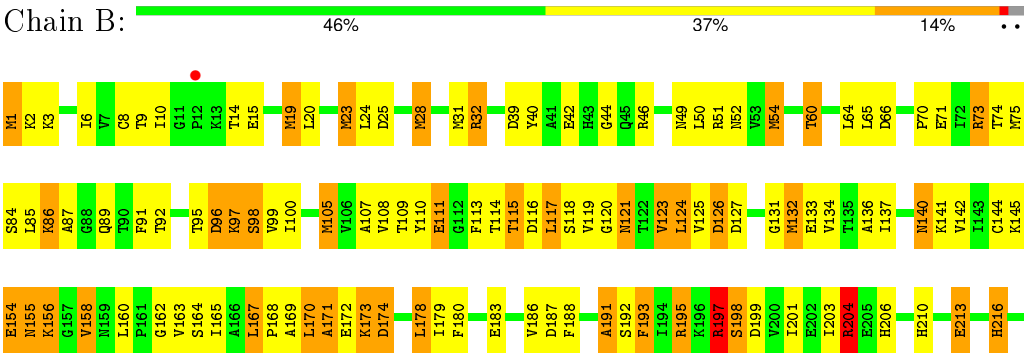
- Molecule 1: PYRUVATE KINASE

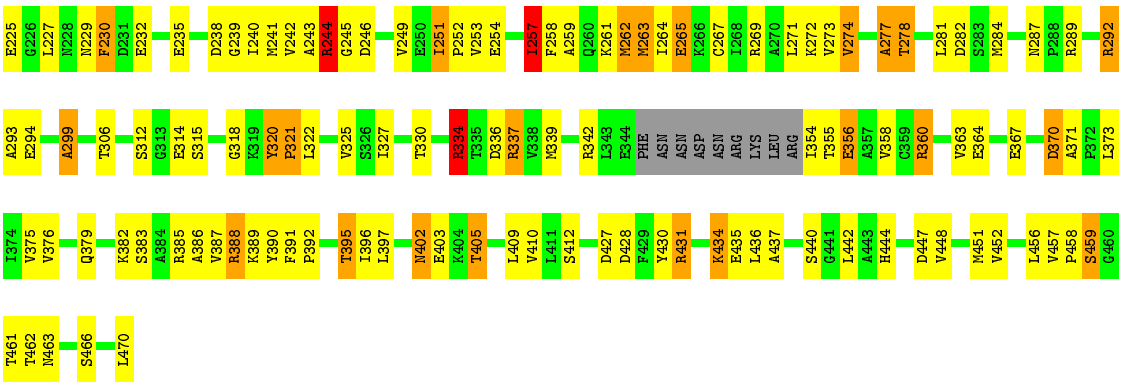
Chain A:



- Molecule 1: PYRUVATE KINASE

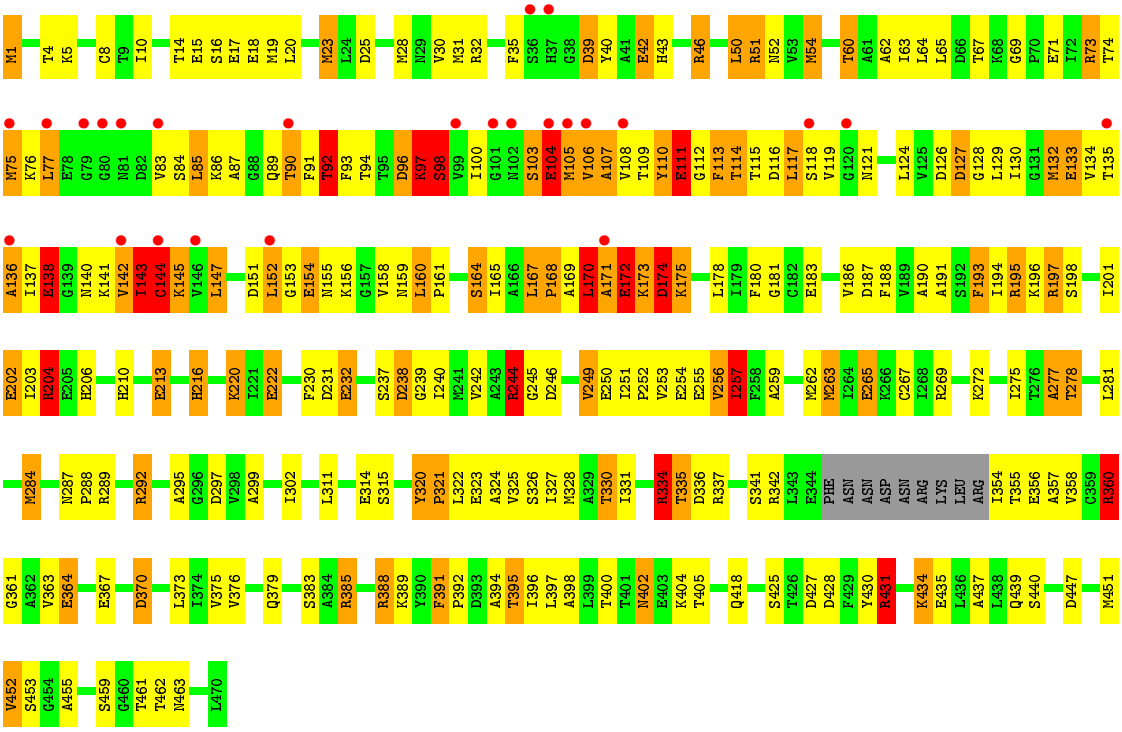
Chain B:





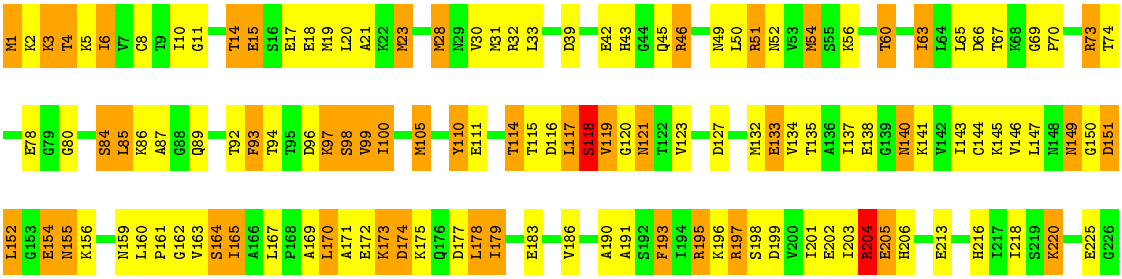
- Molecule 1: PYRUVATE KINASE

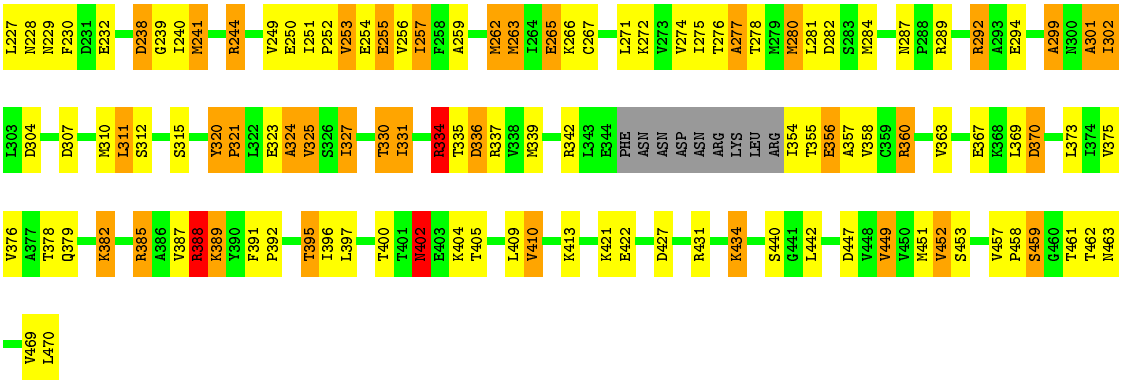
Chain C:



- Molecule 1: PYRUVATE KINASE

Chain D:




L227 N228 N229 F230 D231 E232 D238 G239 I240 M241 R244 V249 E250 I251 P252 V253 E254 E255 V256 I257 F258 A259 M262 M263 I264 E265 K266 C267 L271 K272 V273 V274 I275 T276 A277 T278 M279 M280 L281 D282 S283 M284 N287 P288 R289 R292 A293 E294 A299 N300 A301 I302
L303 D304 D307 M310 L311 S312 S315 Y320 P321 L322 E323 A324 V325 S326 I327 T330 I331 R334 T335 D336 R337 V338 M339 R342 L343 E344 PHE ASN ASN ASP ASN ARG LYS LEU ARG I354 T355 E356 A357 V358 C359 R360 V363 E367 K368 L369 D370 L373 I374 V375
V376 A377 T378 Q379 K382 R385 A386 V387 R388 K389 Y390 F391 P392 T395 I396 L397 T400 T401 N402 E403 K404 T405 L409 V410 K413 K421 E422 D427 R431 K434 S440 G441 L442 D447 V448 V449 V450 M451 V452 S453 V457 P458 S459 G460 T461 T462 N463
V469 L470

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.01Å 129.59Å 241.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.80) 97.9 (14.93-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	5.83 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.245 , 0.312 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	3 of 56604 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14000	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.32 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1649e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.92	2/3479 (0.1%)	2.48	161/4695 (3.4%)
1	B	0.96	3/3479 (0.1%)	2.67	186/4695 (4.0%)
1	C	2.31	6/3479 (0.2%)	2.71	209/4695 (4.5%)
1	D	0.99	1/3479 (0.0%)	2.68	192/4695 (4.1%)
All	All	1.42	12/13916 (0.1%)	2.64	748/18780 (4.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	3
1	D	0	5
All	All	0	14

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	GLU	CD-OE1	81.24	2.15	1.25
1	C	145	LYS	CD-CE	79.59	3.50	1.51
1	C	111	GLU	CD-OE2	50.21	1.80	1.25
1	D	225	GLU	CD-OE1	7.12	1.33	1.25
1	C	97	LYS	CE-NZ	-6.65	1.32	1.49
1	B	198	SER	CB-OG	5.50	1.49	1.42
1	A	197	ARG	CA-CB	-5.50	1.41	1.53
1	C	43	HIS	CE1-NE2	-5.42	1.20	1.32
1	A	244	ARG	NE-CZ	-5.34	1.26	1.33
1	B	277	ALA	C-O	5.25	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	GLU	CD-OE1	5.16	1.31	1.25
1	C	277	ALA	C-O	5.01	1.32	1.23

All (748) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	244	ARG	NE-CZ-NH1	35.92	138.26	120.30
1	C	385	ARG	CD-NE-CZ	34.00	171.20	123.60
1	B	385	ARG	NE-CZ-NH2	-32.17	104.22	120.30
1	D	265	GLU	OE1-CD-OE2	-30.92	86.20	123.30
1	B	360	ARG	NE-CZ-NH2	-28.51	106.04	120.30
1	A	73	ARG	CD-NE-CZ	28.21	163.09	123.60
1	A	342	ARG	NE-CZ-NH2	-27.82	106.39	120.30
1	A	342	ARG	NE-CZ-NH1	27.54	134.07	120.30
1	D	385	ARG	NE-CZ-NH2	-27.47	106.57	120.30
1	A	265	GLU	OE1-CD-OE2	-27.46	90.34	123.30
1	A	385	ARG	CD-NE-CZ	26.93	161.30	123.60
1	D	360	ARG	NE-CZ-NH1	26.21	133.41	120.30
1	C	342	ARG	NE-CZ-NH2	-26.04	107.28	120.30
1	B	32	ARG	NE-CZ-NH1	25.78	133.19	120.30
1	C	265	GLU	OE1-CD-OE2	-25.65	92.52	123.30
1	B	244	ARG	NE-CZ-NH1	25.53	133.07	120.30
1	C	138	GLU	OE1-CD-OE2	-25.25	93.00	123.30
1	B	360	ARG	NE-CZ-NH1	24.94	132.77	120.30
1	B	265	GLU	OE1-CD-OE2	-24.88	93.45	123.30
1	C	342	ARG	NE-CZ-NH1	24.56	132.58	120.30
1	B	342	ARG	NE-CZ-NH2	-24.45	108.07	120.30
1	D	360	ARG	NE-CZ-NH2	-23.67	108.47	120.30
1	D	292	ARG	NE-CZ-NH2	-23.62	108.49	120.30
1	C	197	ARG	NE-CZ-NH1	-21.55	109.53	120.30
1	D	342	ARG	NE-CZ-NH2	-21.43	109.58	120.30
1	B	342	ARG	NE-CZ-NH1	21.19	130.90	120.30
1	C	111	GLU	CB-CG-CD	20.54	169.66	114.20
1	C	244	ARG	NE-CZ-NH1	19.69	130.14	120.30
1	B	292	ARG	NE-CZ-NH1	18.65	129.62	120.30
1	D	204	ARG	NE-CZ-NH2	18.61	129.60	120.30
1	C	145	LYS	CG-CD-CE	-18.52	56.34	111.90
1	A	337	ARG	NE-CZ-NH2	-18.30	111.15	120.30
1	C	244	ARG	NE-CZ-NH2	-18.04	111.28	120.30
1	B	292	ARG	NE-CZ-NH2	-17.98	111.31	120.30
1	B	197	ARG	NE-CZ-NH2	17.90	129.25	120.30
1	D	385	ARG	CD-NE-CZ	17.40	147.96	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	138	GLU	CG-CD-OE1	-17.34	83.61	118.30
1	C	111	GLU	CG-CD-OE1	17.32	152.93	118.30
1	C	337	ARG	NE-CZ-NH2	-17.11	111.75	120.30
1	D	342	ARG	NE-CZ-NH1	17.08	128.84	120.30
1	B	204	ARG	NE-CZ-NH2	17.05	128.83	120.30
1	D	265	GLU	CG-CD-OE1	16.61	151.52	118.30
1	B	385	ARG	NE-CZ-NH1	16.38	128.49	120.30
1	D	46	ARG	NE-CZ-NH1	16.35	128.47	120.30
1	D	151	ASP	CB-CG-OD2	-16.33	103.61	118.30
1	A	360	ARG	NE-CZ-NH2	-16.30	112.15	120.30
1	D	46	ARG	NE-CZ-NH2	-16.29	112.16	120.30
1	D	334	ARG	CD-NE-CZ	16.22	146.31	123.60
1	C	43	HIS	ND1-CG-CD2	-16.11	83.44	106.00
1	C	111	GLU	OE1-CD-OE2	-16.07	104.01	123.30
1	B	334	ARG	CD-NE-CZ	15.88	145.83	123.60
1	D	32	ARG	NE-CZ-NH1	15.79	128.19	120.30
1	B	174	ASP	CB-CG-OD1	15.58	132.32	118.30
1	A	232	GLU	OE1-CD-OE2	15.52	141.93	123.30
1	B	427	ASP	CB-CG-OD1	15.11	131.90	118.30
1	C	334	ARG	CD-NE-CZ	14.98	144.57	123.60
1	C	246	ASP	CB-CG-OD1	14.96	131.77	118.30
1	C	402	ASN	OD1-CG-ND2	-14.88	87.68	121.90
1	B	320	TYR	CB-CG-CD1	-14.75	112.15	121.00
1	D	51	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	C	46	ARG	NE-CZ-NH1	14.57	127.58	120.30
1	C	1	MET	CA-CB-CG	14.53	138.01	113.30
1	A	334	ARG	CD-NE-CZ	14.50	143.90	123.60
1	A	210	HIS	ND1-CG-CD2	-14.47	85.74	106.00
1	B	15	GLU	OE1-CD-OE2	-14.37	106.06	123.30
1	D	244	ARG	NE-CZ-NH2	-14.33	113.14	120.30
1	B	32	ARG	NH1-CZ-NH2	-14.24	103.73	119.40
1	B	385	ARG	CD-NE-CZ	14.21	143.50	123.60
1	C	360	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	C	43	HIS	CG-ND1-CE1	13.89	127.65	108.20
1	A	1	MET	CA-CB-CG	13.83	136.81	113.30
1	D	292	ARG	NE-CZ-NH1	13.80	127.20	120.30
1	A	265	GLU	CG-CD-OE1	13.78	145.86	118.30
1	C	232	GLU	OE1-CD-OE2	13.73	139.78	123.30
1	D	427	ASP	CB-CG-OD1	13.73	130.66	118.30
1	B	1	MET	CA-CB-CG	13.68	136.55	113.30
1	D	320	TYR	CB-CG-CD1	-13.45	112.93	121.00
1	A	197	ARG	NE-CZ-NH1	-13.42	113.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	183	GLU	OE1-CD-OE2	13.12	139.04	123.30
1	B	216	HIS	ND1-CG-CD2	-13.10	87.66	106.00
1	C	402	ASN	CB-CG-ND2	13.04	148.00	116.70
1	A	244	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	B	342	ARG	CD-NE-CZ	12.75	141.45	123.60
1	D	334	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	C	164	SER	N-CA-CB	12.53	129.30	110.50
1	B	96	ASP	CB-CG-OD1	12.27	129.34	118.30
1	D	145	LYS	CA-CB-CG	12.14	140.11	113.40
1	A	210	HIS	CG-ND1-CE1	12.11	125.15	108.20
1	C	32	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	B	197	ARG	NE-CZ-NH1	-11.78	114.41	120.30
1	C	342	ARG	CD-NE-CZ	11.74	140.03	123.60
1	C	174	ASP	CB-CG-OD2	11.71	128.84	118.30
1	B	96	ASP	CB-CG-OD2	-11.69	107.78	118.30
1	B	172	GLU	OE1-CD-OE2	-11.57	109.42	123.30
1	A	244	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	A	385	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	C	104	GLU	CG-CD-OE1	-11.44	95.42	118.30
1	C	265	GLU	CG-CD-OE2	11.44	141.17	118.30
1	C	127	ASP	CB-CG-OD1	11.43	128.59	118.30
1	B	105	MET	CA-CB-CG	11.36	132.62	113.30
1	B	337	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	B	204	ARG	NE-CZ-NH1	-11.29	114.66	120.30
1	A	154	GLU	OE1-CD-OE2	-11.26	109.78	123.30
1	D	1	MET	CA-CB-CG	11.07	132.11	113.30
1	A	342	ARG	CD-NE-CZ	11.06	139.09	123.60
1	C	204	ARG	NE-CZ-NH2	11.05	125.83	120.30
1	C	142	VAL	N-CA-CB	10.96	135.61	111.50
1	B	216	HIS	CG-CD2-NE2	10.85	129.81	109.20
1	D	342	ARG	CD-NE-CZ	10.84	138.78	123.60
1	D	172	GLU	OE1-CD-OE2	-10.81	110.33	123.30
1	B	151	ASP	CB-CG-OD2	-10.69	108.68	118.30
1	A	360	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	C	111	GLU	CA-CB-CG	10.59	136.71	113.40
1	B	337	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	B	265	GLU	CG-CD-OE2	10.58	139.46	118.30
1	C	277	ALA	CA-C-N	10.58	140.47	117.20
1	A	195	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	334	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	B	244	ARG	NH1-CZ-NH2	-10.32	108.05	119.40
1	B	115	THR	CA-CB-CG2	-10.29	97.99	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	393	ASP	CB-CG-OD2	-10.22	109.10	118.30
1	B	82	ASP	CB-CG-OD2	-10.20	109.12	118.30
1	B	277	ALA	CA-C-N	10.14	139.51	117.20
1	D	225	GLU	OE1-CD-OE2	10.13	135.46	123.30
1	D	299	ALA	N-CA-CB	-10.02	96.08	110.10
1	C	427	ASP	CB-CG-OD1	9.94	127.25	118.30
1	C	174	ASP	CB-CG-OD1	-9.88	109.40	118.30
1	C	292	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	D	244	ARG	NH1-CZ-NH2	-9.86	108.55	119.40
1	C	435	GLU	OE1-CD-OE2	9.86	135.13	123.30
1	C	277	ALA	O-C-N	-9.85	106.94	122.70
1	C	320	TYR	CB-CG-CD1	-9.83	115.10	121.00
1	B	370	ASP	CB-CG-OD1	9.81	127.13	118.30
1	C	292	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	A	435	GLU	OE1-CD-OE2	9.73	134.97	123.30
1	D	232	GLU	OE1-CD-OE2	9.64	134.87	123.30
1	A	111	GLU	N-CA-CB	-9.61	93.31	110.60
1	D	278	THR	CA-CB-CG2	-9.54	99.04	112.40
1	C	202	GLU	OE1-CD-OE2	-9.48	111.92	123.30
1	C	222	GLU	OE1-CD-OE2	-9.47	111.94	123.30
1	B	15	GLU	CG-CD-OE2	9.41	137.13	118.30
1	B	151	ASP	CB-CG-OD1	9.41	126.77	118.30
1	A	32	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	D	277	ALA	CA-C-N	9.38	137.82	117.20
1	B	126	ASP	CB-CG-OD2	9.37	126.73	118.30
1	D	370	ASP	CB-CG-OD1	9.32	126.69	118.30
1	D	93	PHE	CB-CG-CD1	-9.30	114.29	120.80
1	C	43	HIS	CG-CD2-NE2	9.28	126.83	109.20
1	C	197	ARG	NH1-CZ-NH2	9.19	129.51	119.40
1	C	195	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	D	385	ARG	NH1-CZ-NH2	9.18	129.49	119.40
1	A	197	ARG	N-CA-CB	-9.17	94.10	110.60
1	B	356	GLU	OE1-CD-OE2	-9.12	112.36	123.30
1	C	104	GLU	CG-CD-OE2	9.08	136.47	118.30
1	D	174	ASP	CB-CG-OD1	9.06	126.46	118.30
1	C	32	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	C	51	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	D	356	GLU	OE1-CD-OE2	-8.99	112.51	123.30
1	A	190	ALA	O-C-N	8.90	136.94	122.70
1	C	111	GLU	CG-CD-OE2	-8.90	100.50	118.30
1	C	216	HIS	CG-ND1-CE1	8.89	120.65	108.20
1	D	244	ARG	CA-CB-CG	-8.88	93.86	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	172	GLU	OE1-CD-OE2	-8.77	112.78	123.30
1	B	370	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	D	135	THR	CA-CB-CG2	-8.69	100.23	112.40
1	B	447	ASP	CB-CG-OD2	8.65	126.09	118.30
1	D	277	ALA	N-CA-C	8.65	134.35	111.00
1	D	195	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	A	111	GLU	CB-CA-C	8.62	127.63	110.40
1	B	46	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	C	127	ASP	OD1-CG-OD2	-8.58	107.00	123.30
1	A	210	HIS	CG-CD2-NE2	8.54	125.42	109.20
1	C	202	GLU	CG-CD-OE1	8.52	135.34	118.30
1	D	51	ARG	NH1-CZ-NH2	-8.51	110.04	119.40
1	C	106	VAL	N-CA-CB	8.50	130.20	111.50
1	A	115	THR	CA-CB-CG2	-8.43	100.60	112.40
1	D	280	MET	CG-SD-CE	8.43	113.68	100.20
1	A	282	ASP	CB-CG-OD1	8.38	125.84	118.30
1	D	123	VAL	CA-CB-CG1	-8.36	98.37	110.90
1	A	277	ALA	CA-C-N	8.33	135.53	117.20
1	B	390	TYR	CB-CG-CD1	8.33	126.00	121.00
1	D	177	ASP	CB-CG-OD1	8.33	125.79	118.30
1	A	337	ARG	NH1-CZ-NH2	8.32	128.55	119.40
1	D	105	MET	CG-SD-CE	8.32	113.51	100.20
1	A	126	ASP	CB-CG-OD2	8.32	125.79	118.30
1	B	171	ALA	CB-CA-C	8.29	122.53	110.10
1	D	204	ARG	NH1-CZ-NH2	-8.28	110.29	119.40
1	A	277	ALA	O-C-N	-8.27	109.46	122.70
1	D	97	LYS	N-CA-CB	-8.25	95.76	110.60
1	B	447	ASP	CA-CB-CG	8.18	131.40	113.40
1	B	172	GLU	CG-CD-OE1	8.17	134.64	118.30
1	D	321	PRO	N-CD-CG	-8.16	90.96	103.20
1	B	277	ALA	O-C-N	-8.14	109.67	122.70
1	B	222	GLU	OE1-CD-OE2	-8.07	113.61	123.30
1	B	25	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	B	158	VAL	CA-CB-CG2	-8.04	98.84	110.90
1	A	278	THR	CA-CB-CG2	-8.04	101.14	112.40
1	B	292	ARG	CA-CB-CG	8.03	131.08	113.40
1	C	216	HIS	ND1-CG-CD2	-7.96	94.85	106.00
1	B	66	ASP	CB-CG-OD1	7.95	125.45	118.30
1	D	277	ALA	O-C-N	-7.84	110.16	122.70
1	C	96	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	C	238	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	431	ARG	NE-CZ-NH2	7.76	124.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	238	ASP	CB-CG-OD2	-7.75	111.33	118.30
1	D	197	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	B	169	ALA	N-CA-CB	-7.72	99.30	110.10
1	A	235	GLU	OE1-CD-OE2	-7.69	114.07	123.30
1	C	73	ARG	CB-CA-C	-7.69	95.02	110.40
1	A	277	ALA	N-CA-C	7.68	131.74	111.00
1	A	216	HIS	CG-ND1-CE1	7.66	118.93	108.20
1	B	427	ASP	OD1-CG-OD2	-7.65	108.77	123.30
1	D	143	ILE	CA-CB-CG2	7.65	126.19	110.90
1	D	263	MET	CA-CB-CG	7.64	126.29	113.30
1	D	256	VAL	CA-C-N	7.64	134.01	117.20
1	B	127	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	244	ARG	CD-NE-CZ	7.61	134.25	123.60
1	C	136	ALA	CB-CA-C	-7.60	98.70	110.10
1	B	82	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	435	GLU	OE1-CD-OE2	7.54	132.35	123.30
1	B	216	HIS	CB-CG-ND1	7.54	142.04	123.20
1	A	51	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	222	GLU	OE1-CD-OE2	-7.51	114.28	123.30
1	D	357	ALA	O-C-N	7.49	134.68	122.70
1	B	51	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	C	18	GLU	O-C-N	7.46	134.65	122.70
1	B	259	ALA	CB-CA-C	7.46	121.29	110.10
1	C	167	LEU	CA-CB-CG	-7.44	98.19	115.30
1	D	45	GLN	CG-CD-OE1	-7.42	106.77	121.60
1	A	289	ARG	CD-NE-CZ	7.39	133.94	123.60
1	B	170	LEU	CA-C-O	7.38	135.60	120.10
1	B	277	ALA	N-CA-C	7.38	130.91	111.00
1	B	40	TYR	CB-CG-CD1	7.34	125.41	121.00
1	C	164	SER	CB-CA-C	-7.34	96.15	110.10
1	A	172	GLU	OE1-CD-OE2	-7.32	114.51	123.30
1	B	73	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	D	253	VAL	CB-CA-C	-7.29	97.55	111.40
1	B	108	VAL	CA-CB-CG2	7.29	121.83	110.90
1	A	356	GLU	OE1-CD-OE2	-7.29	114.56	123.30
1	A	151	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	D	385	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	183	GLU	CG-CD-OE2	-7.27	103.76	118.30
1	B	123	VAL	CA-CB-CG2	-7.26	100.01	110.90
1	D	73	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	243	ALA	N-CA-CB	-7.22	100.00	110.10
1	C	334	ARG	NE-CZ-NH1	7.21	123.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	403	GLU	O-C-N	7.21	134.24	122.70
1	B	46	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	C	28	MET	CA-CB-CG	-7.20	101.06	113.30
1	C	92	THR	N-CA-CB	-7.19	96.65	110.30
1	C	43	HIS	CB-CG-ND1	7.17	141.12	123.20
1	B	385	ARG	NH1-CZ-NH2	7.13	127.24	119.40
1	C	357	ALA	O-C-N	7.12	134.10	122.70
1	D	427	ASP	OD1-CG-OD2	-7.12	109.78	123.30
1	C	337	ARG	NH1-CZ-NH2	7.12	127.23	119.40
1	D	110	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	B	170	LEU	O-C-N	-7.10	111.34	122.70
1	D	123	VAL	CG1-CB-CG2	7.09	122.25	110.90
1	C	151	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	210	HIS	CB-CG-ND1	7.07	140.86	123.20
1	D	155	ASN	OD1-CG-ND2	7.06	138.15	121.90
1	A	171	ALA	O-C-N	-7.05	111.42	122.70
1	C	145	LYS	CD-CE-NZ	-7.03	95.53	111.70
1	C	107	ALA	N-CA-CB	-7.03	100.26	110.10
1	C	39	ASP	CB-CG-OD2	7.03	124.63	118.30
1	C	360	ARG	CG-CD-NE	-7.03	97.04	111.80
1	C	335	THR	CA-CB-CG2	-7.02	102.57	112.40
1	B	263	MET	CA-CB-CG	7.01	125.22	113.30
1	D	255	GLU	OE1-CD-OE2	6.99	131.69	123.30
1	B	225	GLU	OE1-CD-OE2	6.98	131.68	123.30
1	D	307	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	B	6	ILE	O-C-N	6.97	133.85	122.70
1	C	138	GLU	CB-CG-CD	6.97	133.02	114.20
1	C	334	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	282	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	B	123	VAL	O-C-N	6.94	133.81	122.70
1	A	335	THR	CA-CB-CG2	-6.93	102.70	112.40
1	D	54	MET	CG-SD-CE	-6.91	89.15	100.20
1	B	364	GLU	OE1-CD-OE2	6.90	131.58	123.30
1	D	170	LEU	CA-CB-CG	6.90	131.16	115.30
1	B	173	LYS	CB-CG-CD	6.89	129.52	111.60
1	A	169	ALA	N-CA-CB	-6.88	100.47	110.10
1	C	277	ALA	N-CA-C	6.87	129.55	111.00
1	B	187	ASP	CB-CG-OD1	6.87	124.48	118.30
1	D	447	ASP	CA-CB-CG	6.85	128.47	113.40
1	C	370	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	D	262	MET	CG-SD-CE	6.83	111.13	100.20
1	C	144	CYS	CB-CA-C	6.82	124.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	SER	O-C-N	6.80	133.58	122.70
1	C	168	PRO	N-CA-CB	6.80	111.46	103.30
1	C	385	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	170	LEU	N-CA-CB	-6.79	96.81	110.40
1	A	42	GLU	N-CA-CB	6.78	122.81	110.60
1	D	127	ASP	N-CA-CB	6.78	122.80	110.60
1	D	15	GLU	OE1-CD-OE2	-6.75	115.20	123.30
1	D	32	ARG	NH1-CZ-NH2	-6.75	111.98	119.40
1	C	111	GLU	N-CA-CB	6.74	122.74	110.60
1	C	278	THR	N-CA-CB	-6.74	97.49	110.30
1	A	307	ASP	CB-CG-OD1	-6.74	112.23	118.30
1	A	292	ARG	CA-CB-CG	6.74	128.22	113.40
1	C	127	ASP	CB-CG-OD2	6.72	124.35	118.30
1	C	174	ASP	CB-CA-C	6.71	123.83	110.40
1	C	186	VAL	CA-CB-CG1	-6.71	100.84	110.90
1	A	268	ILE	O-C-N	6.71	133.43	122.70
1	D	140	ASN	N-CA-CB	-6.71	98.53	110.60
1	B	172	GLU	CA-C-O	-6.70	106.03	120.10
1	D	206	HIS	N-CA-CB	-6.70	98.54	110.60
1	C	269	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	40	TYR	CB-CG-CD1	6.69	125.01	121.00
1	A	284	MET	CG-SD-CE	6.67	110.88	100.20
1	A	336	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	D	244	ARG	CD-NE-CZ	6.66	132.92	123.60
1	B	293	ALA	N-CA-CB	6.66	119.42	110.10
1	D	149	ASN	OD1-CG-ND2	6.65	137.19	121.90
1	A	183	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	C	154	GLU	CB-CA-C	6.63	123.66	110.40
1	B	146	VAL	CA-CB-CG2	-6.63	100.96	110.90
1	D	395	THR	CA-CB-OG1	-6.63	95.08	109.00
1	C	54	MET	CG-SD-CE	-6.61	89.63	100.20
1	C	73	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	B	444	HIS	CA-CB-CG	-6.60	102.39	113.60
1	A	306	THR	O-C-N	-6.59	112.15	122.70
1	C	171	ALA	N-CA-CB	-6.57	100.90	110.10
1	B	382	LYS	CD-CE-NZ	6.56	126.78	111.70
1	C	259	ALA	CB-CA-C	6.54	119.92	110.10
1	B	123	VAL	CA-C-O	-6.54	106.36	120.10
1	D	179	ILE	CB-CG1-CD1	6.53	132.18	113.90
1	B	71	GLU	N-CA-CB	-6.52	98.86	110.60
1	A	436	LEU	CB-CA-C	6.51	122.57	110.20
1	C	284	MET	CG-SD-CE	6.51	110.62	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	321	PRO	N-CD-CG	-6.51	93.43	103.20
1	D	292	ARG	CD-NE-CZ	6.51	132.72	123.60
1	A	126	ASP	N-CA-CB	6.51	122.31	110.60
1	A	236	ALA	CA-C-N	6.50	131.51	117.20
1	A	334	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	230	PHE	O-C-N	-6.50	112.31	122.70
1	B	66	ASP	CA-C-O	-6.49	106.47	120.10
1	A	292	ARG	CD-NE-CZ	6.49	132.68	123.60
1	D	67	THR	N-CA-CB	6.47	122.60	110.30
1	A	110	TYR	CA-C-N	-6.46	102.98	117.20
1	C	87	ALA	CB-CA-C	-6.46	100.41	110.10
1	B	216	HIS	CG-ND1-CE1	6.45	117.23	108.20
1	D	164	SER	CB-CA-C	-6.45	97.85	110.10
1	D	28	MET	CA-CB-CG	-6.45	102.34	113.30
1	C	197	ARG	CD-NE-CZ	-6.43	114.60	123.60
1	C	92	THR	OG1-CB-CG2	6.43	124.78	110.00
1	D	73	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	455	ALA	CB-CA-C	6.42	119.73	110.10
1	D	190	ALA	N-CA-CB	6.42	119.09	110.10
1	B	224	GLN	CG-CD-OE1	6.40	134.40	121.60
1	A	95	THR	N-CA-CB	6.39	122.44	110.30
1	A	400	THR	CA-CB-CG2	6.39	121.34	112.40
1	C	210	HIS	O-C-N	-6.39	112.34	123.20
1	C	370	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	199	ASP	O-C-N	-6.38	112.49	122.70
1	B	264	ILE	O-C-N	-6.38	112.49	122.70
1	C	32	ARG	CD-NE-CZ	6.38	132.53	123.60
1	A	51	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	B	336	ASP	CA-CB-CG	6.35	127.36	113.40
1	B	222	GLU	CG-CD-OE1	6.35	130.99	118.30
1	B	282	ASP	CB-CG-OD1	6.35	124.01	118.30
1	D	304	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	B	140	ASN	N-CA-CB	-6.34	99.19	110.60
1	D	14	THR	CA-CB-CG2	-6.33	103.53	112.40
1	C	98	SER	CA-CB-OG	6.33	128.30	111.20
1	C	231	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	354	ILE	N-CA-CB	6.33	125.36	110.80
1	B	336	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	A	132	MET	CG-SD-CE	6.31	110.29	100.20
1	A	427	ASP	CB-CG-OD1	6.31	123.98	118.30
1	C	364	GLU	OE1-CD-OE2	6.30	130.86	123.30
1	C	257	ILE	O-C-N	6.30	132.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	127	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	D	320	TYR	CG-CD1-CE1	-6.29	116.27	121.30
1	D	389	LYS	CD-CE-NZ	-6.29	97.23	111.70
1	D	370	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	C	389	LYS	O-C-N	-6.28	112.66	122.70
1	C	385	ARG	CG-CD-NE	-6.27	98.64	111.80
1	B	1	MET	CB-CG-SD	6.26	131.18	112.40
1	B	186	VAL	CA-CB-CG1	-6.26	101.51	110.90
1	A	197	ARG	NH1-CZ-NH2	6.25	126.28	119.40
1	D	52	ASN	CA-CB-CG	-6.25	99.65	113.40
1	B	87	ALA	N-CA-CB	-6.25	101.36	110.10
1	D	400	THR	O-C-N	6.24	132.69	122.70
1	B	195	ARG	CG-CD-NE	6.24	124.91	111.80
1	D	241	MET	CG-SD-CE	6.24	110.19	100.20
1	D	294	GLU	CA-CB-CG	6.24	127.13	113.40
1	A	217	ILE	O-C-N	6.24	132.68	122.70
1	B	155	ASN	CB-CG-OD1	-6.23	109.14	121.60
1	B	49	ASN	O-C-N	6.22	132.65	122.70
1	D	339	MET	CG-SD-CE	6.21	110.14	100.20
1	C	187	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	387	VAL	CG1-CB-CG2	6.21	120.83	110.90
1	C	110	TYR	CA-C-O	6.21	133.13	120.10
1	A	216	HIS	ND1-CG-CD2	-6.20	97.32	106.00
1	D	218	ILE	O-C-N	6.20	132.62	122.70
1	B	292	ARG	CD-NE-CZ	6.19	132.27	123.60
1	D	307	ASP	OD1-CG-OD2	6.19	135.07	123.30
1	A	40	TYR	CB-CG-CD2	-6.19	117.28	121.00
1	C	97	LYS	N-CA-CB	6.18	121.73	110.60
1	A	87	ALA	N-CA-CB	-6.18	101.44	110.10
1	A	238	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	B	320	TYR	CD1-CG-CD2	6.17	124.69	117.90
1	C	97	LYS	CA-CB-CG	6.17	126.96	113.40
1	D	205	GLU	OE1-CD-OE2	6.15	130.68	123.30
1	C	25	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	52	ASN	CA-CB-CG	-6.13	99.92	113.40
1	D	78	GLU	OE1-CD-OE2	6.12	130.65	123.30
1	B	52	ASN	CA-CB-CG	-6.12	99.94	113.40
1	D	197	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	B	269	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	1	MET	CB-CG-SD	6.12	130.74	112.40
1	C	453	SER	CB-CA-C	-6.12	98.48	110.10
1	C	105	MET	CA-CB-CG	6.11	123.68	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ILE	CA-C-O	-6.10	107.28	120.10
1	B	123	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	A	177	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	320	TYR	CG-CD1-CE1	-6.06	116.45	121.30
1	C	250	GLU	N-CA-CB	-6.06	99.69	110.60
1	A	195	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	32	ARG	CD-NE-CZ	6.05	132.07	123.60
1	B	262	MET	CG-SD-CE	6.05	109.88	100.20
1	D	169	ALA	N-CA-CB	-6.05	101.63	110.10
1	B	210	HIS	CG-ND1-CE1	6.04	116.66	108.20
1	C	269	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	162	GLY	CA-C-O	-6.03	109.75	120.60
1	B	51	ARG	CD-NE-CZ	6.01	132.02	123.60
1	D	325	VAL	CA-CB-CG2	-6.00	101.89	110.90
1	A	32	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	449	VAL	CA-C-N	6.00	130.39	117.20
1	C	142	VAL	CA-C-N	-6.00	104.01	117.20
1	C	439	GLN	N-CA-CB	6.00	121.39	110.60
1	D	307	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	321	PRO	N-CD-CG	-5.99	94.21	103.20
1	B	322	LEU	O-C-N	-5.98	113.13	122.70
1	A	190	ALA	CA-C-O	-5.98	107.54	120.10
1	D	470	LEU	CA-C-O	-5.98	107.54	120.10
1	B	105	MET	O-C-N	5.98	132.27	122.70
1	C	151	ASP	CB-CG-OD1	5.97	123.68	118.30
1	D	145	LYS	CD-CE-NZ	5.97	125.44	111.70
1	A	388	ARG	CG-CD-NE	5.97	124.34	111.80
1	C	190	ALA	N-CA-CB	5.97	118.45	110.10
1	C	395	THR	CA-CB-OG1	-5.96	96.48	109.00
1	D	216	HIS	CG-ND1-CE1	5.96	116.54	108.20
1	D	289	ARG	CD-NE-CZ	5.95	131.93	123.60
1	B	163	VAL	CB-CA-C	-5.94	100.12	111.40
1	C	398	ALA	N-CA-CB	5.93	118.41	110.10
1	A	422	GLU	O-C-N	5.93	132.19	122.70
1	C	52	ASN	CA-CB-CG	-5.92	100.37	113.40
1	C	389	LYS	CD-CE-NZ	-5.92	98.08	111.70
1	B	60	THR	CA-CB-CG2	-5.92	104.12	112.40
1	B	321	PRO	N-CD-CG	-5.92	94.32	103.20
1	D	93	PHE	CG-CD1-CE1	-5.91	114.30	120.80
1	D	186	VAL	O-C-N	-5.91	113.24	122.70
1	D	78	GLU	CG-CD-OE2	-5.89	106.52	118.30
1	D	152	LEU	CA-CB-CG	-5.89	101.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	254	GLU	OE1-CD-OE2	5.89	130.36	123.30
1	C	361	GLY	O-C-N	5.89	132.12	122.70
1	D	119	VAL	CB-CA-C	-5.88	100.22	111.40
1	D	324	ALA	N-CA-CB	5.88	118.34	110.10
1	B	277	ALA	CA-C-O	-5.88	107.75	120.10
1	A	238	ASP	CA-CB-CG	-5.88	100.47	113.40
1	D	225	GLU	N-CA-CB	-5.88	100.02	110.60
1	A	231	ASP	CB-CG-OD1	-5.87	113.01	118.30
1	A	342	ARG	CB-CG-CD	5.87	126.87	111.60
1	C	46	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	C	1	MET	CB-CG-SD	5.86	129.99	112.40
1	D	382	LYS	CD-CE-NZ	5.86	125.17	111.70
1	A	28	MET	CA-CB-CG	-5.86	103.34	113.30
1	A	231	ASP	C-N-CA	-5.85	107.06	121.70
1	D	161	PRO	N-CA-CB	5.85	110.32	103.30
1	C	263	MET	CA-CB-CG	5.85	123.24	113.30
1	C	398	ALA	CB-CA-C	-5.84	101.33	110.10
1	A	26	ALA	CA-C-O	-5.84	107.83	120.10
1	A	62	ALA	CB-CA-C	5.84	118.86	110.10
1	B	294	GLU	CA-CB-CG	5.83	126.24	113.40
1	D	66	ASP	CA-C-O	-5.83	107.85	120.10
1	D	173	LYS	O-C-N	-5.83	113.38	122.70
1	D	173	LYS	CA-C-N	5.82	130.01	117.20
1	C	110	TYR	CA-C-N	-5.81	104.42	117.20
1	C	320	TYR	CG-CD2-CE2	-5.81	116.66	121.30
1	A	66	ASP	CA-C-O	-5.80	107.92	120.10
1	C	63	ILE	O-C-N	5.80	131.98	122.70
1	A	232	GLU	CG-CD-OE2	-5.79	106.71	118.30
1	B	339	MET	O-C-N	-5.79	113.43	122.70
1	B	254	GLU	CA-C-O	-5.79	107.94	120.10
1	B	167	LEU	CA-C-O	5.79	132.25	120.10
1	B	224	GLN	CA-C-O	-5.79	107.94	120.10
1	C	238	ASP	OD1-CG-OD2	5.79	134.29	123.30
1	D	150	GLY	O-C-N	5.78	131.95	122.70
1	D	311	LEU	CA-C-O	5.78	132.23	120.10
1	B	44	GLY	O-C-N	5.76	131.92	122.70
1	D	73	ARG	CG-CD-NE	5.76	123.89	111.80
1	C	388	ARG	CB-CG-CD	5.75	126.56	111.60
1	A	236	ALA	CA-C-O	-5.75	108.02	120.10
1	C	289	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	C	142	VAL	CA-CB-CG1	-5.75	102.28	110.90
1	C	210	HIS	CG-ND1-CE1	5.74	116.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	402	ASN	N-CA-CB	-5.74	100.27	110.60
1	D	127	ASP	CB-CG-OD1	5.73	123.45	118.30
1	C	361	GLY	CA-C-O	-5.73	110.29	120.60
1	C	447	ASP	CA-CB-CG	5.72	125.99	113.40
1	A	233	ILE	CA-CB-CG2	5.72	122.33	110.90
1	A	71	GLU	CA-CB-CG	5.71	125.96	113.40
1	B	19	MET	N-CA-CB	-5.71	100.33	110.60
1	B	49	ASN	CB-CA-C	-5.70	98.99	110.40
1	B	95	THR	N-CA-CB	5.70	121.12	110.30
1	D	453	SER	N-CA-CB	-5.70	101.95	110.50
1	B	180	PHE	O-C-N	5.70	132.88	123.20
1	C	391	PHE	CZ-CE2-CD2	-5.68	113.29	120.10
1	D	232	GLU	CB-CA-C	5.67	121.75	110.40
1	B	162	GLY	CA-C-O	-5.67	110.39	120.60
1	B	156	LYS	CA-CB-CG	-5.67	100.93	113.40
1	C	292	ARG	CD-NE-CZ	5.67	131.53	123.60
1	A	187	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	190	ALA	N-CA-CB	5.66	118.03	110.10
1	C	143	ILE	N-CA-CB	-5.66	97.78	110.80
1	D	404	LYS	CB-CG-CD	5.66	126.31	111.60
1	B	223	ASN	CA-C-N	-5.66	104.76	117.20
1	C	194	ILE	CA-CB-CG1	-5.66	100.25	111.00
1	C	242	VAL	CG1-CB-CG2	5.65	119.95	110.90
1	C	110	TYR	CB-CG-CD2	5.65	124.39	121.00
1	D	193	PHE	CB-CG-CD1	5.65	124.75	120.80
1	C	357	ALA	N-CA-CB	5.64	118.00	110.10
1	D	115	THR	N-CA-CB	-5.64	99.58	110.30
1	C	5	LYS	CD-CE-NZ	5.64	124.67	111.70
1	C	73	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	434	LYS	CB-CG-CD	5.63	126.25	111.60
1	D	282	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	99	VAL	CA-C-O	5.62	131.91	120.10
1	C	138	GLU	CG-CD-OE2	5.62	129.55	118.30
1	D	178	LEU	CB-CG-CD2	5.62	120.56	111.00
1	D	388	ARG	CA-CB-CG	5.62	125.76	113.40
1	A	360	ARG	CG-CD-NE	-5.61	100.02	111.80
1	A	253	VAL	CB-CA-C	-5.61	100.74	111.40
1	D	155	ASN	CB-CG-OD1	-5.61	110.38	121.60
1	B	405	THR	CA-CB-CG2	-5.61	104.55	112.40
1	A	246	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	30	VAL	CB-CA-C	-5.59	100.78	111.40
1	A	19	MET	N-CA-CB	-5.58	100.55	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	436	LEU	N-CA-CB	-5.58	99.23	110.40
1	C	400	THR	O-C-N	5.57	131.62	122.70
1	D	133	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	C	67	THR	OG1-CB-CG2	5.57	122.81	110.00
1	A	250	GLU	N-CA-CB	-5.57	100.58	110.60
1	C	133	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	A	390	TYR	CG-CD2-CE2	-5.56	116.85	121.30
1	C	73	ARG	NH1-CZ-NH2	5.56	125.52	119.40
1	B	32	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	16	SER	O-C-N	-5.55	113.82	122.70
1	C	246	ASP	OD1-CG-OD2	-5.55	112.75	123.30
1	B	383	SER	CB-CA-C	5.54	120.64	110.10
1	A	30	VAL	O-C-N	5.54	131.57	122.70
1	D	118	SER	N-CA-CB	-5.54	102.19	110.50
1	D	331	ILE	CB-CA-C	-5.54	100.52	111.60
1	A	225	GLU	CG-CD-OE2	-5.54	107.23	118.30
1	A	73	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	395	THR	CA-CB-OG1	-5.53	97.39	109.00
1	D	265	GLU	CA-CB-CG	5.53	125.56	113.40
1	B	167	LEU	CB-CA-C	-5.52	99.71	110.20
1	B	388	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	9	THR	CA-CB-CG2	-5.52	104.68	112.40
1	D	254	GLU	CA-C-O	-5.51	108.52	120.10
1	B	124	LEU	CA-CB-CG	5.51	127.97	115.30
1	C	297	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	64	LEU	CB-CG-CD1	-5.50	101.64	111.00
1	D	469	VAL	CA-C-O	-5.50	108.54	120.10
1	D	99	VAL	CG1-CB-CG2	5.50	119.69	110.90
1	B	3	LYS	O-C-N	5.50	131.49	122.70
1	A	78	GLU	CB-CA-C	-5.49	99.42	110.40
1	A	268	ILE	CA-C-O	-5.49	108.57	120.10
1	C	87	ALA	N-CA-CB	5.49	117.78	110.10
1	A	3	LYS	O-C-N	5.48	131.47	122.70
1	A	389	LYS	CD-CE-NZ	-5.48	99.10	111.70
1	C	257	ILE	N-CA-CB	5.48	123.41	110.80
1	B	86	LYS	CB-CA-C	5.48	121.36	110.40
1	D	175	LYS	O-C-N	5.48	131.46	122.70
1	A	418	GLN	CG-CD-OE1	5.48	132.55	121.60
1	B	193	PHE	CB-CG-CD2	5.48	124.63	120.80
1	B	360	ARG	CG-CD-NE	-5.47	100.30	111.80
1	D	4	THR	CA-CB-CG2	5.47	120.06	112.40
1	C	92	THR	CB-CA-C	5.46	126.33	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	297	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	322	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	C	62	ALA	CB-CA-C	5.45	118.28	110.10
1	A	207	LEU	O-C-N	5.45	131.42	122.70
1	A	295	ALA	N-CA-CB	5.45	117.73	110.10
1	A	66	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	192	SER	CA-CB-OG	5.44	125.89	111.20
1	B	146	VAL	O-C-N	5.44	131.40	122.70
1	A	277	ALA	CA-C-O	-5.43	108.69	120.10
1	D	259	ALA	CB-CA-C	5.43	118.25	110.10
1	C	431	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	420	VAL	CA-CB-CG1	5.42	119.03	110.90
1	B	388	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	216	HIS	CE1-NE2-CD2	-5.41	93.07	106.60
1	D	202	GLU	CG-CD-OE2	5.41	129.11	118.30
1	D	320	TYR	CD1-CG-CD2	5.41	123.85	117.90
1	D	60	THR	OG1-CB-CG2	5.40	122.42	110.00
1	D	257	ILE	CB-CG1-CD1	-5.40	98.78	113.90
1	A	435	GLU	CG-CD-OE2	-5.40	107.51	118.30
1	C	171	ALA	CB-CA-C	5.39	118.19	110.10
1	D	60	THR	CA-CB-CG2	-5.39	104.86	112.40
1	A	116	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	17	GLU	CA-C-N	-5.38	105.35	117.20
1	D	151	ASP	OD1-CG-OD2	5.38	133.53	123.30
1	D	422	GLU	O-C-N	5.38	131.30	122.70
1	B	126	ASP	OD1-CG-OD2	-5.37	113.09	123.30
1	A	78	GLU	CB-CG-CD	5.37	128.71	114.20
1	C	245	GLY	O-C-N	-5.37	114.11	122.70
1	D	301	ALA	CB-CA-C	5.36	118.15	110.10
1	B	278	THR	N-CA-CB	-5.36	100.11	110.30
1	C	196	LYS	CB-CG-CD	5.36	125.53	111.60
1	C	289	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	86	LYS	N-CA-CB	-5.36	100.96	110.60
1	C	170	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	D	228	ASN	O-C-N	-5.35	114.15	122.70
1	D	256	VAL	O-C-N	-5.34	114.15	122.70
1	D	63	ILE	C-N-CA	5.34	135.05	121.70
1	D	15	GLU	CG-CD-OE1	5.34	128.97	118.30
1	A	356	GLU	CA-CB-CG	5.33	125.13	113.40
1	A	390	TYR	CA-CB-CG	-5.33	103.28	113.40
1	B	54	MET	CG-SD-CE	-5.33	91.68	100.20
1	A	151	ASP	CB-CG-OD1	5.33	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	LEU	CB-CG-CD1	5.32	120.05	111.00
1	D	277	ALA	CA-C-O	-5.32	108.93	120.10
1	C	277	ALA	CA-C-O	-5.31	108.94	120.10
1	C	124	LEU	O-C-N	5.31	131.20	122.70
1	C	142	VAL	O-C-N	5.31	131.20	122.70
1	C	42	GLU	N-CA-CB	5.31	120.16	110.60
1	A	225	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	B	213	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	D	257	ILE	N-CA-CB	5.30	123.00	110.80
1	C	142	VAL	CA-CB-CG2	5.30	118.85	110.90
1	B	136	ALA	O-C-N	-5.29	114.24	122.70
1	C	295	ALA	N-CA-CB	5.29	117.50	110.10
1	B	257	ILE	N-CA-CB	5.28	122.95	110.80
1	B	242	VAL	CG1-CB-CG2	5.28	119.35	110.90
1	C	434	LYS	CD-CE-NZ	5.28	123.84	111.70
1	D	330	THR	CA-CB-OG1	5.28	120.08	109.00
1	B	206	HIS	CB-CA-C	5.27	120.94	110.40
1	C	110	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	B	111	GLU	N-CA-CB	-5.26	101.12	110.60
1	C	425	SER	N-CA-CB	-5.26	102.61	110.50
1	A	199	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	249	VAL	CA-C-O	5.26	131.15	120.10
1	C	418	GLN	CA-C-O	5.26	131.15	120.10
1	A	179	ILE	CA-CB-CG1	-5.25	101.02	111.00
1	B	132	MET	CA-CB-CG	-5.25	104.38	113.30
1	C	92	THR	CA-C-N	-5.25	105.65	117.20
1	B	156	LYS	CA-C-N	-5.24	105.73	116.20
1	B	299	ALA	N-CA-CB	-5.23	102.77	110.10
1	A	154	GLU	CB-CA-C	-5.23	99.94	110.40
1	D	413	LYS	CB-CG-CD	5.22	125.18	111.60
1	D	6	ILE	O-C-N	5.21	131.04	122.70
1	D	43	HIS	ND1-CG-CD2	-5.21	98.70	106.00
1	A	216	HIS	O-C-N	5.20	131.02	122.70
1	C	30	VAL	O-C-N	5.20	131.01	122.70
1	D	33	LEU	O-C-N	5.20	131.01	122.70
1	C	427	ASP	OD1-CG-OD2	-5.19	113.43	123.30
1	C	262	MET	CA-CB-CG	5.19	122.13	113.30
1	A	184	GLN	C-N-CA	-5.19	111.41	122.30
1	A	74	THR	CA-CB-CG2	5.18	119.66	112.40
1	C	42	GLU	O-C-N	5.18	131.00	122.70
1	B	388	ARG	CA-CB-CG	5.18	124.80	113.40
1	C	238	ASP	CA-CB-CG	-5.18	102.01	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	257	ILE	CB-CA-C	-5.18	101.25	111.60
1	D	336	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	B	434	LYS	CB-CG-CD	5.17	125.05	111.60
1	C	106	VAL	CA-C-N	-5.17	105.83	117.20
1	D	205	GLU	CA-CB-CG	-5.17	102.03	113.40
1	C	231	ASP	OD1-CG-OD2	-5.17	113.48	123.30
1	D	165	ILE	CA-CB-CG1	-5.17	101.18	111.00
1	C	292	ARG	CA-CB-CG	5.17	124.76	113.40
1	D	155	ASN	N-CA-CB	-5.16	101.31	110.60
1	D	186	VAL	CA-CB-CG1	-5.16	103.16	110.90
1	B	178	LEU	CB-CG-CD2	5.16	119.77	111.00
1	B	273	VAL	O-C-N	5.16	130.95	122.70
1	D	225	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	257	ILE	CB-CA-C	-5.15	101.29	111.60
1	C	388	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	116	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	365	THR	O-C-N	5.15	130.94	122.70
1	B	174	ASP	OD1-CG-OD2	-5.15	113.52	123.30
1	B	210	HIS	ND1-CG-CD2	-5.14	98.81	106.00
1	D	11	GLY	CA-C-O	5.14	129.85	120.60
1	D	150	GLY	CA-C-O	-5.14	111.36	120.60
1	D	46	ARG	CD-NE-CZ	-5.13	116.41	123.60
1	D	434	LYS	CB-CG-CD	5.13	124.94	111.60
1	B	132	MET	CB-CG-SD	-5.13	97.02	112.40
1	D	302	ILE	O-C-N	-5.13	114.50	122.70
1	D	51	ARG	CD-NE-CZ	5.13	130.78	123.60
1	B	164	SER	CB-CA-C	-5.12	100.36	110.10
1	A	133	GLU	CB-CA-C	5.12	120.64	110.40
1	C	8	CYS	CA-C-O	-5.12	109.34	120.10
1	A	159	ASN	OD1-CG-ND2	5.12	133.67	121.90
1	B	110	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	241	MET	CG-SD-CE	5.12	108.39	100.20
1	D	339	MET	O-C-N	-5.11	114.52	122.70
1	C	143	ILE	CA-CB-CG1	-5.11	101.30	111.00
1	C	181	GLY	CA-C-O	5.11	129.79	120.60
1	A	278	THR	N-CA-CB	-5.10	100.60	110.30
1	A	141	LYS	CB-CG-CD	5.10	124.86	111.60
1	D	49	ASN	O-C-N	5.10	130.86	122.70
1	C	17	GLU	O-C-N	5.09	130.85	122.70
1	C	452	VAL	CB-CA-C	-5.09	101.72	111.40
1	D	449	VAL	N-CA-CB	-5.09	100.30	111.50
1	B	269	ARG	CD-NE-CZ	5.09	130.72	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	282	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	173	LYS	CA-C-N	-5.09	106.01	117.20
1	C	388	ARG	CG-CD-NE	5.08	122.46	111.80
1	B	191	ALA	O-C-N	-5.07	114.58	122.70
1	A	197	ARG	CD-NE-CZ	-5.07	116.50	123.60
1	B	412	SER	O-C-N	5.07	130.81	122.70
1	C	256	VAL	CA-C-O	-5.07	109.46	120.10
1	D	151	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	280	MET	CA-C-N	5.06	128.34	117.20
1	A	47	ILE	CA-CB-CG1	-5.06	101.39	111.00
1	D	277	ALA	CB-CA-C	-5.06	102.52	110.10
1	C	360	ARG	NH1-CZ-NH2	5.05	124.96	119.40
1	B	155	ASN	OD1-CG-ND2	5.05	133.52	121.90
1	C	437	ALA	CA-C-O	5.05	130.71	120.10
1	B	172	GLU	CA-C-N	5.05	128.31	117.20
1	B	403	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	C	8	CYS	O-C-N	5.05	130.78	122.70
1	A	143	ILE	CA-CB-CG1	-5.04	101.42	111.00
1	A	336	ASP	OD1-CG-OD2	5.04	132.88	123.30
1	A	4	THR	O-C-N	5.04	130.76	122.70
1	A	237	SER	N-CA-CB	-5.04	102.94	110.50
1	A	197	ARG	CA-CB-CG	5.04	124.48	113.40
1	C	360	ARG	CA-C-N	-5.03	106.13	116.20
1	D	60	THR	CB-CA-C	-5.03	98.01	111.60
1	B	99	VAL	CB-CA-C	5.03	120.96	111.40
1	B	274	VAL	CA-C-O	5.03	130.67	120.10
1	D	49	ASN	CB-CG-OD1	5.03	131.66	121.60
1	C	175	LYS	N-CA-CB	5.03	119.65	110.60
1	D	311	LEU	O-C-N	-5.03	114.66	122.70
1	C	60	THR	CB-CA-C	-5.02	98.03	111.60
1	B	389	LYS	CB-CA-C	-5.02	100.36	110.40
1	D	100	ILE	CA-CB-CG1	-5.02	101.46	111.00
1	D	457	VAL	CA-CB-CG2	5.02	118.43	110.90
1	A	361	GLY	CA-C-O	-5.02	111.56	120.60
1	B	155	ASN	N-CA-CB	-5.02	101.57	110.60
1	C	50	LEU	O-C-N	5.02	130.73	122.70
1	D	250	GLU	OE1-CD-OE2	5.01	129.32	123.30
1	A	78	GLU	CG-CD-OE2	-5.01	108.28	118.30
1	A	168	PRO	N-CA-CB	5.01	109.31	103.30
1	D	320	TYR	CA-CB-CG	-5.00	103.89	113.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ASP	Mainchain
1	A	277	ALA	Mainchain
1	B	2	LYS	Mainchain
1	B	223	ASN	Mainchain
1	B	277	ALA	Mainchain
1	B	28	MET	Mainchain
1	C	104	GLU	Sidechain
1	C	138	GLU	Sidechain
1	C	277	ALA	Mainchain
1	D	277	ALA	Mainchain
1	D	3	LYS	Mainchain
1	D	30	VAL	Mainchain
1	D	410	VAL	Mainchain
1	D	452	VAL	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	A	3445	0	3533	176	0
1	B	3445	0	3533	134	0
1	C	3445	0	3533	300	1
1	D	3445	0	3533	142	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	38	0	0	4	0
3	B	55	0	0	2	0
3	C	48	0	0	10	0
3	D	59	0	0	5	0
All	All	14000	0	14132	736	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (736) 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:C:92:THR:HG22	1:C:105:MET:SD	1.35	1.62
1:C:136:ALA:CB	1:C:143:ILE:CG2	1.82	1.58
1:C:77:LEU:CD1	1:C:154:GLU:HB3	1.33	1.58
1:C:136:ALA:CB	1:C:143:ILE:HG21	1.36	1.51
1:C:92:THR:CG2	1:C:105:MET:SD	2.05	1.45
1:C:136:ALA:HB3	1:C:143:ILE:CG2	0.94	1.41
1:A:88:GLY:HA2	1:A:145:LYS:CE	1.49	1.40
1:A:88:GLY:CA	1:A:145:LYS:HE3	1.52	1.39
1:C:92:THR:O	1:C:105:MET:HB2	1.31	1.26
1:C:106:VAL:CG2	1:C:107:ALA:H	1.36	1.25
1:C:119:VAL:HA	1:C:134:VAL:CG1	1.67	1.24
1:C:137:ILE:CG1	1:C:142:VAL:HG13	1.68	1.21
1:C:197:ARG:HB3	1:C:232:GLU:HG3	1.19	1.19
1:C:106:VAL:HG22	1:C:107:ALA:N	1.38	1.17
1:C:92:THR:OG1	1:C:143:ILE:HA	1.46	1.16
1:D:354:ILE:N	3:D:2048:HOH:O	1.76	1.14
1:C:137:ILE:HG13	1:C:142:VAL:HG13	1.26	1.12
1:C:77:LEU:HD11	1:C:154:GLU:HB3	1.22	1.12
1:C:77:LEU:CD1	1:C:154:GLU:CB	2.30	1.10
1:C:165:ILE:HG22	1:C:167:LEU:H	1.10	1.10
1:C:77:LEU:HD12	1:C:154:GLU:CB	1.81	1.09
1:B:70:PRO:HB2	1:B:167:LEU:HD13	1.25	1.09
1:A:170:LEU:HD22	1:A:174:ASP:HB3	1.33	1.06
1:C:136:ALA:CB	1:C:143:ILE:HG22	1.62	1.05
1:A:69:GLY:HA2	1:A:174:ASP:OD2	1.57	1.05
1:C:130:ILE:HG22	1:C:132:MET:HE2	1.35	1.04
1:D:10:ILE:HG12	1:D:31:MET:HG3	1.40	1.03
1:A:118:SER:N	1:A:121:ASN:OD1	1.90	1.03
1:C:113:PHE:CE1	1:C:117:LEU:CD2	2.43	1.02
1:A:99:VAL:HG11	1:A:105:MET:HE3	1.43	1.01
1:C:119:VAL:HA	1:C:134:VAL:HG12	1.01	1.01
1:C:137:ILE:CG1	1:C:142:VAL:CG1	2.39	1.00
1:C:137:ILE:HG12	1:C:142:VAL:CG1	1.92	1.00
1:D:80:GLY:HA2	1:D:154:GLU:OE2	1.60	0.99
1:C:90:THR:HG23	1:C:144:CYS:O	1.61	0.99
1:C:69:GLY:N	1:C:174:ASP:OD2	1.94	0.99
1:C:77:LEU:HD12	1:C:154:GLU:HB3	0.98	0.98
1:A:45:GLN:HB2	3:A:2007:HOH:O	1.63	0.97
1:C:73:ARG:HB2	1:C:109:THR:HG23	1.42	0.97
1:C:191:ALA:O	1:C:220:LYS:HG3	1.63	0.97
1:C:175:LYS:HG2	1:C:206:HIS:CE1	1.98	0.97
1:C:133:GLU:O	1:C:144:CYS:HB3	1.65	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:CD2	1:A:174:ASP:HB3	1.93	0.97
1:C:136:ALA:HB3	1:C:143:ILE:HG22	0.99	0.96
1:C:114:THR:HG22	1:C:137:ILE:HG21	1.47	0.96
1:D:140:ASN:OD1	1:D:141:LYS:HG3	1.64	0.96
1:C:204:ARG:NH2	1:C:238:ASP:OD2	1.99	0.95
1:C:114:THR:HG22	1:C:137:ILE:CG2	1.97	0.95
1:D:39:ASP:OD1	1:D:42:GLU:HG3	1.67	0.95
1:C:158:VAL:HG12	1:C:160:LEU:HD21	1.47	0.94
1:C:136:ALA:HB3	1:C:143:ILE:CB	1.97	0.94
1:C:137:ILE:HG12	1:C:142:VAL:HG22	1.46	0.94
1:C:159:ASN:C	1:C:160:LEU:HD23	1.89	0.93
1:C:113:PHE:CE1	1:C:117:LEU:HD21	2.04	0.93
1:C:113:PHE:HE1	1:C:117:LEU:HD21	1.33	0.92
1:C:251:ILE:HB	1:C:252:PRO:HD2	1.51	0.92
1:C:171:ALA:HB3	1:C:174:ASP:HB2	1.47	0.92
1:C:90:THR:CG2	1:C:144:CYS:O	2.17	0.92
1:C:130:ILE:HG22	1:C:132:MET:CE	1.99	0.92
1:C:354:ILE:N	3:C:2036:HOH:O	2.03	0.92
1:C:354:ILE:N	3:C:2035:HOH:O	2.01	0.90
1:A:51:ARG:HA	1:A:54:MET:HE3	1.51	0.90
1:B:14:THR:HG21	1:B:315:SER:O	1.73	0.89
1:C:133:GLU:O	1:C:144:CYS:CB	2.20	0.89
1:C:137:ILE:HG13	1:C:142:VAL:CG1	2.03	0.88
1:C:92:THR:O	1:C:105:MET:CB	2.21	0.88
1:C:137:ILE:HG12	1:C:142:VAL:CG2	2.03	0.87
1:C:136:ALA:HB2	1:C:143:ILE:HG21	1.52	0.87
1:C:152:LEU:HD12	1:C:153:GLY:O	1.75	0.87
1:C:159:ASN:O	1:C:160:LEU:HD23	1.75	0.87
1:C:202:GLU:CG	3:C:2016:HOH:O	2.23	0.87
1:C:137:ILE:HG23	1:C:141:LYS:O	1.74	0.86
1:D:87:ALA:HA	1:D:146:VAL:HG12	1.57	0.86
1:C:137:ILE:HG12	1:C:142:VAL:HG13	1.47	0.86
1:B:191:ALA:O	1:B:220:LYS:HG3	1.75	0.86
1:A:191:ALA:O	1:A:220:LYS:HG3	1.75	0.86
1:A:10:ILE:CG1	1:A:31:MET:HG3	2.06	0.85
1:B:97:LYS:NZ	1:B:109:THR:O	2.08	0.85
1:C:77:LEU:HD11	1:C:154:GLU:CB	2.01	0.85
1:C:165:ILE:HG22	1:C:167:LEU:N	1.91	0.85
1:D:402:ASN:ND2	1:D:405:THR:H	1.74	0.85
1:C:136:ALA:CA	1:C:143:ILE:HG22	2.07	0.84
1:A:204:ARG:NH2	1:A:238:ASP:OD2	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:HA2	1:A:154:GLU:OE2	1.77	0.84
1:C:170:LEU:O	1:C:175:LYS:HE3	1.77	0.83
1:C:73:ARG:HB2	1:C:109:THR:CG2	2.07	0.83
1:B:8:CYS:HB2	1:B:28:MET:HE3	1.60	0.83
1:C:10:ILE:HG12	1:C:31:MET:HG3	1.58	0.83
1:C:51:ARG:HA	1:C:54:MET:HE3	1.58	0.83
1:D:204:ARG:NH2	1:D:238:ASP:OD2	2.11	0.83
1:C:113:PHE:HE1	1:C:117:LEU:CD2	1.84	0.82
1:C:106:VAL:HG22	1:C:107:ALA:H	0.67	0.82
1:A:99:VAL:HG11	1:A:105:MET:CE	2.10	0.82
1:C:136:ALA:N	1:C:143:ILE:HG22	1.95	0.82
1:C:14:THR:HG21	1:C:315:SER:O	1.79	0.81
1:B:204:ARG:NH2	1:B:238:ASP:OD2	2.11	0.81
1:C:119:VAL:CA	1:C:134:VAL:CG1	2.57	0.81
1:C:119:VAL:CA	1:C:134:VAL:HG12	1.98	0.81
1:C:170:LEU:HD13	1:C:175:LYS:HG3	1.61	0.81
1:C:136:ALA:HB3	1:C:143:ILE:HG21	0.84	0.80
1:A:299:ALA:CB	1:C:257:ILE:HD11	2.12	0.80
1:B:80:GLY:HA2	1:B:154:GLU:OE2	1.80	0.80
1:C:136:ALA:HB2	1:C:143:ILE:CG2	2.09	0.80
1:A:10:ILE:HG12	1:A:31:MET:HG3	1.64	0.79
1:C:155:ASN:O	1:C:156:LYS:HD3	1.82	0.79
1:D:160:LEU:HD12	1:D:165:ILE:CD1	2.13	0.79
1:D:402:ASN:HD22	1:D:405:THR:H	1.29	0.78
1:B:10:ILE:HG12	1:B:31:MET:HG3	1.63	0.78
1:C:202:GLU:HG2	3:C:2016:HOH:O	1.82	0.77
1:C:173:LYS:N	3:C:2012:HOH:O	2.18	0.77
1:D:140:ASN:OD1	1:D:141:LYS:HE3	1.84	0.77
1:B:170:LEU:CD2	1:B:174:ASP:HB3	2.15	0.77
1:A:135:THR:OG1	1:A:143:ILE:HG22	1.85	0.77
1:B:10:ILE:CG1	1:B:31:MET:HG3	2.13	0.76
1:C:92:THR:HG1	1:C:143:ILE:HA	1.50	0.76
1:D:191:ALA:O	1:D:220:LYS:HG3	1.85	0.75
1:A:434:LYS:HG3	1:A:451:MET:CE	2.16	0.75
1:D:334:ARG:HD2	1:D:337:ARG:NH1	2.03	0.74
1:D:10:ILE:CG1	1:D:31:MET:HG3	2.17	0.74
1:A:117:LEU:HD12	1:A:121:ASN:OD1	1.88	0.74
1:C:142:VAL:HG12	1:C:143:ILE:H	1.52	0.73
1:D:50:LEU:HG	1:D:54:MET:HE1	1.68	0.73
1:C:142:VAL:HG12	1:C:143:ILE:N	2.02	0.73
1:C:158:VAL:CG1	1:C:160:LEU:HD21	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LYS:HG3	1:A:451:MET:HE3	1.71	0.73
1:C:197:ARG:HB3	1:C:232:GLU:CG	2.10	0.73
1:C:92:THR:HG21	1:C:105:MET:SD	2.25	0.73
1:A:171:ALA:HB3	1:A:174:ASP:CG	2.09	0.73
1:D:170:LEU:CD2	1:D:174:ASP:HB3	2.19	0.73
1:C:75:MET:HG3	1:C:107:ALA:HB3	1.70	0.72
1:C:113:PHE:CD1	1:C:117:LEU:CD2	2.72	0.72
1:C:244:ARG:NH1	1:C:278:THR:O	2.22	0.72
1:C:188:PHE:CD1	1:C:216:HIS:HB2	2.24	0.72
1:B:402:ASN:HD22	1:B:405:THR:H	1.38	0.72
1:A:171:ALA:O	1:A:174:ASP:HB2	1.90	0.72
1:B:402:ASN:ND2	1:B:405:THR:H	1.89	0.71
1:C:10:ILE:CG1	1:C:31:MET:HG3	2.20	0.71
1:C:86:LYS:O	1:C:89:GLN:HB3	1.91	0.71
1:C:106:VAL:HG22	1:C:107:ALA:CA	2.20	0.71
1:D:50:LEU:HG	1:D:54:MET:CE	2.20	0.71
1:C:119:VAL:HA	1:C:134:VAL:HG11	1.72	0.70
1:D:402:ASN:HA	3:D:2053:HOH:O	1.90	0.70
1:A:188:PHE:CD1	1:A:216:HIS:HB2	2.26	0.70
1:D:358:VAL:HG21	1:D:463:ASN:HA	1.72	0.70
1:B:23:MET:CE	1:B:325:VAL:HG21	2.21	0.70
1:C:75:MET:CG	1:C:107:ALA:HB3	2.21	0.70
1:D:170:LEU:HD22	1:D:174:ASP:HB3	1.73	0.70
1:A:89:GLN:HG3	1:A:90:THR:O	1.90	0.70
1:C:106:VAL:HG22	1:C:107:ALA:CB	2.22	0.70
1:C:169:ALA:HB3	3:C:2017:HOH:O	1.91	0.69
1:C:130:ILE:CG2	1:C:132:MET:HE2	2.17	0.69
1:D:160:LEU:HD12	1:D:165:ILE:HD13	1.74	0.69
1:C:175:LYS:HG2	1:C:206:HIS:HE1	1.55	0.69
1:A:10:ILE:HG13	1:A:31:MET:HG3	1.72	0.69
1:D:251:ILE:HB	1:D:252:PRO:HD2	1.75	0.69
1:A:402:ASN:HD22	1:A:402:ASN:C	1.97	0.68
1:A:244:ARG:NH1	1:A:278:THR:O	2.26	0.68
1:B:358:VAL:HG21	1:B:463:ASN:HA	1.75	0.68
1:A:93:PHE:CE2	1:A:123:VAL:HG11	2.29	0.68
1:A:75:MET:HG3	1:A:107:ALA:HB3	1.75	0.68
1:D:376:VAL:HG22	1:D:452:VAL:HB	1.75	0.68
1:A:96:ASP:O	1:A:98:SER:N	2.26	0.68
1:B:86:LYS:O	1:B:89:GLN:HB3	1.94	0.68
1:A:358:VAL:HG21	1:A:463:ASN:HA	1.76	0.68
1:D:80:GLY:CA	1:D:154:GLU:OE2	2.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:HG2	1:C:138:GLU:OE1	1.94	0.68
1:B:39:ASP:OD1	1:B:42:GLU:HG3	1.92	0.68
1:C:138:GLU:O	1:C:141:LYS:HB2	1.93	0.67
1:C:108:VAL:HG21	1:C:113:PHE:CD2	2.29	0.67
1:C:92:THR:OG1	1:C:143:ILE:HG13	1.93	0.67
1:A:44:GLY:O	3:A:2006:HOH:O	2.12	0.67
1:C:135:THR:OG1	1:C:143:ILE:HG23	1.95	0.67
1:D:74:THR:O	1:D:155:ASN:HA	1.94	0.67
1:C:130:ILE:CG2	1:C:132:MET:CE	2.72	0.67
1:C:251:ILE:HB	1:C:252:PRO:CD	2.24	0.66
1:A:175:LYS:HG2	1:A:206:HIS:CE1	2.30	0.66
1:C:434:LYS:HG3	1:C:451:MET:CE	2.25	0.66
1:D:69:GLY:HA2	1:D:174:ASP:OD2	1.96	0.66
1:D:50:LEU:O	1:D:54:MET:HE2	1.95	0.66
1:B:125:VAL:HG12	1:B:126:ASP:N	2.11	0.66
1:B:334:ARG:HD2	1:B:337:ARG:NH1	2.11	0.66
1:B:92:THR:O	1:B:105:MET:HB2	1.96	0.66
1:C:170:LEU:HD13	1:C:175:LYS:CG	2.26	0.65
1:A:124:LEU:HD23	1:A:131:GLY:HA2	1.78	0.65
1:A:124:LEU:HD23	1:A:131:GLY:CA	2.27	0.65
1:D:2:LYS:HE2	1:D:6:ILE:HD12	1.77	0.65
1:C:39:ASP:OD1	1:C:42:GLU:HG3	1.97	0.65
1:C:434:LYS:HG3	1:C:451:MET:HE3	1.79	0.65
1:A:197:ARG:HB3	1:A:232:GLU:HG3	1.78	0.64
1:C:113:PHE:CE1	1:C:117:LEU:HD23	2.32	0.64
1:C:138:GLU:CG	1:C:138:GLU:OE1	2.45	0.64
1:A:383:SER:HB3	1:A:462:THR:OG1	1.97	0.64
1:B:125:VAL:HG22	1:B:158:VAL:HG22	1.78	0.64
1:C:191:ALA:HB1	1:C:203:ILE:CD1	2.27	0.64
1:D:191:ALA:HB1	1:D:203:ILE:CD1	2.27	0.64
1:D:51:ARG:HA	1:D:54:MET:HE3	1.78	0.64
1:B:125:VAL:CG1	1:B:126:ASP:N	2.60	0.64
1:A:135:THR:OG1	1:A:143:ILE:O	2.13	0.64
1:C:104:GLU:O	1:C:105:MET:HB3	1.97	0.64
1:C:158:VAL:HG12	1:C:160:LEU:CD2	2.25	0.64
1:C:376:VAL:HG22	1:C:452:VAL:HB	1.80	0.63
1:C:92:THR:HG23	1:C:105:MET:SD	2.31	0.63
1:C:175:LYS:CD	1:C:206:HIS:HE1	2.11	0.63
1:C:133:GLU:N	1:C:147:LEU:HD21	2.12	0.63
1:B:50:LEU:HG	1:B:54:MET:CE	2.29	0.63
1:B:191:ALA:CB	1:B:203:ILE:CD1	2.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:CB	1:A:232:GLU:HG3	2.29	0.63
1:B:131:GLY:C	1:B:132:MET:HG3	2.19	0.63
1:C:137:ILE:N	3:C:2010:HOH:O	2.31	0.63
1:C:137:ILE:CG2	1:C:142:VAL:HG22	2.28	0.63
1:C:50:LEU:HG	1:C:54:MET:HE1	1.82	0.62
1:B:402:ASN:HB3	1:B:405:THR:HB	1.81	0.62
1:A:163:VAL:O	1:A:165:ILE:HD12	1.99	0.62
1:B:118:SER:O	1:B:121:ASN:HB2	1.99	0.62
1:C:136:ALA:H	1:C:143:ILE:HG22	1.62	0.62
1:B:318:GLY:HA3	3:B:2040:HOH:O	2.00	0.62
1:C:358:VAL:HG21	1:C:463:ASN:HA	1.82	0.62
1:B:197:ARG:HB3	1:B:232:GLU:HG3	1.81	0.62
1:B:251:ILE:HB	1:B:252:PRO:HD2	1.82	0.62
1:B:284:MET:HA	1:B:287:ASN:O	2.00	0.62
1:D:191:ALA:CB	1:D:203:ILE:CD1	2.77	0.62
1:B:434:LYS:HG3	1:B:451:MET:HE3	1.80	0.62
1:C:106:VAL:CG2	1:C:107:ALA:N	2.13	0.61
1:B:267:CYS:HB3	1:B:272:LYS:O	2.00	0.61
1:C:75:MET:CG	1:C:107:ALA:CB	2.77	0.61
1:B:376:VAL:HG22	1:B:452:VAL:HB	1.81	0.61
1:C:428:ASP:OD1	1:C:431:ARG:NH1	2.33	0.61
1:D:378:THR:OG1	2:D:704:SO4:O3	2.14	0.61
1:B:299:ALA:HB1	1:D:257:ILE:HD11	1.81	0.61
1:B:257:ILE:HD11	1:D:299:ALA:HB1	1.83	0.61
1:C:85:LEU:HD23	1:C:85:LEU:N	2.16	0.61
1:C:92:THR:HG21	1:C:143:ILE:HD11	1.82	0.61
1:A:193:PHE:CE2	1:A:195:ARG:HD3	2.36	0.61
1:C:77:LEU:HD11	1:C:154:GLU:CA	2.31	0.60
1:D:86:LYS:O	1:D:89:GLN:HB3	2.00	0.60
1:C:175:LYS:CG	1:C:206:HIS:CE1	2.81	0.60
1:D:160:LEU:HB2	1:D:163:VAL:HB	1.82	0.60
1:B:75:MET:HG3	1:B:107:ALA:O	2.01	0.60
1:B:131:GLY:C	1:B:132:MET:CG	2.70	0.60
1:C:111:GLU:HG2	1:C:111:GLU:OE2	2.01	0.60
1:C:136:ALA:HB3	1:C:143:ILE:HB	1.82	0.60
1:D:4:THR:HG21	1:D:302:ILE:HG12	1.84	0.60
1:A:69:GLY:CA	1:A:174:ASP:OD2	2.44	0.60
1:C:159:ASN:C	1:C:161:PRO:HD3	2.22	0.60
1:C:140:ASN:OD1	1:C:141:LYS:HE3	2.02	0.59
1:A:170:LEU:HD22	1:A:174:ASP:CB	2.22	0.59
1:B:244:ARG:NH1	1:B:278:THR:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HD11	1:B:91:PHE:CE1	2.38	0.59
1:D:201:ILE:O	1:D:205:GLU:HG3	2.02	0.59
1:C:92:THR:C	1:C:105:MET:HB2	2.17	0.59
1:C:74:THR:HG22	1:C:93:PHE:HE1	1.66	0.59
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.84	0.59
1:C:50:LEU:HG	1:C:54:MET:CE	2.32	0.59
1:B:170:LEU:HD23	1:B:174:ASP:HB3	1.83	0.59
1:A:23:MET:CE	1:A:325:VAL:HG21	2.32	0.59
1:C:111:GLU:CG	1:C:111:GLU:OE2	2.51	0.59
1:D:23:MET:CE	1:D:325:VAL:HG21	2.33	0.59
1:C:90:THR:HG22	1:C:144:CYS:O	2.00	0.59
1:A:74:THR:O	1:A:155:ASN:HA	2.02	0.59
1:C:106:VAL:HG22	1:C:107:ALA:HB3	1.84	0.58
1:A:321:PRO:HG2	1:A:322:LEU:H	1.68	0.58
1:D:373:LEU:HD11	1:D:397:LEU:HB2	1.85	0.58
1:D:402:ASN:C	1:D:402:ASN:HD22	2.05	0.58
1:B:191:ALA:CB	1:B:203:ILE:HD12	2.33	0.58
1:C:311:LEU:HD22	1:C:314:GLU:HB2	1.84	0.58
1:B:387:VAL:HG12	1:B:396:ILE:CD1	2.34	0.58
1:C:152:LEU:CD1	1:C:153:GLY:O	2.51	0.58
1:B:92:THR:HG23	1:B:142:VAL:O	2.03	0.58
1:D:375:VAL:HG22	1:D:397:LEU:HB3	1.85	0.58
1:A:88:GLY:O	1:A:145:LYS:HD2	2.03	0.58
1:B:14:THR:CG2	1:B:315:SER:O	2.51	0.58
1:A:14:THR:HG21	1:A:315:SER:O	2.03	0.58
1:C:197:ARG:CB	1:C:232:GLU:HG3	2.13	0.58
1:D:239:GLY:C	1:D:240:ILE:HG12	2.23	0.58
1:D:8:CYS:HB2	1:D:28:MET:HE3	1.86	0.58
1:C:170:LEU:HD22	1:C:174:ASP:HB3	1.84	0.58
1:A:299:ALA:HB1	1:C:257:ILE:HD11	1.86	0.58
1:B:74:THR:O	1:B:155:ASN:HA	2.04	0.58
1:D:110:TYR:OH	1:D:116:ASP:OD2	2.17	0.57
1:B:170:LEU:HD22	1:B:174:ASP:HB3	1.84	0.57
1:D:230:PHE:CE1	1:D:263:MET:HG2	2.39	0.57
1:A:191:ALA:HB1	1:A:203:ILE:CD1	2.34	0.57
1:C:175:LYS:CG	1:C:206:HIS:HE1	2.16	0.57
1:D:164:SER:C	1:D:165:ILE:HG13	2.25	0.57
1:C:202:GLU:OE1	3:C:2015:HOH:O	2.18	0.57
1:B:114:THR:HG22	1:B:142:VAL:HG23	1.87	0.57
1:C:373:LEU:HD12	1:C:395:THR:O	2.03	0.57
1:B:23:MET:HE2	1:B:325:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG22	1:A:452:VAL:HB	1.86	0.57
1:C:284:MET:HA	1:C:287:ASN:O	2.04	0.57
1:D:434:LYS:HG3	1:D:451:MET:HE3	1.85	0.57
1:C:430:TYR:O	1:C:434:LYS:HG3	2.05	0.56
1:A:113:PHE:HD2	1:A:142:VAL:HG21	1.68	0.56
1:B:191:ALA:HB1	1:B:203:ILE:CD1	2.36	0.56
1:B:132:MET:HA	1:B:147:LEU:HG	1.87	0.56
1:D:434:LYS:HG3	1:D:451:MET:CE	2.36	0.56
1:A:110:TYR:OH	1:A:166:ALA:HB3	2.05	0.56
1:B:140:ASN:OD1	1:B:141:LYS:HG3	2.05	0.56
1:A:251:ILE:HB	1:A:252:PRO:HD2	1.88	0.56
1:B:133:GLU:O	1:B:144:CYS:HA	2.05	0.56
1:D:160:LEU:HD12	1:D:165:ILE:HD11	1.88	0.56
1:B:50:LEU:HG	1:B:54:MET:HE1	1.88	0.56
1:D:274:VAL:O	1:D:274:VAL:HG13	2.06	0.56
1:C:133:GLU:O	1:C:144:CYS:CA	2.54	0.56
1:D:160:LEU:N	3:D:2020:HOH:O	2.13	0.56
1:A:96:ASP:C	1:A:98:SER:H	2.09	0.56
1:B:387:VAL:HG12	1:B:396:ILE:HD11	1.86	0.56
1:C:75:MET:HG3	1:C:107:ALA:CB	2.34	0.56
1:C:142:VAL:CG1	1:C:143:ILE:H	2.17	0.55
1:C:191:ALA:CB	1:C:203:ILE:HD13	2.36	0.55
1:A:51:ARG:HA	1:A:54:MET:CE	2.29	0.55
1:A:257:ILE:HD11	1:C:299:ALA:CB	2.36	0.55
1:B:155:ASN:C	1:B:156:LYS:HG2	2.27	0.55
1:C:155:ASN:C	1:C:156:LYS:HD3	2.26	0.55
1:C:83:VAL:HG21	1:C:103:SER:HA	1.88	0.55
1:A:39:ASP:OD1	1:A:42:GLU:HG3	2.05	0.55
1:C:198:SER:O	1:C:202:GLU:HG3	2.06	0.55
1:A:402:ASN:ND2	1:A:405:THR:H	2.04	0.55
1:A:73:ARG:O	1:A:109:THR:HG23	2.05	0.55
1:D:17:GLU:OE1	1:D:56:LYS:NZ	2.40	0.55
1:B:73:ARG:HA	1:B:156:LYS:O	2.07	0.55
1:D:159:ASN:HA	3:D:2020:HOH:O	2.06	0.55
1:C:434:LYS:CG	1:C:451:MET:CE	2.84	0.55
1:C:83:VAL:HG23	1:C:85:LEU:CD2	2.36	0.55
1:B:8:CYS:HB2	1:B:28:MET:CE	2.35	0.54
1:A:113:PHE:CD2	1:A:142:VAL:HG21	2.42	0.54
1:A:354:ILE:N	3:A:2032:HOH:O	2.40	0.54
1:C:133:GLU:O	1:C:144:CYS:HA	2.07	0.54
1:A:257:ILE:HD11	1:C:299:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ALA:HB3	1:A:174:ASP:OD2	2.07	0.54
1:A:50:LEU:HG	1:A:54:MET:CE	2.38	0.54
1:B:281:LEU:O	1:B:314:GLU:HG2	2.07	0.54
1:D:391:PHE:N	1:D:392:PRO:CD	2.70	0.54
1:C:50:LEU:O	1:C:54:MET:HE2	2.08	0.54
1:B:23:MET:HE1	1:B:325:VAL:HG21	1.89	0.54
1:A:255:GLU:CD	1:C:334:ARG:HH11	2.10	0.54
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.06	0.54
1:C:383:SER:HB3	1:C:462:THR:OG1	2.07	0.54
1:C:77:LEU:HD12	1:C:154:GLU:CG	2.36	0.54
1:A:434:LYS:HG3	1:A:451:MET:HE1	1.87	0.54
1:D:262:MET:O	1:D:266:LYS:HG3	2.08	0.54
1:C:167:LEU:HD22	1:C:168:PRO:HD2	1.89	0.53
1:C:191:ALA:CB	1:C:203:ILE:CD1	2.86	0.53
1:A:19:MET:O	1:A:22:LYS:N	2.41	0.53
1:C:75:MET:HG2	1:C:107:ALA:O	2.07	0.53
1:C:65:LEU:C	1:C:65:LEU:HD23	2.28	0.53
1:C:119:VAL:HG22	1:C:135:THR:C	2.29	0.53
1:A:133:GLU:HB2	1:A:147:LEU:HD21	1.91	0.53
1:A:284:MET:HA	1:A:287:ASN:O	2.09	0.53
1:B:375:VAL:HG22	1:B:397:LEU:HB3	1.91	0.53
1:A:75:MET:HG2	1:A:107:ALA:O	2.08	0.53
1:C:51:ARG:HA	1:C:54:MET:CE	2.35	0.53
1:C:175:LYS:HD3	1:C:206:HIS:HE1	1.74	0.53
1:B:154:GLU:HA	3:B:2007:HOH:O	2.08	0.53
1:D:74:THR:OG1	1:D:156:LYS:HB2	2.09	0.53
1:C:132:MET:HA	1:C:147:LEU:HG	1.91	0.53
1:C:142:VAL:CG1	1:C:143:ILE:N	2.71	0.53
1:C:373:LEU:HA	1:C:394:ALA:HB1	1.91	0.53
1:C:136:ALA:O	1:C:142:VAL:HG13	2.09	0.53
1:A:320:TYR:HB3	1:A:323:GLU:HB2	1.90	0.53
1:C:92:THR:OG1	1:C:143:ILE:CA	2.39	0.52
1:A:172:GLU:OE1	1:A:175:LYS:HD2	2.09	0.52
1:D:284:MET:HA	1:D:287:ASN:O	2.09	0.52
1:A:334:ARG:HH11	1:C:255:GLU:CD	2.12	0.52
1:A:299:ALA:HB3	1:C:257:ILE:HD11	1.91	0.52
1:C:96:ASP:O	1:C:98:SER:N	2.43	0.52
1:B:402:ASN:C	1:B:402:ASN:HD22	2.13	0.52
1:C:230:PHE:CE1	1:C:263:MET:HG2	2.44	0.52
1:C:110:TYR:O	1:C:112:GLY:N	2.43	0.52
1:C:137:ILE:CG1	1:C:142:VAL:HG11	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:LYS:HD2	1:D:241:MET:SD	2.49	0.52
1:B:452:VAL:CG1	1:B:462:THR:CG2	2.88	0.52
1:A:140:ASN:C	1:A:141:LYS:HG2	2.30	0.52
1:B:434:LYS:HG3	1:B:451:MET:CE	2.40	0.52
1:A:88:GLY:CA	1:A:145:LYS:CE	2.38	0.52
1:C:172:GLU:HG2	1:C:175:LYS:HZ1	1.75	0.52
1:D:160:LEU:HB2	1:D:165:ILE:HD11	1.91	0.52
1:B:391:PHE:N	1:B:392:PRO:CD	2.73	0.52
1:D:114:THR:HG22	1:D:137:ILE:HG23	1.91	0.52
1:B:65:LEU:HD23	1:B:65:LEU:C	2.30	0.52
1:D:229:ASN:O	1:D:230:PHE:C	2.48	0.52
1:D:118:SER:O	1:D:121:ASN:HB2	2.08	0.51
1:C:113:PHE:CD1	1:C:117:LEU:HD23	2.43	0.51
1:C:137:ILE:HG12	1:C:142:VAL:CB	2.41	0.51
1:D:274:VAL:HG22	1:D:275:ILE:N	2.24	0.51
1:C:320:TYR:HB3	1:C:323:GLU:HB2	1.91	0.51
1:A:206:HIS:O	1:A:207:LEU:C	2.48	0.51
1:B:363:VAL:O	1:B:367:GLU:HG3	2.10	0.51
1:C:137:ILE:HG21	1:C:142:VAL:HG22	1.93	0.51
1:B:23:MET:HE1	1:B:325:VAL:CG2	2.40	0.51
1:B:133:GLU:O	1:B:144:CYS:CA	2.59	0.51
1:A:240:ILE:O	1:A:275:ILE:N	2.38	0.51
1:C:170:LEU:HD13	1:C:175:LYS:HA	1.93	0.51
1:B:354:ILE:O	1:B:358:VAL:HG23	2.11	0.51
1:A:311:LEU:HD22	1:A:314:GLU:HB2	1.93	0.51
1:A:25:ASP:OD1	1:A:59:LYS:NZ	2.32	0.51
1:D:159:ASN:CG	1:D:249:VAL:HG11	2.31	0.50
1:D:17:GLU:O	1:D:21:ALA:N	2.36	0.50
1:B:80:GLY:CA	1:B:154:GLU:OE2	2.56	0.50
1:B:387:VAL:CG1	1:B:396:ILE:HD13	2.41	0.50
1:B:10:ILE:HG13	1:B:31:MET:HG3	1.91	0.50
1:B:193:PHE:CE2	1:B:195:ARG:HD3	2.46	0.50
1:A:15:GLU:HB2	1:A:46:ARG:HG3	1.93	0.50
1:C:94:THR:HA	1:C:140:ASN:O	2.12	0.50
1:B:220:LYS:HE2	1:B:222:GLU:OE2	2.12	0.50
1:D:133:GLU:O	1:D:144:CYS:HA	2.12	0.50
1:C:133:GLU:C	1:C:144:CYS:HB3	2.31	0.50
1:A:88:GLY:HA2	1:A:145:LYS:CD	2.36	0.50
1:D:191:ALA:CB	1:D:203:ILE:HD13	2.41	0.50
1:A:70:PRO:CB	1:A:167:LEU:HD13	2.42	0.50
1:C:240:ILE:O	1:C:275:ILE:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:THR:HG21	1:C:302:ILE:HG12	1.94	0.50
1:C:167:LEU:HD22	1:C:168:PRO:CD	2.42	0.50
1:C:251:ILE:CB	1:C:252:PRO:CD	2.88	0.50
1:A:50:LEU:HG	1:A:54:MET:HE2	1.94	0.50
1:C:118:SER:N	1:C:121:ASN:OD1	2.45	0.50
1:D:160:LEU:CB	1:D:163:VAL:HB	2.42	0.50
1:A:436:LEU:O	1:A:440:SER:HB3	2.12	0.50
1:B:9:THR:HG23	1:B:32:ARG:HG2	1.93	0.50
1:B:174:ASP:O	1:B:178:LEU:HG	2.12	0.49
1:A:440:SER:OG	1:A:442:LEU:HB2	2.12	0.49
1:C:325:VAL:O	1:C:328:MET:HB3	2.12	0.49
1:C:74:THR:HA	1:C:108:VAL:HG12	1.93	0.49
1:A:45:GLN:CG	3:A:2007:HOH:O	2.59	0.49
1:B:19:MET:O	1:B:20:LEU:C	2.49	0.49
1:D:334:ARG:HD2	1:D:337:ARG:HH12	1.76	0.49
1:D:230:PHE:CZ	1:D:263:MET:HG2	2.46	0.49
1:C:195:ARG:NH2	3:C:2014:HOH:O	2.46	0.49
1:D:28:MET:CE	1:D:31:MET:HA	2.43	0.49
1:B:171:ALA:O	1:B:174:ASP:HB2	2.12	0.49
1:C:360:ARG:NH2	1:C:364:GLU:OE1	2.46	0.49
1:C:137:ILE:CG2	1:C:141:LYS:O	2.54	0.49
1:A:133:GLU:O	1:A:144:CYS:HB3	2.12	0.49
1:A:281:LEU:HB3	1:A:284:MET:HG3	1.93	0.49
1:D:267:CYS:HB3	1:D:272:LYS:O	2.12	0.49
1:A:132:MET:HG2	1:A:146:VAL:HA	1.94	0.49
1:A:402:ASN:ND2	1:A:402:ASN:C	2.64	0.49
1:B:312:SER:N	1:B:314:GLU:OE1	2.44	0.49
1:C:75:MET:HG2	1:C:107:ALA:HB3	1.94	0.49
1:A:35:PHE:CZ	1:A:43:HIS:CD2	3.01	0.49
1:A:402:ASN:HD22	1:A:405:THR:H	1.60	0.49
1:A:191:ALA:CB	1:A:203:ILE:CD1	2.91	0.48
1:C:10:ILE:HG22	1:C:46:ARG:HD3	1.94	0.48
1:C:92:THR:OG1	1:C:143:ILE:CG1	2.62	0.48
1:D:99:VAL:CG1	1:D:100:ILE:N	2.76	0.48
1:D:65:LEU:C	1:D:65:LEU:HD23	2.34	0.48
1:C:119:VAL:CA	1:C:134:VAL:HG11	2.35	0.48
1:A:299:ALA:HB3	1:C:257:ILE:CD1	2.43	0.48
1:C:373:LEU:HD11	1:C:397:LEU:HB2	1.95	0.48
1:D:119:VAL:HG12	1:D:120:GLY:N	2.28	0.48
1:D:320:TYR:HB3	1:D:323:GLU:HB2	1.95	0.48
1:A:76:LYS:HA	1:A:154:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:SER:OG	1:D:442:LEU:HG	2.13	0.48
1:C:434:LYS:HG3	1:C:451:MET:HE1	1.94	0.48
1:C:281:LEU:O	1:C:314:GLU:HG2	2.12	0.48
1:B:123:VAL:HG12	1:B:124:LEU:N	2.29	0.48
1:D:327:ILE:O	1:D:331:ILE:HG13	2.14	0.48
1:C:119:VAL:HG22	1:C:134:VAL:HG12	1.96	0.48
1:C:355:THR:HG23	1:C:462:THR:HB	1.96	0.48
1:A:23:MET:HE2	1:A:325:VAL:HG21	1.95	0.48
1:C:287:ASN:HB3	1:C:288:PRO:HD2	1.95	0.48
1:C:434:LYS:CG	1:C:451:MET:HE1	2.44	0.48
1:D:281:LEU:HD12	1:D:311:LEU:HD21	1.96	0.48
1:C:175:LYS:HG2	1:C:206:HIS:ND1	2.26	0.48
1:A:96:ASP:C	1:A:98:SER:N	2.67	0.48
1:A:463:ASN:O	1:B:466:SER:HA	2.14	0.48
1:A:133:GLU:HB2	1:A:147:LEU:CD2	2.43	0.47
1:C:172:GLU:HG2	1:C:175:LYS:NZ	2.30	0.47
1:D:179:ILE:O	1:D:183:GLU:HG3	2.15	0.47
1:D:132:MET:HA	1:D:147:LEU:HG	1.96	0.47
1:C:16:SER:O	1:C:20:LEU:HG	2.14	0.47
1:D:171:ALA:O	1:D:174:ASP:HB2	2.14	0.47
1:B:154:GLU:O	1:B:155:ASN:HB3	2.14	0.47
1:A:135:THR:O	1:A:136:ALA:HB2	2.15	0.47
1:C:140:ASN:OD1	1:C:141:LYS:CD	2.62	0.47
1:C:170:LEU:HD11	1:C:178:LEU:HD12	1.96	0.47
1:A:161:PRO:O	1:A:163:VAL:N	2.48	0.47
1:C:83:VAL:CG2	1:C:103:SER:HA	2.44	0.47
1:B:229:ASN:O	1:B:230:PHE:C	2.53	0.47
1:C:117:LEU:HD12	1:C:121:ASN:OD1	2.14	0.47
1:A:118:SER:O	1:A:119:VAL:C	2.52	0.47
1:A:428:ASP:OD1	1:A:431:ARG:NH1	2.48	0.47
1:A:75:MET:HB2	1:A:76:LYS:H	1.46	0.47
1:B:118:SER:O	1:B:119:VAL:C	2.53	0.47
1:A:181:GLY:O	1:A:185:GLY:N	2.48	0.47
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.82	0.47
1:A:9:THR:HG23	1:A:32:ARG:HG2	1.96	0.47
1:B:434:LYS:CG	1:B:451:MET:HE3	2.45	0.46
1:B:96:ASP:O	1:B:98:SER:N	2.49	0.46
1:C:15:GLU:HB2	1:C:46:ARG:HG3	1.97	0.46
1:A:86:LYS:O	1:A:87:ALA:C	2.53	0.46
1:B:50:LEU:O	1:B:54:MET:HE2	2.15	0.46
1:A:466:SER:OG	1:A:468:HIS:NE2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:LYS:HG3	1:D:410:VAL:O	2.16	0.46
1:B:188:PHE:CD1	1:B:216:HIS:HB2	2.50	0.46
1:C:110:TYR:O	1:C:113:PHE:N	2.45	0.46
1:C:191:ALA:HB2	1:C:203:ILE:HD13	1.97	0.46
1:B:191:ALA:HB2	1:B:203:ILE:CD1	2.45	0.46
1:C:341:SER:HA	1:C:391:PHE:O	2.15	0.46
1:A:89:GLN:CG	1:A:90:THR:N	2.79	0.46
1:D:373:LEU:HD12	1:D:395:THR:O	2.16	0.46
1:A:140:ASN:OD1	1:A:141:LYS:NZ	2.43	0.46
1:C:118:SER:C	1:C:134:VAL:HG11	2.36	0.46
1:B:14:THR:HA	1:B:19:MET:HG2	1.97	0.46
1:B:133:GLU:O	1:B:144:CYS:HB3	2.14	0.46
1:C:326:SER:O	1:C:330:THR:HG23	2.16	0.46
1:C:74:THR:HG22	1:C:93:PHE:CE1	2.49	0.46
1:C:15:GLU:O	1:C:16:SER:C	2.53	0.46
1:C:324:ALA:O	1:C:325:VAL:C	2.48	0.46
1:D:402:ASN:ND2	1:D:402:ASN:C	2.69	0.46
1:B:354:ILE:O	1:B:355:THR:C	2.53	0.46
1:C:452:VAL:CG1	1:C:462:THR:CG2	2.94	0.46
1:C:321:PRO:HG2	1:C:322:LEU:H	1.80	0.46
1:D:196:LYS:O	1:D:199:ASP:HB2	2.16	0.46
1:C:159:ASN:ND2	1:C:249:VAL:CG1	2.79	0.46
1:C:23:MET:CE	1:C:325:VAL:HG21	2.45	0.46
1:D:409:LEU:O	1:D:410:VAL:C	2.51	0.46
1:B:258:PHE:HZ	1:D:335:THR:HG23	1.81	0.46
1:D:363:VAL:O	1:D:367:GLU:HG3	2.16	0.46
1:D:10:ILE:HG13	1:D:31:MET:SD	2.56	0.45
1:C:202:GLU:HG3	3:C:2016:HOH:O	2.06	0.45
1:A:64:LEU:C	1:A:64:LEU:HD23	2.37	0.45
1:C:14:THR:CG2	1:C:315:SER:O	2.59	0.45
1:A:281:LEU:HB2	1:A:314:GLU:HG2	1.97	0.45
1:A:4:THR:HG21	1:A:302:ILE:HG12	1.98	0.45
1:B:274:VAL:O	1:B:274:VAL:HG13	2.16	0.45
1:C:140:ASN:OD1	1:C:141:LYS:CE	2.63	0.45
1:C:267:CYS:HB3	1:C:272:LYS:O	2.15	0.45
1:C:320:TYR:N	1:C:321:PRO:CD	2.80	0.45
1:D:152:LEU:HA	1:D:152:LEU:HD12	1.65	0.45
1:D:198:SER:HB3	3:D:2029:HOH:O	2.16	0.45
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.68	0.45
1:B:428:ASP:OD1	1:B:431:ARG:NH1	2.49	0.45
1:B:440:SER:OG	1:B:442:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LYS:O	1:B:262:MET:C	2.55	0.45
1:A:440:SER:OG	1:A:442:LEU:HG	2.17	0.45
1:D:271:LEU:O	1:D:385:ARG:HD2	2.17	0.45
1:A:105:MET:CG	1:A:106:VAL:N	2.79	0.44
1:A:203:ILE:HG21	1:A:203:ILE:HD13	1.75	0.44
1:A:452:VAL:CG1	1:A:462:THR:CG2	2.95	0.44
1:A:176:GLN:HG3	1:A:176:GLN:H	1.59	0.44
1:B:409:LEU:O	1:B:410:VAL:C	2.55	0.44
1:D:387:VAL:HG12	1:D:396:ILE:CD1	2.47	0.44
1:A:395:THR:CG2	1:A:396:ILE:N	2.80	0.44
1:D:230:PHE:CD1	1:D:263:MET:HG2	2.53	0.44
1:A:171:ALA:CB	1:A:174:ASP:OD2	2.66	0.44
1:A:284:MET:C	1:A:286:LYS:N	2.68	0.44
1:A:287:ASN:HB3	1:A:288:PRO:CD	2.48	0.44
1:D:388:ARG:O	1:D:389:LYS:C	2.56	0.44
1:C:113:PHE:CD1	1:C:117:LEU:HD22	2.50	0.44
1:C:73:ARG:HA	1:C:73:ARG:HD3	1.85	0.44
1:A:75:MET:HB3	1:A:75:MET:HE3	1.86	0.44
1:A:434:LYS:CG	1:A:451:MET:CE	2.92	0.44
1:B:391:PHE:N	1:B:392:PRO:HD2	2.32	0.44
1:D:119:VAL:HA	1:D:134:VAL:HG12	2.00	0.44
1:D:320:TYR:N	1:D:321:PRO:CD	2.80	0.44
1:A:24:LEU:HA	1:A:28:MET:HB3	1.98	0.44
1:D:402:ASN:ND2	1:D:405:THR:N	2.56	0.44
1:A:76:LYS:HG2	1:A:154:GLU:OE1	2.18	0.44
1:A:124:LEU:O	1:A:158:VAL:HA	2.18	0.44
1:B:452:VAL:CG1	1:B:462:THR:HG21	2.48	0.44
1:A:320:TYR:N	1:A:321:PRO:CD	2.80	0.44
1:C:395:THR:CG2	1:C:396:ILE:N	2.80	0.44
1:C:110:TYR:OH	1:C:116:ASP:OD2	2.36	0.44
1:B:50:LEU:HG	1:B:54:MET:HE2	1.99	0.44
1:B:75:MET:HG3	1:B:107:ALA:C	2.37	0.44
1:D:99:VAL:HG12	1:D:100:ILE:N	2.33	0.44
1:A:126:ASP:O	1:A:127:ASP:C	2.56	0.44
1:A:191:ALA:HB1	1:A:203:ILE:HD11	1.99	0.43
1:A:426:THR:HG22	1:A:430:TYR:CE2	2.52	0.43
1:C:119:VAL:CG2	1:C:134:VAL:HG12	2.48	0.43
1:C:191:ALA:C	1:C:220:LYS:HG3	2.35	0.43
1:A:50:LEU:O	1:A:54:MET:HE2	2.18	0.43
1:D:324:ALA:O	1:D:325:VAL:C	2.56	0.43
1:A:354:ILE:HG21	1:A:354:ILE:HD13	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.88	0.43
1:C:363:VAL:O	1:C:367:GLU:HG3	2.18	0.43
1:A:395:THR:HG22	1:A:396:ILE:N	2.32	0.43
1:D:193:PHE:CE2	1:D:195:ARG:HD3	2.54	0.43
1:D:96:ASP:O	1:D:98:SER:N	2.51	0.43
1:C:64:LEU:C	1:C:64:LEU:HD23	2.39	0.43
1:D:165:ILE:HG22	1:D:167:LEU:H	1.82	0.43
1:C:188:PHE:CE1	1:C:216:HIS:HB2	2.53	0.43
1:D:375:VAL:HA	1:D:397:LEU:O	2.18	0.43
1:C:159:ASN:ND2	1:C:249:VAL:HG11	2.33	0.43
1:D:117:LEU:HD11	1:D:160:LEU:HD22	2.00	0.43
1:D:174:ASP:O	1:D:178:LEU:HG	2.18	0.43
1:C:434:LYS:CG	1:C:451:MET:HE3	2.45	0.43
1:B:456:LEU:O	1:B:457:VAL:HG13	2.19	0.43
1:B:179:ILE:O	1:B:183:GLU:HG3	2.18	0.43
1:D:227:LEU:HD12	1:D:227:LEU:HA	1.67	0.43
1:B:23:MET:CE	1:B:325:VAL:CG2	2.92	0.43
1:B:160:LEU:HD12	1:B:165:ILE:HD13	2.01	0.43
1:C:335:THR:O	1:C:336:ASP:C	2.56	0.43
1:D:8:CYS:HB2	1:D:28:MET:CE	2.49	0.43
1:A:117:LEU:HD21	1:A:123:VAL:HG23	2.00	0.43
1:A:10:ILE:HG13	1:A:31:MET:CG	2.44	0.43
1:C:430:TYR:HA	1:C:451:MET:SD	2.58	0.43
1:D:387:VAL:HG12	1:D:396:ILE:HD11	2.00	0.43
1:D:84:SER:C	1:D:85:LEU:HD23	2.39	0.43
1:A:152:LEU:HG	1:A:153:GLY:O	2.18	0.43
1:B:334:ARG:HH11	1:D:255:GLU:CD	2.21	0.43
1:B:251:ILE:HB	1:B:252:PRO:CD	2.49	0.43
1:A:19:MET:O	1:A:20:LEU:C	2.57	0.43
1:D:14:THR:HA	1:D:19:MET:HG2	2.01	0.43
1:C:281:LEU:HD12	1:C:311:LEU:HD21	2.00	0.43
1:C:77:LEU:HD11	1:C:154:GLU:N	2.33	0.43
1:A:67:THR:CG2	1:A:178:LEU:HD21	2.49	0.43
1:C:193:PHE:CE2	1:C:195:ARG:HD3	2.54	0.42
1:B:124:LEU:HD12	1:B:249:VAL:HG13	1.99	0.42
1:A:335:THR:O	1:A:336:ASP:C	2.57	0.42
1:A:10:ILE:HD13	1:A:10:ILE:HA	1.75	0.42
1:C:287:ASN:HB3	1:C:288:PRO:CD	2.48	0.42
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.75	0.42
1:C:171:ALA:O	1:C:173:LYS:N	2.51	0.42
1:C:160:LEU:N	1:C:161:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:PRO:HB2	1:D:167:LEU:HD13	2.01	0.42
1:A:110:TYR:O	1:A:112:GLY:N	2.52	0.42
1:C:239:GLY:C	1:C:240:ILE:HG12	2.40	0.42
1:C:171:ALA:O	1:C:174:ASP:N	2.52	0.42
1:C:220:LYS:HB2	1:C:222:GLU:OE2	2.19	0.42
1:C:19:MET:O	1:C:20:LEU:C	2.55	0.42
1:D:251:ILE:HB	1:D:252:PRO:CD	2.48	0.42
1:A:165:ILE:HG22	1:A:167:LEU:H	1.84	0.42
1:A:23:MET:CE	1:A:325:VAL:CG2	2.97	0.42
1:C:136:ALA:O	1:C:143:ILE:HB	2.19	0.42
1:D:138:GLU:O	1:D:141:LYS:HB2	2.19	0.42
1:A:160:LEU:HB2	1:A:163:VAL:HB	2.02	0.42
1:C:230:PHE:CZ	1:C:263:MET:HG2	2.53	0.42
1:A:240:ILE:O	1:A:274:VAL:HA	2.19	0.42
1:C:140:ASN:OD1	1:C:140:ASN:N	2.50	0.42
1:C:134:VAL:HA	1:C:144:CYS:HB3	2.01	0.42
1:D:10:ILE:HG22	1:D:46:ARG:HD3	2.00	0.42
1:A:220:LYS:HB2	1:A:222:GLU:OE2	2.19	0.42
1:A:197:ARG:HB2	1:A:232:GLU:HG3	1.99	0.42
1:A:94:THR:HA	1:A:140:ASN:O	2.19	0.42
1:D:118:SER:O	1:D:119:VAL:C	2.57	0.42
1:C:126:ASP:O	1:C:127:ASP:C	2.56	0.42
1:C:75:MET:HG2	1:C:107:ALA:CB	2.48	0.42
1:D:10:ILE:HD11	1:D:28:MET:HE1	2.02	0.42
1:D:15:GLU:HB2	1:D:46:ARG:HG3	2.01	0.42
1:C:160:LEU:N	1:C:160:LEU:HD23	2.34	0.42
1:A:430:TYR:HA	1:A:451:MET:SD	2.60	0.42
1:A:188:PHE:CD1	1:A:216:HIS:CB	3.01	0.42
1:A:147:LEU:O	1:A:148:ASN:HB3	2.18	0.42
1:A:146:VAL:HG12	1:A:148:ASN:H	1.84	0.42
1:B:430:TYR:O	1:B:434:LYS:HG3	2.19	0.42
1:C:84:SER:C	1:C:85:LEU:HD23	2.40	0.42
1:C:137:ILE:CG1	1:C:142:VAL:HG22	2.34	0.42
1:D:31:MET:HE2	1:D:63:ILE:HG12	2.01	0.42
1:A:159:ASN:C	1:A:161:PRO:HD3	2.41	0.42
1:D:391:PHE:N	1:D:392:PRO:HD2	2.33	0.42
1:C:402:ASN:HB3	1:C:405:THR:HB	2.01	0.42
1:B:245:GLY:O	1:B:246:ASP:C	2.57	0.42
1:A:65:LEU:HD23	1:A:65:LEU:C	2.41	0.42
1:C:173:LYS:HG3	1:C:174:ASP:N	2.30	0.41
1:B:10:ILE:HA	1:B:10:ILE:HD13	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:THR:HG22	1:D:396:ILE:N	2.35	0.41
1:B:373:LEU:HD11	1:B:397:LEU:HB2	2.02	0.41
1:C:341:SER:HB3	1:C:367:GLU:OE2	2.20	0.41
1:A:391:PHE:N	1:A:392:PRO:CD	2.83	0.41
1:C:119:VAL:CG2	1:C:135:THR:C	2.89	0.41
1:B:402:ASN:C	1:B:402:ASN:ND2	2.73	0.41
1:C:126:ASP:HB3	1:C:129:LEU:HB2	2.02	0.41
1:C:118:SER:O	1:C:119:VAL:C	2.58	0.41
1:C:119:VAL:HG21	1:C:135:THR:O	2.21	0.41
1:C:135:THR:OG1	1:C:143:ILE:CG2	2.66	0.41
1:C:93:PHE:N	1:C:142:VAL:O	2.36	0.41
1:C:94:THR:O	1:C:94:THR:HG23	2.19	0.41
1:D:354:ILE:O	1:D:355:THR:C	2.58	0.41
1:A:50:LEU:HG	1:A:54:MET:HE1	2.02	0.41
1:A:163:VAL:O	1:A:165:ILE:CD1	2.68	0.41
1:B:227:LEU:HA	1:B:227:LEU:HD12	1.71	0.41
1:C:331:ILE:HG21	1:C:331:ILE:HD13	1.75	0.41
1:D:271:LEU:HD12	1:D:382:LYS:HE2	2.03	0.41
1:D:280:MET:HG3	1:D:310:MET:O	2.20	0.41
1:B:458:PRO:O	1:B:459:SER:C	2.58	0.41
1:B:320:TYR:N	1:B:321:PRO:CD	2.83	0.41
1:C:140:ASN:OD1	1:C:141:LYS:HD2	2.21	0.41
1:B:24:LEU:HD23	1:B:24:LEU:HA	1.86	0.41
1:B:239:GLY:C	1:B:240:ILE:HG12	2.40	0.41
1:A:288:PRO:HB3	1:A:320:TYR:CE1	2.54	0.41
1:D:387:VAL:CG1	1:D:396:ILE:HD13	2.50	0.41
1:B:395:THR:HG22	1:B:396:ILE:N	2.34	0.41
1:A:257:ILE:O	1:A:261:LYS:HG3	2.20	0.41
1:B:258:PHE:CZ	1:D:335:THR:HA	2.55	0.41
1:B:271:LEU:HD22	1:B:386:ALA:HA	2.03	0.41
1:D:458:PRO:O	1:D:459:SER:C	2.58	0.41
1:C:73:ARG:O	1:C:108:VAL:HA	2.20	0.41
1:C:174:ASP:O	1:C:175:LYS:C	2.59	0.41
1:B:387:VAL:CG1	1:B:396:ILE:CD1	2.98	0.41
1:D:85:LEU:N	1:D:85:LEU:HD23	2.35	0.41
1:D:92:THR:HG22	1:D:93:PHE:N	2.35	0.41
1:C:110:TYR:O	1:C:113:PHE:HB2	2.21	0.41
1:C:251:ILE:HD11	1:C:256:VAL:HG22	2.02	0.41
1:A:86:LYS:O	1:A:89:GLN:HB3	2.20	0.41
1:B:137:ILE:HG12	1:B:142:VAL:HG22	2.03	0.41
1:D:14:THR:HG21	1:D:315:SER:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LYS:N	1:D:336:ASP:OD2	2.48	0.41
1:C:75:MET:CG	1:C:107:ALA:HB1	2.50	0.41
1:D:94:THR:HA	1:D:140:ASN:O	2.20	0.41
1:B:299:ALA:CB	1:D:257:ILE:HD11	2.48	0.41
1:C:85:LEU:HD13	1:C:91:PHE:CD1	2.56	0.41
1:B:371:ALA:HB1	1:B:448:VAL:O	2.20	0.41
1:D:369:LEU:O	1:D:370:ASP:HB2	2.20	0.41
1:B:120:GLY:N	1:B:134:VAL:O	2.47	0.41
1:C:35:PHE:HZ	1:C:180:PHE:CE2	2.38	0.41
1:C:213:GLU:H	1:C:213:GLU:HG3	1.12	0.41
1:B:113:PHE:O	1:B:117:LEU:HB2	2.21	0.41
1:C:373:LEU:HD11	1:C:397:LEU:CB	2.51	0.41
1:C:395:THR:HG22	1:C:396:ILE:N	2.34	0.41
1:C:375:VAL:HG22	1:C:397:LEU:HB3	2.03	0.41
1:D:276:THR:HG21	1:D:301:ALA:CB	2.51	0.41
1:A:230:PHE:CE1	1:A:263:MET:HG2	2.56	0.41
1:C:92:THR:HG21	1:C:143:ILE:CD1	2.50	0.40
1:D:191:ALA:HB2	1:D:203:ILE:HD13	2.03	0.40
1:D:452:VAL:CG1	1:D:462:THR:CG2	2.99	0.40
1:C:83:VAL:HG23	1:C:85:LEU:HD21	2.02	0.40
1:A:255:GLU:OE1	1:C:334:ARG:NH1	2.54	0.40
1:C:391:PHE:N	1:C:392:PRO:CD	2.84	0.40
1:D:19:MET:O	1:D:20:LEU:C	2.59	0.40
1:C:128:GLY:O	1:C:129:LEU:C	2.59	0.40
1:B:436:LEU:O	1:B:437:ALA:C	2.58	0.40
1:A:88:GLY:C	1:A:145:LYS:HD2	2.41	0.40
1:B:230:PHE:CE1	1:B:263:MET:HG2	2.56	0.40
1:C:140:ASN:C	1:C:141:LYS:HG3	2.41	0.40
1:A:89:GLN:HG2	1:A:146:VAL:HG23	2.03	0.40
1:B:92:THR:O	1:B:105:MET:HA	2.22	0.40
1:C:197:ARG:HD3	1:C:197:ARG:HH11	1.34	0.40
1:A:105:MET:HG3	1:A:106:VAL:N	2.36	0.40
1:C:188:PHE:HD1	1:C:216:HIS:HB2	1.81	0.40
1:A:23:MET:HE1	1:A:325:VAL:CG2	2.51	0.40
1:A:229:ASN:O	1:A:230:PHE:C	2.60	0.40
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.67	0.40
1:D:23:MET:HE2	1:D:325:VAL:HG21	2.02	0.40
1:A:194:ILE:HG13	1:A:219:SER:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:THR:CG2	1:D:18:GLU:OE2[4_446]	1.86	0.34

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/470 (97%)	434 (95%)	19 (4%)	4 (1%)	21	55
1	B	457/470 (97%)	432 (94%)	24 (5%)	1 (0%)	52	84
1	C	457/470 (97%)	430 (94%)	24 (5%)	3 (1%)	26	62
1	D	457/470 (97%)	441 (96%)	15 (3%)	1 (0%)	52	84
All	All	1828/1880 (97%)	1737 (95%)	82 (4%)	9 (0%)	34	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	162	GLY
1	B	97	LYS
1	C	97	LYS
1	C	172	GLU
1	D	97	LYS
1	A	171	ALA
1	A	111	GLU
1	C	111	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	377/389 (97%)	337 (89%)	40 (11%)	8 24
1	B	377/389 (97%)	339 (90%)	38 (10%)	9 27
1	C	377/389 (97%)	322 (85%)	55 (15%)	4 11
1	D	377/389 (97%)	338 (90%)	39 (10%)	9 26
All	All	1508/1556 (97%)	1336 (89%)	172 (11%)	7 21

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	SER
1	A	23	MET
1	A	60	THR
1	A	75	MET
1	A	84	SER
1	A	89	GLN
1	A	115	THR
1	A	118	SER
1	A	122	THR
1	A	133	GLU
1	A	137	ILE
1	A	145	LYS
1	A	147	LEU
1	A	172	GLU
1	A	196	LYS
1	A	197	ARG
1	A	198	SER
1	A	204	ARG
1	A	213	GLU
1	A	220	LYS
1	A	244	ARG
1	A	251	ILE
1	A	253	VAL
1	A	265	GLU
1	A	292	ARG
1	A	327	ILE
1	A	330	THR
1	A	334	ARG
1	A	356	GLU
1	A	360	ARG
1	A	370	ASP
1	A	379	GLN

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Mol	Chain	Res	Type
1	A	388	ARG
1	A	402	ASN
1	A	404	LYS
1	A	431	ARG
1	A	440	SER
1	A	459	SER
1	A	461	THR
1	B	1	MET
1	B	23	MET
1	B	60	THR
1	B	84	SER
1	B	100	ILE
1	B	111	GLU
1	B	115	THR
1	B	117	LEU
1	B	121	ASN
1	B	145	LYS
1	B	154	GLU
1	B	173	LYS
1	B	197	ARG
1	B	198	SER
1	B	201	ILE
1	B	204	ARG
1	B	213	GLU
1	B	220	LYS
1	B	244	ARG
1	B	251	ILE
1	B	253	VAL
1	B	257	ILE
1	B	265	GLU
1	B	289	ARG
1	B	292	ARG
1	B	306	THR
1	B	327	ILE
1	B	330	THR
1	B	334	ARG
1	B	356	GLU
1	B	360	ARG
1	B	370	ASP
1	B	379	GLN
1	B	388	ARG
1	B	402	ASN

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Mol	Chain	Res	Type
1	B	431	ARG
1	B	459	SER
1	B	461	THR
1	C	1	MET
1	C	23	MET
1	C	60	THR
1	C	71	GLU
1	C	75	MET
1	C	76	LYS
1	C	77	LEU
1	C	85	LEU
1	C	90	THR
1	C	92	THR
1	C	97	LYS
1	C	98	SER
1	C	100	ILE
1	C	103	SER
1	C	104	GLU
1	C	111	GLU
1	C	113	PHE
1	C	114	THR
1	C	117	LEU
1	C	132	MET
1	C	143	ILE
1	C	144	CYS
1	C	145	LYS
1	C	147	LEU
1	C	152	LEU
1	C	160	LEU
1	C	164	SER
1	C	170	LEU
1	C	173	LYS
1	C	174	ASP
1	C	193	PHE
1	C	201	ILE
1	C	204	ARG
1	C	213	GLU
1	C	220	LYS
1	C	237	SER
1	C	244	ARG
1	C	253	VAL
1	C	257	ILE

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Mol	Chain	Res	Type
1	C	265	GLU
1	C	292	ARG
1	C	327	ILE
1	C	330	THR
1	C	334	ARG
1	C	356	GLU
1	C	360	ARG
1	C	370	ASP
1	C	379	GLN
1	C	385	ARG
1	C	388	ARG
1	C	404	LYS
1	C	431	ARG
1	C	440	SER
1	C	459	SER
1	C	461	THR
1	D	1	MET
1	D	23	MET
1	D	60	THR
1	D	73	ARG
1	D	84	SER
1	D	85	LEU
1	D	98	SER
1	D	105	MET
1	D	111	GLU
1	D	114	THR
1	D	117	LEU
1	D	118	SER
1	D	121	ASN
1	D	149	ASN
1	D	151	ASP
1	D	154	GLU
1	D	173	LYS
1	D	197	ARG
1	D	204	ARG
1	D	213	GLU
1	D	220	LYS
1	D	244	ARG
1	D	253	VAL
1	D	265	GLU
1	D	292	ARG
1	D	312	SER

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Mol	Chain	Res	Type
1	D	327	ILE
1	D	330	THR
1	D	334	ARG
1	D	356	GLU
1	D	360	ARG
1	D	379	GLN
1	D	388	ARG
1	D	402	ASN
1	D	421	LYS
1	D	431	ARG
1	D	449	VAL
1	D	459	SER
1	D	461	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	155	ASN
1	A	206	HIS
1	A	287	ASN
1	A	402	ASN
1	B	224	GLN
1	B	402	ASN
1	C	159	ASN
1	C	206	HIS
1	C	224	GLN
1	C	444	HIS
1	D	402	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	701	-	4,4,4	0.88	0	6,6,6	1.36	1 (16%)
2	SO4	B	702	-	4,4,4	0.75	0	6,6,6	0.95	1 (16%)
2	SO4	C	703	-	4,4,4	1.20	1 (25%)	6,6,6	0.81	0
2	SO4	D	704	-	4,4,4	0.96	0	6,6,6	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	701	-	-	0/0/0/0	0/0/0/0
2	SO4	B	702	-	-	0/0/0/0	0/0/0/0
2	SO4	C	703	-	-	0/0/0/0	0/0/0/0
2	SO4	D	704	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	703	SO4	O4-S	2.04	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	702	SO4	O2-S-O1	2.20	116.46	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	SO4	O2-S-O1	3.05	119.18	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	704	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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^2)	Q<0.9
1	A	461/470 (98%)	-0.48	1 (0%) 95 94	5, 18, 50, 75	0
1	B	461/470 (98%)	-0.59	1 (0%) 95 94	5, 13, 37, 73	0
1	C	461/470 (98%)	-0.24	25 (5%) 29 19	5, 17, 71, 100	6 (1%)
1	D	461/470 (98%)	-0.65	0 100 100	4, 11, 33, 69	0
All	All	1844/1880 (98%)	-0.49	27 (1%) 76 68	4, 14, 53, 100	6 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	36	SER	4.9
1	C	77	LEU	4.8
1	C	106	VAL	4.0
1	C	80	GLY	3.9
1	C	81	ASN	3.5
1	C	146	VAL	3.2
1	C	142	VAL	3.1
1	C	135	THR	3.0
1	C	90	THR	3.0
1	C	105	MET	2.9
1	C	118	SER	2.7
1	C	79	GLY	2.7
1	A	118	SER	2.6
1	C	102	ASN	2.5
1	C	37	HIS	2.5
1	C	75	MET	2.4
1	B	12	PRO	2.4
1	C	171	ALA	2.4
1	C	152	LEU	2.4
1	C	104	GLU	2.3
1	C	136	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	101	GLY	2.1
1	C	108	VAL	2.1
1	C	144	CYS	2.0
1	C	83	VAL	2.0
1	C	120	GLY	2.0
1	C	99	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	D	704	5/5	0.99	0.13	-0.48	44,44,45,46	0
2	SO4	A	701	5/5	0.97	0.11	-0.68	21,22,23,23	0
2	SO4	B	702	5/5	0.97	0.12	-0.84	18,19,20,20	0
2	SO4	C	703	5/5	0.98	0.10	-1.12	10,11,12,14	0

6.5 Other polymers (i)

There are no such residues in this entry.