WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:42 PM EDT

PDB ID : 1LDB
Title : STRUCTURE DETERMINATION AND REFINEMENT OF BACILLUS STEAROTHERMOPHILUS LACTATE DEHYDROGENASE
Authors : Piontek, K.; Rossmann, M.G.
Deposited on : 1989-03-27
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
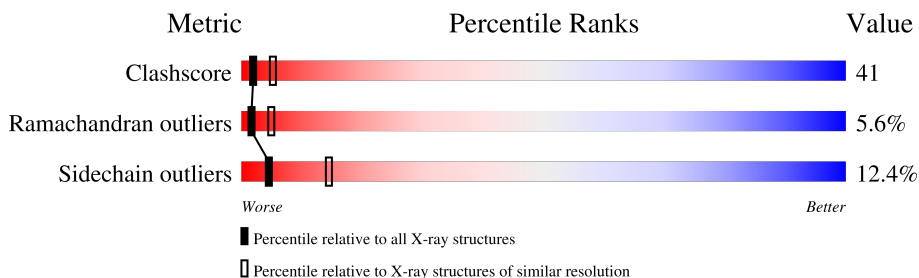Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		41
Ramachandran outliers		5.6%
Sidechain outliers		12.4%

Worse   *Better*

▐ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	317	28% / 36% / 20% / 9% / 7%
1	B	317	28% / 34% / 21% / 9% / 7%
1	C	317	27% / 37% / 21% / 8% / 7%
1	D	317	27% / 36% / 21% / 8% / 7%

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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9119 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 APO-L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total 2277	C 1457	N 390	O 422	S 8	0	0	0
1	B	294	Total 2277	C 1457	N 390	O 422	S 8	0	0	0
1	C	294	Total 2277	C 1457	N 390	O 422	S 8	0	0	0
1	D	294	Total 2277	C 1457	N 390	O 422	S 8	0	0	0

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

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

- Molecule 3 is water.

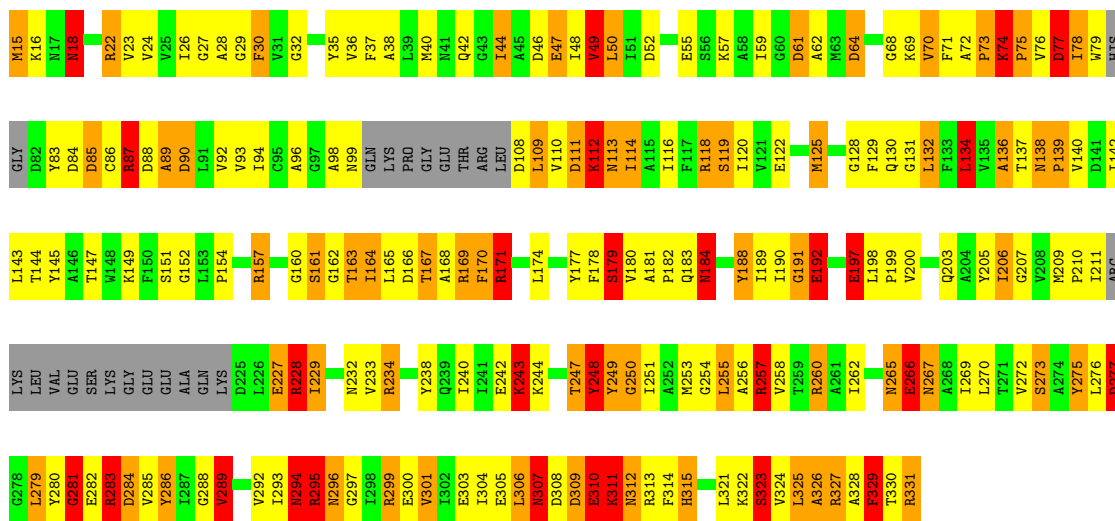| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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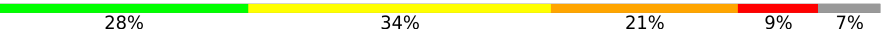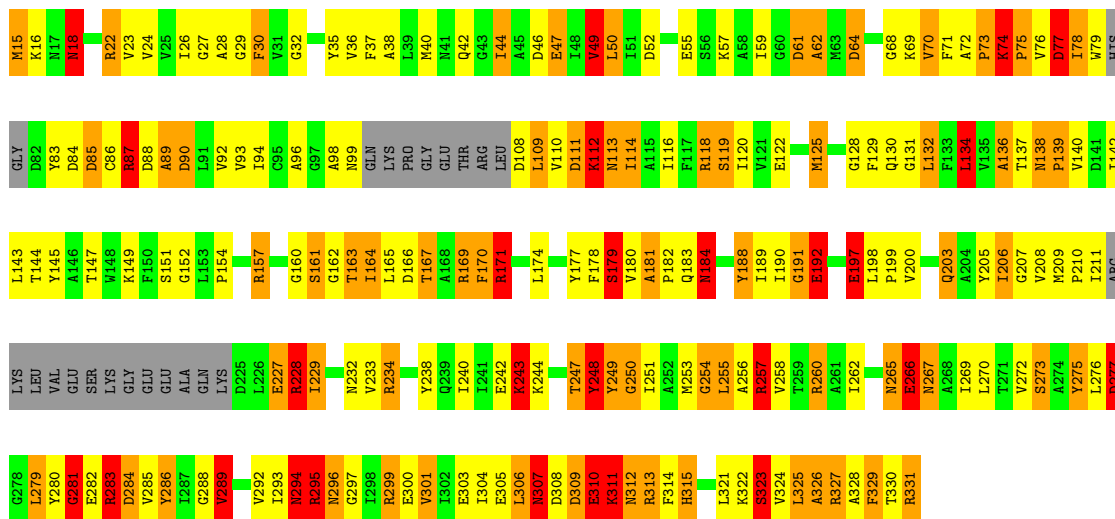
Note EDS was not executed.

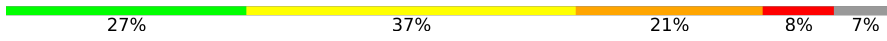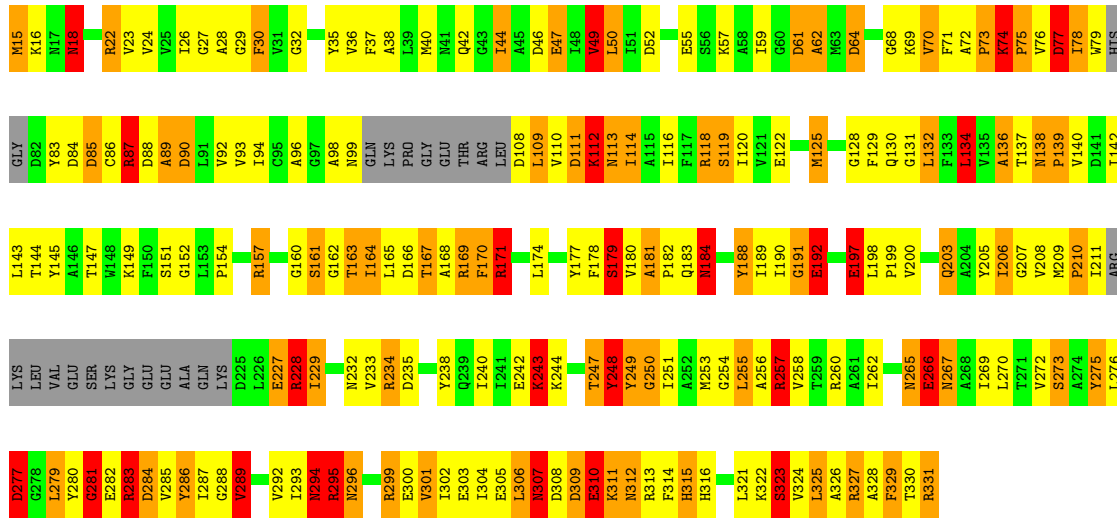• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain A:

• Molecule 1: APO-L-LACTATE DEHYDROGENASE

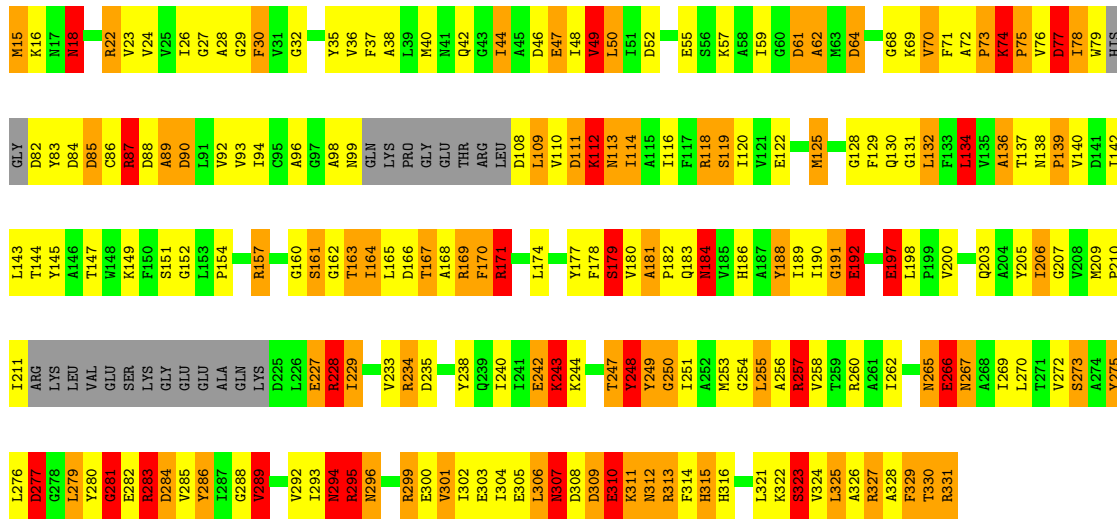Chain B:

• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain C: 27% 37% 21% 8% 7%

M15 K16 N17 N18 R22 V23 V24 V25 I26 G27 A28 G29 F30 V31 G32 Y35 V36 F37 A38 L39 M40 N41 Q42 G43 I44 A45 D46 E47 I48 V49 L50 I51 D52 E55 S56 K57 A58 I59 G60 D61 A62 M63 D64 G68 K69 V70 F71 A72 P73 K74 P75 V76 D77 I78 W79 HIS

GLY D82 Y83 D84 D85 C86 R87 D88 A89 D90 L91 V92 V93 I94 C95 A96 G97 A98 N99 GLN LYS PRO GLY GLU THR ARG LEU D108 L109 V110 D111 K112 N113 I114 A115 I116 F117 R118 S119 I120 V121 E122 M125 G128 F129 Q130 G131 L132 F133 L134 V135 A136 T137 N138 P139 V140 D141 I142

L143 T144 Y145 A146 T147 W148 K149 F150 S151 G152 L153 P154 R157 G160 S161 G162 T163 I164 L165 D166 T167 A168 R169 F170 R171 L174 Y177 F178 S179 V180 A181 P182 Q183 N184 Y188 I189 I190 G191 E192 E197 L198 P199 V200 Q203 A204 Y205 I206 G207 V208 M209 P210 I211 ARG

LYS LEU VAL GLU SER LYS GLY GLU GLU ALA GLN LYS D225 L226 E227 R228 I229 N232 V233 R234 D235 Y238 Q239 I240 I241 E242 K243 K244 T247 Y248 Y249 G250 I251 A252 M253 G254 L255 A256 R267 V258 T259 R260 A261 I262 N265 E266 N267 A268 I269 L270 T271 V272 S273 A274 Y275 L276

D277 G278 L279 Y280 G281 E282 R283 D284 V285 Y286 I287 G288 V289 V292 I293 N294 R295 N296 R299 E300 V301 I302 E303 I304 E305 L306 N307 D308 D309 E310 K311 N312 R313 F314 H315 H316 L321 K322 S323 V324 L325 A326 R327 A328 F329 T330 R331

• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain D: 27% 36% 21% 8% 7%

M15 K16 N17 N18 R22 V23 V24 V25 I26 G27 A28 G29 F30 V31 G32 Y35 V36 F37 A38 L39 M40 N41 Q42 G43 I44 A45 D46 E47 I48 V49 L50 I51 D52 E55 S56 K57 A58 I59 G60 D61 A62 M63 D64 G68 K69 V70 F71 A72 P73 K74 P75 V76 D77 I78 W79 HIS

GLY D82 Y83 D84 D85 C86 R87 D88 A89 D90 L91 V92 V93 I94 C95 A96 G97 A98 N99 GLN LYS PRO GLY GLU THR ARG LEU D108 L109 V110 D111 K112 N113 I114 A115 I116 F117 R118 S119 I120 V121 E122 M125 G128 F129 Q130 G131 L132 F133 L134 V135 A136 T137 N138 P139 V140 D141 I142

L143 T144 Y145 A146 T147 W148 K149 F150 S151 G152 L153 P154 R157 G160 S161 G162 T163 I164 L165 D166 T167 A168 R169 F170 R171 L174 Y177 F178 S179 V180 A181 P182 Q183 N184 V185 H186 A187 Y188 I189 I190 G191 E192 E197 L198 P199 V200 Q203 A204 Y205 I206 G207 V208 M209 P210

I211 ARG LYS LEU VAL GLU SER LYS GLY GLU GLU ALA GLN LYS D225 L226 E227 R228 I229 V233 R234 D235 Y238 Q239 I240 I241 E242 K243 K244 T247 Y248 Y249 G250 I251 A252 M253 G254 L255 A256 R267 V258 T259 R260 A261 I262 N265 E266 N267 A268 I269 L270 T271 V272 S273 A274 Y275

L276 D277 G278 L279 Y280 G281 E282 R283 D284 V285 Y286 I287 G288 V289 V292 I293 N294 R295 N296 R299 E300 V301 I302 E303 I304 E305 L306 N307 D308 D309 E310 K311 N312 R313 F314 H315 H316 L321 K322 S323 V324 L325 A326 R327 A328 F329 T330 R331

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	86.90Å 86.90Å 357.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.286 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9119	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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:
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	1.56	15/2320 (0.6%)	2.68	142/3146 (4.5%)
1	B	1.56	15/2320 (0.6%)	2.69	143/3146 (4.5%)
1	C	1.56	15/2320 (0.6%)	2.69	141/3146 (4.5%)
1	D	1.56	15/2320 (0.6%)	2.69	141/3146 (4.5%)
All	All	1.56	60/9280 (0.6%)	2.69	567/12584 (4.5%)

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	31
1	B	0	32
1	C	0	31
1	D	0	31
All	All	0	125

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	188	TYR	CG-CD1	8.15	1.49	1.39
1	A	188	TYR	CG-CD1	8.14	1.49	1.39
1	C	188	TYR	CG-CD1	8.13	1.49	1.39
1	B	188	TYR	CG-CD1	8.03	1.49	1.39
1	C	192	GLU	CD-OE1	-6.89	1.18	1.25
1	D	192	GLU	CD-OE1	-6.84	1.18	1.25
1	A	192	GLU	CD-OE1	-6.79	1.18	1.25
1	B	192	GLU	CD-OE1	-6.74	1.18	1.25
1	B	119	SER	CB-OG	6.24	1.50	1.42
1	D	44	ILE	C-O	6.24	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ILE	C-O	6.18	1.35	1.23
1	A	119	SER	CB-OG	6.17	1.50	1.42
1	C	119	SER	CB-OG	6.16	1.50	1.42
1	C	44	ILE	C-O	6.14	1.35	1.23
1	D	119	SER	CB-OG	6.14	1.50	1.42
1	B	44	ILE	C-O	6.10	1.34	1.23
1	C	134	LEU	N-CA	6.03	1.58	1.46
1	D	134	LEU	N-CA	6.00	1.58	1.46
1	A	134	LEU	N-CA	6.00	1.58	1.46
1	B	134	LEU	N-CA	5.98	1.58	1.46
1	C	151	SER	CB-OG	5.96	1.50	1.42
1	A	151	SER	CB-OG	5.82	1.49	1.42
1	B	151	SER	CB-OG	5.82	1.49	1.42
1	D	151	SER	CB-OG	5.81	1.49	1.42
1	A	283	ARG	C-O	5.71	1.34	1.23
1	D	283	ARG	C-O	5.67	1.34	1.23
1	D	179	SER	CB-OG	5.65	1.49	1.42
1	C	283	ARG	C-O	5.65	1.34	1.23
1	C	254	GLY	C-O	5.64	1.32	1.23
1	D	254	GLY	C-O	5.64	1.32	1.23
1	C	179	SER	CB-OG	5.64	1.49	1.42
1	A	254	GLY	C-O	5.64	1.32	1.23
1	B	283	ARG	C-O	5.64	1.34	1.23
1	A	179	SER	CB-OG	5.59	1.49	1.42
1	B	179	SER	CB-OG	5.54	1.49	1.42
1	B	254	GLY	C-O	5.54	1.32	1.23
1	C	30	PHE	C-O	5.53	1.33	1.23
1	B	30	PHE	C-O	5.52	1.33	1.23
1	B	281	GLY	N-CA	5.46	1.54	1.46
1	D	30	PHE	C-O	5.45	1.33	1.23
1	A	30	PHE	C-O	5.43	1.33	1.23
1	A	281	GLY	N-CA	5.40	1.54	1.46
1	C	281	GLY	N-CA	5.39	1.54	1.46
1	D	281	GLY	N-CA	5.30	1.53	1.46
1	B	277	ASP	CA-CB	5.28	1.65	1.53
1	C	277	ASP	CA-CB	5.26	1.65	1.53
1	A	277	ASP	CA-CB	5.25	1.65	1.53
1	D	162	GLY	C-O	5.19	1.31	1.23
1	D	277	ASP	CA-CB	5.19	1.65	1.53
1	A	162	GLY	C-O	5.12	1.31	1.23
1	C	163	THR	C-O	5.12	1.33	1.23
1	C	162	GLY	C-O	5.12	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	GLY	C-O	5.08	1.31	1.23
1	B	163	THR	C-O	5.07	1.32	1.23
1	A	138	ASN	N-CA	5.04	1.56	1.46
1	A	163	THR	C-O	5.03	1.32	1.23
1	C	138	ASN	N-CA	5.02	1.56	1.46
1	D	163	THR	C-O	5.01	1.32	1.23
1	B	138	ASN	N-CA	5.01	1.56	1.46
1	D	282	GLU	CD-OE1	-5.01	1.20	1.25

All (567) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH1	35.23	137.92	120.30
1	B	169	ARG	NE-CZ-NH1	35.19	137.90	120.30
1	D	169	ARG	NE-CZ-NH1	35.12	137.86	120.30
1	C	169	ARG	NE-CZ-NH1	35.09	137.84	120.30
1	C	260	ARG	NE-CZ-NH1	-24.25	108.17	120.30
1	B	260	ARG	NE-CZ-NH1	-24.15	108.22	120.30
1	D	260	ARG	NE-CZ-NH1	-24.15	108.22	120.30
1	A	260	ARG	NE-CZ-NH1	-24.02	108.29	120.30
1	A	171	ARG	NE-CZ-NH1	-20.99	109.81	120.30
1	B	171	ARG	NE-CZ-NH1	-20.94	109.83	120.30
1	C	171	ARG	NE-CZ-NH1	-20.94	109.83	120.30
1	D	171	ARG	NE-CZ-NH1	-20.80	109.90	120.30
1	D	228	ARG	NE-CZ-NH1	-18.72	110.94	120.30
1	A	228	ARG	NE-CZ-NH1	-18.66	110.97	120.30
1	C	228	ARG	NE-CZ-NH1	-18.64	110.98	120.30
1	B	228	ARG	NE-CZ-NH1	-18.60	111.00	120.30
1	B	111	ASP	CB-CG-OD1	17.88	134.39	118.30
1	A	111	ASP	CB-CG-OD1	17.87	134.38	118.30
1	C	111	ASP	CB-CG-OD1	17.84	134.36	118.30
1	D	111	ASP	CB-CG-OD1	17.81	134.33	118.30
1	D	249	TYR	CB-CG-CD1	16.55	130.93	121.00
1	C	249	TYR	CB-CG-CD1	16.48	130.88	121.00
1	B	249	TYR	CB-CG-CD1	16.41	130.85	121.00
1	A	249	TYR	CB-CG-CD1	16.37	130.82	121.00
1	A	249	TYR	CB-CG-CD2	-14.44	112.34	121.00
1	B	249	TYR	CB-CG-CD2	-14.43	112.34	121.00
1	D	249	TYR	CB-CG-CD2	-14.42	112.35	121.00
1	A	276	LEU	C-N-CA	14.35	157.57	121.70
1	D	276	LEU	C-N-CA	14.35	157.57	121.70
1	C	276	LEU	C-N-CA	14.34	157.54	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	LEU	C-N-CA	14.32	157.51	121.70
1	C	249	TYR	CB-CG-CD2	-14.30	112.42	121.00
1	B	309	ASP	CB-CG-OD2	14.18	131.06	118.30
1	C	309	ASP	CB-CG-OD2	14.16	131.04	118.30
1	A	309	ASP	CB-CG-OD2	14.07	130.97	118.30
1	D	309	ASP	CB-CG-OD2	14.06	130.96	118.30
1	A	52	ASP	CB-CG-OD1	13.44	130.39	118.30
1	B	52	ASP	CB-CG-OD1	13.36	130.32	118.30
1	D	52	ASP	CB-CG-OD1	13.33	130.30	118.30
1	C	52	ASP	CB-CG-OD1	13.30	130.27	118.30
1	B	87	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	C	87	ARG	NE-CZ-NH1	13.09	126.84	120.30
1	D	87	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	A	87	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	C	77	ASP	CB-CG-OD2	-12.82	106.76	118.30
1	B	77	ASP	CB-CG-OD2	-12.79	106.79	118.30
1	D	77	ASP	CB-CG-OD2	-12.75	106.83	118.30
1	A	125	MET	CG-SD-CE	12.74	120.59	100.20
1	D	125	MET	CG-SD-CE	12.73	120.57	100.20
1	A	77	ASP	CB-CG-OD2	-12.72	106.85	118.30
1	B	125	MET	CG-SD-CE	12.72	120.56	100.20
1	C	125	MET	CG-SD-CE	12.71	120.54	100.20
1	B	169	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	A	169	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	D	169	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	C	169	ARG	NE-CZ-NH2	-12.17	114.21	120.30
1	C	169	ARG	CD-NE-CZ	11.88	140.22	123.60
1	B	169	ARG	CD-NE-CZ	11.86	140.20	123.60
1	A	169	ARG	CD-NE-CZ	11.83	140.16	123.60
1	D	169	ARG	CD-NE-CZ	11.83	140.16	123.60
1	B	308	ASP	CB-CG-OD1	11.74	128.87	118.30
1	D	308	ASP	CB-CG-OD1	11.71	128.84	118.30
1	A	308	ASP	CB-CG-OD1	11.69	128.82	118.30
1	A	260	ARG	NE-CZ-NH2	11.69	126.14	120.30
1	C	308	ASP	CB-CG-OD1	11.68	128.82	118.30
1	C	260	ARG	NE-CZ-NH2	11.65	126.13	120.30
1	B	260	ARG	NE-CZ-NH2	11.63	126.12	120.30
1	D	260	ARG	NE-CZ-NH2	11.60	126.10	120.30
1	B	228	ARG	CD-NE-CZ	-11.59	107.38	123.60
1	C	228	ARG	CD-NE-CZ	-11.58	107.39	123.60
1	D	228	ARG	CD-NE-CZ	-11.58	107.39	123.60
1	A	228	ARG	CD-NE-CZ	-11.56	107.41	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	ARG	NH1-CZ-NH2	-11.31	106.96	119.40
1	A	169	ARG	NH1-CZ-NH2	-11.29	106.99	119.40
1	B	169	ARG	NH1-CZ-NH2	-11.27	107.01	119.40
1	D	169	ARG	NH1-CZ-NH2	-11.26	107.02	119.40
1	D	234	ARG	NE-CZ-NH2	-11.11	114.74	120.30
1	B	234	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	C	234	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	234	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	B	69	LYS	CA-CB-CG	10.51	136.52	113.40
1	D	69	LYS	CA-CB-CG	10.51	136.53	113.40
1	A	69	LYS	CA-CB-CG	10.50	136.50	113.40
1	C	69	LYS	CA-CB-CG	10.46	136.41	113.40
1	B	85	ASP	CB-CG-OD2	-10.26	109.07	118.30
1	A	85	ASP	CB-CG-OD2	-10.25	109.08	118.30
1	D	85	ASP	CB-CG-OD2	-10.21	109.11	118.30
1	C	85	ASP	CB-CG-OD2	-10.16	109.16	118.30
1	D	277	ASP	CB-CG-OD1	9.97	127.27	118.30
1	C	277	ASP	CB-CG-OD1	9.96	127.26	118.30
1	C	46	ASP	CB-CG-OD1	9.86	127.18	118.30
1	B	277	ASP	CB-CG-OD1	9.86	127.17	118.30
1	A	277	ASP	CB-CG-OD1	9.82	127.14	118.30
1	D	46	ASP	CB-CG-OD1	9.78	127.10	118.30
1	C	286	TYR	CB-CG-CD1	9.70	126.82	121.00
1	A	46	ASP	CB-CG-OD1	9.70	127.03	118.30
1	B	46	ASP	CB-CG-OD1	9.70	127.03	118.30
1	D	118	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	D	286	TYR	CB-CG-CD1	9.65	126.79	121.00
1	A	286	TYR	CB-CG-CD1	9.64	126.78	121.00
1	B	286	TYR	CB-CG-CD1	9.62	126.77	121.00
1	B	309	ASP	CA-CB-CG	9.61	134.55	113.40
1	C	118	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	D	310	GLU	CA-CB-CG	9.59	134.50	113.40
1	B	118	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	310	GLU	CA-CB-CG	9.57	134.46	113.40
1	C	310	GLU	CA-CB-CG	9.57	134.45	113.40
1	C	309	ASP	CA-CB-CG	9.56	134.43	113.40
1	A	309	ASP	CA-CB-CG	9.54	134.39	113.40
1	B	310	GLU	CA-CB-CG	9.54	134.39	113.40
1	D	309	ASP	CA-CB-CG	9.51	134.32	113.40
1	A	118	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	C	87	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	C	228	ARG	NE-CZ-NH2	9.36	124.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	87	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	C	309	ASP	OD1-CG-OD2	-9.35	105.53	123.30
1	A	309	ASP	OD1-CG-OD2	-9.35	105.54	123.30
1	D	309	ASP	OD1-CG-OD2	-9.34	105.55	123.30
1	B	228	ARG	NE-CZ-NH2	9.34	124.97	120.30
1	D	228	ARG	NE-CZ-NH2	9.34	124.97	120.30
1	B	309	ASP	OD1-CG-OD2	-9.33	105.58	123.30
1	A	228	ARG	NE-CZ-NH2	9.29	124.94	120.30
1	A	87	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	D	276	LEU	O-C-N	-9.14	108.08	122.70
1	A	276	LEU	O-C-N	-9.13	108.10	122.70
1	B	22	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	C	276	LEU	O-C-N	-9.12	108.11	122.70
1	B	276	LEU	O-C-N	-9.11	108.13	122.70
1	C	22	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	D	22	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	D	87	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	A	22	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	D	326	ALA	CB-CA-C	8.99	123.59	110.10
1	C	326	ALA	CB-CA-C	8.99	123.58	110.10
1	A	326	ALA	CB-CA-C	8.93	123.49	110.10
1	B	326	ALA	CB-CA-C	8.92	123.48	110.10
1	D	299	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	D	281	GLY	CA-C-O	-8.68	104.98	120.60
1	A	281	GLY	CA-C-O	-8.64	105.05	120.60
1	C	281	GLY	CA-C-O	-8.63	105.06	120.60
1	B	281	GLY	CA-C-O	-8.62	105.09	120.60
1	C	111	ASP	N-CA-CB	8.60	126.08	110.60
1	C	299	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	B	111	ASP	N-CA-CB	8.59	126.06	110.60
1	D	111	ASP	N-CA-CB	8.58	126.04	110.60
1	A	111	ASP	N-CA-CB	8.56	126.02	110.60
1	C	89	ALA	N-CA-CB	-8.54	98.15	110.10
1	B	89	ALA	N-CA-CB	-8.51	98.18	110.10
1	B	248	TYR	CB-CG-CD2	8.49	126.09	121.00
1	A	299	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	B	299	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	D	89	ALA	N-CA-CB	-8.47	98.24	110.10
1	D	248	TYR	CB-CG-CD2	8.47	126.08	121.00
1	A	89	ALA	N-CA-CB	-8.46	98.26	110.10
1	C	248	TYR	CB-CG-CD2	8.42	126.05	121.00
1	A	74	LYS	N-CA-C	8.40	133.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	74	LYS	N-CA-C	8.40	133.68	111.00
1	D	74	LYS	N-CA-C	8.39	133.65	111.00
1	B	74	LYS	N-CA-C	8.38	133.64	111.00
1	A	248	TYR	CB-CG-CD2	8.37	126.02	121.00
1	C	171	ARG	CD-NE-CZ	-8.18	112.15	123.60
1	B	171	ARG	CD-NE-CZ	-8.15	112.19	123.60
1	D	171	ARG	CD-NE-CZ	-8.15	112.19	123.60
1	B	84	ASP	CB-CG-OD1	8.14	125.62	118.30
1	A	171	ARG	CD-NE-CZ	-8.13	112.22	123.60
1	C	84	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	84	ASP	CB-CG-OD1	8.07	125.56	118.30
1	D	260	ARG	CD-NE-CZ	-8.06	112.31	123.60
1	A	260	ARG	CD-NE-CZ	-8.06	112.32	123.60
1	B	260	ARG	CD-NE-CZ	-8.06	112.32	123.60
1	D	84	ASP	CB-CG-OD1	8.05	125.54	118.30
1	C	260	ARG	CD-NE-CZ	-8.05	112.34	123.60
1	C	308	ASP	CA-CB-CG	7.91	130.79	113.40
1	D	308	ASP	CA-CB-CG	7.89	130.75	113.40
1	B	308	ASP	CA-CB-CG	7.86	130.69	113.40
1	A	308	ASP	CA-CB-CG	7.85	130.67	113.40
1	C	57	LYS	CD-CE-NZ	7.79	129.62	111.70
1	D	57	LYS	CD-CE-NZ	7.79	129.62	111.70
1	B	57	LYS	CD-CE-NZ	7.78	129.59	111.70
1	A	57	LYS	CD-CE-NZ	7.74	129.51	111.70
1	A	197	GLU	OE1-CD-OE2	-7.71	114.05	123.30
1	D	197	GLU	OE1-CD-OE2	-7.69	114.07	123.30
1	B	197	GLU	OE1-CD-OE2	-7.68	114.09	123.30
1	C	197	GLU	OE1-CD-OE2	-7.64	114.13	123.30
1	D	242	GLU	CA-CB-CG	7.63	130.18	113.40
1	A	242	GLU	CA-CB-CG	7.62	130.16	113.40
1	C	242	GLU	CA-CB-CG	7.61	130.14	113.40
1	B	108	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	108	ASP	CB-CG-OD1	7.57	125.12	118.30
1	B	242	GLU	CA-CB-CG	7.57	130.06	113.40
1	B	174	LEU	CA-CB-CG	7.57	132.71	115.30
1	C	174	LEU	CA-CB-CG	7.57	132.71	115.30
1	A	174	LEU	CA-CB-CG	7.55	132.66	115.30
1	D	174	LEU	CA-CB-CG	7.55	132.66	115.30
1	D	108	ASP	CB-CG-OD1	7.54	125.09	118.30
1	C	108	ASP	CB-CG-OD1	7.49	125.04	118.30
1	D	47	GLU	OE1-CD-OE2	7.49	132.29	123.30
1	C	47	GLU	OE1-CD-OE2	7.47	132.26	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	47	GLU	OE1-CD-OE2	7.46	132.26	123.30
1	A	47	GLU	OE1-CD-OE2	7.45	132.24	123.30
1	D	46	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	C	46	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	A	111	ASP	OD1-CG-OD2	-7.38	109.28	123.30
1	A	46	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	B	111	ASP	OD1-CG-OD2	-7.36	109.31	123.30
1	B	46	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	D	111	ASP	OD1-CG-OD2	-7.30	109.42	123.30
1	D	277	ASP	OD1-CG-OD2	-7.29	109.46	123.30
1	C	277	ASP	OD1-CG-OD2	-7.28	109.47	123.30
1	C	111	ASP	OD1-CG-OD2	-7.28	109.47	123.30
1	B	277	ASP	OD1-CG-OD2	-7.27	109.48	123.30
1	A	277	ASP	OD1-CG-OD2	-7.26	109.51	123.30
1	A	87	ARG	O-C-N	7.21	134.23	122.70
1	B	87	ARG	O-C-N	7.20	134.21	122.70
1	D	308	ASP	CB-CA-C	7.20	124.79	110.40
1	C	308	ASP	CB-CA-C	7.19	124.77	110.40
1	B	308	ASP	CB-CA-C	7.17	124.74	110.40
1	D	87	ARG	O-C-N	7.17	134.18	122.70
1	C	87	ARG	O-C-N	7.14	134.13	122.70
1	D	305	GLU	CG-CD-OE2	-7.14	104.01	118.30
1	A	305	GLU	CG-CD-OE2	-7.14	104.02	118.30
1	C	305	GLU	CG-CD-OE2	-7.14	104.02	118.30
1	A	308	ASP	CB-CA-C	7.12	124.64	110.40
1	B	305	GLU	CG-CD-OE2	-7.11	104.07	118.30
1	B	40	MET	CG-SD-CE	-7.10	88.84	100.20
1	A	40	MET	CG-SD-CE	-7.08	88.87	100.20
1	C	40	MET	CG-SD-CE	-7.07	88.89	100.20
1	B	145	TYR	CB-CG-CD1	7.05	125.23	121.00
1	D	40	MET	CG-SD-CE	-7.03	88.95	100.20
1	A	313	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	D	313	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	C	29	GLY	O-C-N	-7.00	111.50	122.70
1	A	145	TYR	CB-CG-CD1	6.99	125.19	121.00
1	C	145	TYR	CB-CG-CD1	6.98	125.19	121.00
1	A	29	GLY	O-C-N	-6.97	111.54	122.70
1	A	64	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	B	29	GLY	O-C-N	-6.97	111.55	122.70
1	D	238	TYR	CG-CD2-CE2	6.96	126.87	121.30
1	A	238	TYR	CG-CD2-CE2	6.96	126.87	121.30
1	C	327	ARG	CD-NE-CZ	-6.96	113.86	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	GLY	O-C-N	-6.95	111.57	122.70
1	C	64	ASP	CB-CG-OD1	-6.95	112.04	118.30
1	D	327	ARG	CD-NE-CZ	-6.95	113.87	123.60
1	D	64	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	A	327	ARG	CD-NE-CZ	-6.93	113.89	123.60
1	B	64	ASP	CB-CG-OD1	-6.92	112.08	118.30
1	B	313	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	D	145	TYR	CB-CG-CD1	6.91	125.14	121.00
1	B	238	TYR	CG-CD2-CE2	6.90	126.82	121.30
1	B	327	ARG	CD-NE-CZ	-6.89	113.96	123.60
1	C	238	TYR	CG-CD2-CE2	6.88	126.80	121.30
1	D	299	ARG	NH1-CZ-NH2	6.86	126.94	119.40
1	C	313	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	299	ARG	NH1-CZ-NH2	6.84	126.93	119.40
1	B	299	ARG	NH1-CZ-NH2	6.81	126.89	119.40
1	C	299	ARG	NH1-CZ-NH2	6.79	126.87	119.40
1	D	61	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	C	134	LEU	CB-CA-C	6.75	123.02	110.20
1	B	134	LEU	CB-CA-C	6.75	123.02	110.20
1	A	134	LEU	CB-CA-C	6.73	122.99	110.20
1	B	61	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	D	74	LYS	CB-CA-C	-6.72	96.97	110.40
1	A	74	LYS	CB-CA-C	-6.71	96.97	110.40
1	D	134	LEU	CB-CA-C	6.71	122.95	110.20
1	C	74	LYS	CB-CA-C	-6.70	97.01	110.40
1	C	61	ASP	CB-CG-OD2	-6.68	112.28	118.30
1	B	74	LYS	CB-CA-C	-6.66	97.09	110.40
1	A	61	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	163	THR	CA-CB-CG2	6.64	121.70	112.40
1	C	292	VAL	CA-CB-CG2	6.63	120.84	110.90
1	D	292	VAL	CA-CB-CG2	6.63	120.84	110.90
1	A	299	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	313	ARG	CG-CD-NE	6.61	125.67	111.80
1	B	163	THR	CA-CB-CG2	6.60	121.64	112.40
1	D	313	ARG	CG-CD-NE	6.60	125.66	111.80
1	D	163	THR	CA-CB-CG2	6.59	121.63	112.40
1	B	292	VAL	CA-CB-CG2	6.59	120.78	110.90
1	C	163	THR	CA-CB-CG2	6.59	121.62	112.40
1	C	313	ARG	CG-CD-NE	6.57	125.60	111.80
1	B	313	ARG	CG-CD-NE	6.57	125.60	111.80
1	A	292	VAL	CA-CB-CG2	6.57	120.75	110.90
1	D	50	LEU	CA-CB-CG	6.57	130.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	C	22	ARG	CD-NE-CZ	-6.55	114.44	123.60
1	B	22	ARG	CD-NE-CZ	-6.54	114.44	123.60
1	C	50	LEU	CA-CB-CG	6.54	130.35	115.30
1	D	22	ARG	CD-NE-CZ	-6.54	114.45	123.60
1	B	50	LEU	CA-CB-CG	6.53	130.33	115.30
1	B	50	LEU	N-CA-CB	-6.53	97.35	110.40
1	A	50	LEU	CA-CB-CG	6.52	130.31	115.30
1	C	50	LEU	N-CA-CB	-6.50	97.40	110.40
1	A	22	ARG	CD-NE-CZ	-6.50	114.51	123.60
1	A	78	ILE	CA-CB-CG1	6.49	123.33	111.00
1	A	50	LEU	N-CA-CB	-6.49	97.42	110.40
1	A	161	SER	C-N-CA	6.47	135.88	122.30
1	D	50	LEU	N-CA-CB	-6.46	97.48	110.40
1	D	78	ILE	CA-CB-CG1	6.45	123.26	111.00
1	B	161	SER	C-N-CA	6.45	135.85	122.30
1	C	161	SER	C-N-CA	6.45	135.85	122.30
1	D	161	SER	C-N-CA	6.45	135.84	122.30
1	B	78	ILE	CA-CB-CG1	6.44	123.23	111.00
1	C	78	ILE	CA-CB-CG1	6.43	123.22	111.00
1	D	299	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	A	157	ARG	CG-CD-NE	6.41	125.27	111.80
1	C	323	SER	N-CA-CB	-6.41	100.88	110.50
1	B	157	ARG	CG-CD-NE	6.39	125.21	111.80
1	C	299	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	D	323	SER	N-CA-CB	-6.37	100.94	110.50
1	B	323	SER	N-CA-CB	-6.36	100.95	110.50
1	A	323	SER	N-CA-CB	-6.35	100.97	110.50
1	C	157	ARG	CG-CD-NE	6.35	125.13	111.80
1	C	191	GLY	O-C-N	-6.34	112.56	122.70
1	D	157	ARG	CG-CD-NE	6.33	125.09	111.80
1	D	313	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	A	313	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	D	37	PHE	CB-CG-CD2	6.30	125.21	120.80
1	D	191	GLY	O-C-N	-6.30	112.62	122.70
1	C	37	PHE	CB-CG-CD2	6.25	125.18	120.80
1	A	37	PHE	CB-CG-CD2	6.24	125.17	120.80
1	A	191	GLY	O-C-N	-6.24	112.72	122.70
1	B	191	GLY	O-C-N	-6.23	112.73	122.70
1	B	313	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	B	289	VAL	N-CA-CB	-6.22	97.81	111.50
1	C	289	VAL	N-CA-CB	-6.21	97.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ASN	CB-CA-C	6.21	122.81	110.40
1	C	296	ASN	CB-CA-C	6.20	122.81	110.40
1	A	279	LEU	CA-C-O	-6.20	107.09	120.10
1	A	289	VAL	N-CA-CB	-6.19	97.88	111.50
1	D	296	ASN	CB-CA-C	6.19	122.78	110.40
1	B	279	LEU	CA-C-O	-6.19	107.10	120.10
1	D	279	LEU	CA-C-O	-6.19	107.11	120.10
1	B	37	PHE	CB-CG-CD2	6.19	125.13	120.80
1	B	296	ASN	CB-CA-C	6.18	122.76	110.40
1	D	289	VAL	N-CA-CB	-6.17	97.92	111.50
1	C	313	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	C	47	GLU	CG-CD-OE2	-6.16	105.98	118.30
1	C	279	LEU	CA-C-O	-6.16	107.17	120.10
1	D	47	GLU	CG-CD-OE2	-6.15	106.00	118.30
1	B	47	GLU	CG-CD-OE2	-6.15	106.00	118.30
1	A	47	GLU	CG-CD-OE2	-6.12	106.06	118.30
1	A	279	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	279	LEU	CA-CB-CG	6.10	129.33	115.30
1	D	279	LEU	CA-CB-CG	6.09	129.31	115.30
1	C	132	LEU	CA-CB-CG	6.09	129.30	115.30
1	A	132	LEU	CA-CB-CG	6.08	129.28	115.30
1	C	164	ILE	CB-CG1-CD1	-6.08	96.88	113.90
1	B	132	LEU	CA-CB-CG	6.07	129.27	115.30
1	B	76	VAL	C-N-CA	6.07	136.88	121.70
1	B	164	ILE	CB-CG1-CD1	-6.07	96.90	113.90
1	C	279	LEU	CA-CB-CG	6.06	129.25	115.30
1	D	76	VAL	C-N-CA	6.06	136.86	121.70
1	D	132	LEU	CA-CB-CG	6.06	129.25	115.30
1	A	76	VAL	C-N-CA	6.05	136.81	121.70
1	D	164	ILE	CB-CG1-CD1	-6.05	96.97	113.90
1	A	164	ILE	CB-CG1-CD1	-6.04	96.98	113.90
1	C	76	VAL	C-N-CA	6.04	136.80	121.70
1	B	50	LEU	CB-CA-C	5.99	121.57	110.20
1	A	50	LEU	CB-CA-C	5.98	121.56	110.20
1	D	50	LEU	CB-CA-C	5.96	121.53	110.20
1	C	50	LEU	CB-CA-C	5.96	121.52	110.20
1	B	234	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	D	234	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	256	ALA	CB-CA-C	5.89	118.94	110.10
1	C	234	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	256	ALA	CB-CA-C	5.86	118.89	110.10
1	C	276	LEU	CA-C-O	5.84	132.37	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	256	ALA	CB-CA-C	5.84	118.86	110.10
1	B	276	LEU	CA-C-O	5.83	132.35	120.10
1	B	256	ALA	CB-CA-C	5.83	118.85	110.10
1	A	276	LEU	CA-C-O	5.83	132.35	120.10
1	A	234	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	276	LEU	CA-C-O	5.80	132.28	120.10
1	B	205	TYR	CB-CG-CD2	5.77	124.47	121.00
1	C	144	THR	N-CA-CB	5.77	121.26	110.30
1	C	294	ASN	CB-CA-C	5.76	121.93	110.40
1	A	184	ASN	CB-CG-ND2	5.75	130.51	116.70
1	D	205	TYR	CB-CG-CD2	5.75	124.45	121.00
1	C	286	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	D	144	THR	N-CA-CB	5.75	121.22	110.30
1	A	144	THR	N-CA-CB	5.74	121.21	110.30
1	C	184	ASN	CB-CG-ND2	5.74	130.47	116.70
1	B	144	THR	N-CA-CB	5.73	121.19	110.30
1	B	184	ASN	CB-CG-ND2	5.73	130.45	116.70
1	B	294	ASN	CB-CA-C	5.73	121.85	110.40
1	C	181	ALA	CB-CA-C	5.73	118.69	110.10
1	D	184	ASN	CB-CG-ND2	5.73	130.44	116.70
1	B	181	ALA	CB-CA-C	5.72	118.69	110.10
1	A	294	ASN	CB-CA-C	5.71	121.82	110.40
1	D	181	ALA	CB-CA-C	5.70	118.64	110.10
1	C	171	ARG	NH1-CZ-NH2	5.69	125.66	119.40
1	A	181	ALA	CB-CA-C	5.68	118.62	110.10
1	C	205	TYR	CB-CG-CD2	5.68	124.41	121.00
1	D	294	ASN	CB-CA-C	5.68	121.76	110.40
1	B	284	ASP	O-C-N	5.67	131.77	122.70
1	C	166	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	205	TYR	CB-CG-CD2	5.66	124.39	121.00
1	D	286	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	A	166	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	171	ARG	NH1-CZ-NH2	5.65	125.62	119.40
1	A	286	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	D	166	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	286	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	C	284	ASP	O-C-N	5.63	131.72	122.70
1	C	327	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	166	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	171	ARG	NH1-CZ-NH2	5.62	125.58	119.40
1	D	284	ASP	O-C-N	5.61	131.67	122.70
1	D	171	ARG	NH1-CZ-NH2	5.60	125.56	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	ASP	O-C-N	5.59	131.65	122.70
1	B	307	ASN	N-CA-CB	-5.57	100.58	110.60
1	C	315	HIS	CA-C-O	5.56	131.78	120.10
1	B	315	HIS	CA-C-O	5.54	131.74	120.10
1	D	307	ASN	N-CA-CB	-5.54	100.63	110.60
1	A	315	HIS	CA-C-O	5.53	131.72	120.10
1	A	257	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	307	ASN	N-CA-CB	-5.53	100.64	110.60
1	D	315	HIS	CA-C-O	5.53	131.70	120.10
1	B	111	ASP	CA-CB-CG	5.52	125.55	113.40
1	A	307	ASN	N-CA-CB	-5.52	100.67	110.60
1	A	111	ASP	CA-CB-CG	5.51	125.52	113.40
1	B	257	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	111	ASP	CA-CB-CG	5.50	125.50	113.40
1	D	111	ASP	CA-CB-CG	5.49	125.47	113.40
1	C	257	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	136	ALA	CA-C-O	-5.44	108.68	120.10
1	B	243	LYS	N-CA-CB	5.44	120.39	110.60
1	C	243	LYS	N-CA-CB	5.44	120.39	110.60
1	B	136	ALA	CA-C-O	-5.43	108.69	120.10
1	A	243	LYS	N-CA-CB	5.43	120.38	110.60
1	D	255	LEU	CB-CA-C	5.43	120.51	110.20
1	D	136	ALA	CA-C-O	-5.42	108.71	120.10
1	B	136	ALA	CA-C-N	5.42	129.13	117.20
1	B	255	LEU	CB-CA-C	5.42	120.49	110.20
1	C	136	ALA	CA-C-N	5.41	129.11	117.20
1	A	136	ALA	CA-C-N	5.41	129.11	117.20
1	D	243	LYS	N-CA-CB	5.41	120.34	110.60
1	D	136	ALA	CA-C-N	5.41	129.09	117.20
1	A	255	LEU	CB-CA-C	5.40	120.47	110.20
1	A	136	ALA	CA-C-O	-5.40	108.76	120.10
1	A	327	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	139	PRO	CA-C-O	-5.39	107.26	120.20
1	B	139	PRO	CA-C-O	-5.39	107.27	120.20
1	C	255	LEU	CB-CA-C	5.38	120.43	110.20
1	D	327	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	139	PRO	CA-C-O	-5.38	107.29	120.20
1	C	139	PRO	CA-C-O	-5.37	107.30	120.20
1	C	134	LEU	CB-CG-CD1	5.37	120.13	111.00
1	B	134	LEU	CB-CG-CD1	5.36	120.11	111.00
1	D	313	ARG	CB-CA-C	5.35	121.10	110.40
1	B	85	ASP	CB-CG-OD1	5.35	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	SER	N-CA-CB	5.35	118.52	110.50
1	D	257	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	134	LEU	CB-CG-CD1	5.34	120.07	111.00
1	B	306	LEU	CA-C-O	5.34	131.31	120.10
1	C	313	ARG	CB-CA-C	5.34	121.07	110.40
1	B	327	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	281	GLY	CA-C-N	5.33	128.93	117.20
1	A	85	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	281	GLY	CA-C-N	5.33	128.92	117.20
1	A	277	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	273	SER	N-CA-CB	5.32	118.48	110.50
1	C	70	VAL	C-N-CA	5.32	135.00	121.70
1	A	306	LEU	CA-C-O	5.32	131.27	120.10
1	A	313	ARG	CB-CA-C	5.32	121.04	110.40
1	B	277	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	313	ARG	CB-CA-C	5.32	121.03	110.40
1	D	273	SER	N-CA-CB	5.32	118.48	110.50
1	C	273	SER	N-CA-CB	5.31	118.47	110.50
1	D	134	LEU	CB-CG-CD1	5.31	120.03	111.00
1	A	70	VAL	C-N-CA	5.31	134.97	121.70
1	D	70	VAL	C-N-CA	5.31	134.97	121.70
1	C	306	LEU	CA-C-O	5.31	131.24	120.10
1	B	70	VAL	C-N-CA	5.30	134.96	121.70
1	B	281	GLY	CA-C-N	5.30	128.86	117.20
1	D	306	LEU	CA-C-O	5.30	131.23	120.10
1	B	84	ASP	OD1-CG-OD2	-5.30	113.23	123.30
1	A	177	TYR	CB-CG-CD2	-5.29	117.82	121.00
1	A	281	GLY	CA-C-N	5.29	128.84	117.20
1	D	109	LEU	CB-CA-C	-5.29	100.14	110.20
1	A	108	ASP	C-N-CA	5.29	134.92	121.70
1	C	109	LEU	CB-CA-C	-5.28	100.17	110.20
1	B	108	ASP	C-N-CA	5.28	134.90	121.70
1	C	108	ASP	C-N-CA	5.28	134.90	121.70
1	A	109	LEU	CB-CA-C	-5.27	100.18	110.20
1	D	85	ASP	CB-CG-OD1	5.27	123.04	118.30
1	D	108	ASP	C-N-CA	5.26	134.85	121.70
1	B	109	LEU	CB-CA-C	-5.25	100.22	110.20
1	D	266	GLU	CA-CB-CG	5.25	124.95	113.40
1	C	266	GLU	CA-CB-CG	5.25	124.94	113.40
1	C	277	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	277	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	84	ASP	OD1-CG-OD2	-5.24	113.34	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	GLU	CA-CB-CG	5.24	124.92	113.40
1	A	84	ASP	OD1-CG-OD2	-5.24	113.35	123.30
1	B	266	GLU	CA-CB-CG	5.24	124.92	113.40
1	C	85	ASP	CB-CG-OD1	5.23	123.00	118.30
1	C	327	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	84	ASP	OD1-CG-OD2	-5.21	113.41	123.30
1	B	49	VAL	CG1-CB-CG2	5.20	119.22	110.90
1	D	177	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	B	177	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	C	49	VAL	CG1-CB-CG2	5.19	119.20	110.90
1	D	49	VAL	CG1-CB-CG2	5.18	119.19	110.90
1	A	49	VAL	CG1-CB-CG2	5.17	119.17	110.90
1	B	282	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	D	327	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	283	ARG	CA-C-N	5.16	128.56	117.20
1	A	37	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	C	283	ARG	CA-C-N	5.16	128.54	117.20
1	D	227	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	132	LEU	N-CA-CB	-5.14	100.11	110.40
1	C	305	GLU	CG-CD-OE1	5.14	128.59	118.30
1	D	305	GLU	CG-CD-OE1	5.14	128.58	118.30
1	D	282	GLU	CG-CD-OE2	-5.14	108.03	118.30
1	C	282	GLU	CG-CD-OE2	-5.13	108.03	118.30
1	D	248	TYR	CG-CD2-CE2	5.13	125.41	121.30
1	D	114	ILE	CB-CG1-CD1	5.13	128.27	113.90
1	A	227	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	C	114	ILE	CB-CG1-CD1	5.13	128.27	113.90
1	A	283	ARG	CA-C-N	5.13	128.49	117.20
1	B	132	LEU	N-CA-CB	-5.13	100.14	110.40
1	B	248	TYR	CG-CD2-CE2	5.13	125.40	121.30
1	B	77	ASP	OD1-CG-OD2	5.13	133.05	123.30
1	B	114	ILE	CB-CG1-CD1	5.13	128.26	113.90
1	B	283	ARG	CA-C-N	5.13	128.48	117.20
1	A	114	ILE	CB-CG1-CD1	5.12	128.24	113.90
1	B	247	THR	CA-CB-CG2	5.12	119.57	112.40
1	D	132	LEU	N-CA-CB	-5.12	100.16	110.40
1	C	77	ASP	OD1-CG-OD2	5.12	133.03	123.30
1	D	309	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	177	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	309	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	227	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	A	282	GLU	CG-CD-OE2	-5.11	108.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	GLU	CG-CD-OE1	5.11	128.51	118.30
1	D	166	ASP	OD1-CG-OD2	-5.11	113.60	123.30
1	A	77	ASP	OD1-CG-OD2	5.10	133.00	123.30
1	C	166	ASP	OD1-CG-OD2	-5.10	113.61	123.30
1	A	112	LYS	CA-C-N	-5.10	105.98	117.20
1	A	305	GLU	CG-CD-OE1	5.10	128.50	118.30
1	D	77	ASP	OD1-CG-OD2	5.10	132.99	123.30
1	B	227	GLU	CG-CD-OE2	-5.10	108.11	118.30
1	A	327	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	247	THR	CA-CB-CG2	5.09	119.53	112.40
1	D	37	PHE	CB-CG-CD1	-5.09	117.24	120.80
1	D	112	LYS	CA-C-N	-5.09	106.00	117.20
1	C	132	LEU	N-CA-CB	-5.09	100.22	110.40
1	C	247	THR	CA-CB-CG2	5.08	119.52	112.40
1	B	327	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	37	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	B	62	ALA	CB-CA-C	5.07	117.70	110.10
1	C	112	LYS	CA-C-N	-5.07	106.06	117.20
1	A	166	ASP	OD1-CG-OD2	-5.06	113.68	123.30
1	D	247	THR	CA-CB-CG2	5.06	119.48	112.40
1	C	248	TYR	CG-CD2-CE2	5.06	125.35	121.30
1	B	112	LYS	CA-C-N	-5.05	106.08	117.20
1	A	248	TYR	CG-CD2-CE2	5.05	125.34	121.30
1	D	62	ALA	CB-CA-C	5.04	117.66	110.10
1	B	166	ASP	OD1-CG-OD2	-5.04	113.73	123.30
1	C	309	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	37	PHE	CB-CG-CD1	-5.03	117.28	120.80
1	B	311	LYS	O-C-N	5.03	130.75	122.70
1	C	62	ALA	CB-CA-C	5.03	117.64	110.10
1	A	311	LYS	O-C-N	5.01	130.72	122.70
1	B	297	GLY	CA-C-O	-5.01	111.58	120.60
1	B	277	ASP	N-CA-CB	-5.01	101.58	110.60
1	A	297	GLY	CA-C-O	-5.01	111.59	120.60

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Mainchain
1	A	134	LEU	Mainchain
1	A	147	THR	Mainchain
1	A	152	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	154	PRO	Mainchain
1	A	167	THR	Mainchain
1	A	170	PHE	Sidechain
1	A	171	ARG	Sidechain
1	A	184	ASN	Mainchain
1	A	188	TYR	Mainchain
1	A	191	GLY	Mainchain
1	A	206	ILE	Mainchain
1	A	207	GLY	Mainchain
1	A	229	ILE	Mainchain
1	A	23	VAL	Mainchain
1	A	275	TYR	Sidechain
1	A	281	GLY	Mainchain
1	A	285	VAL	Mainchain
1	A	286	TYR	Sidechain
1	A	295	ARG	Mainchain
1	A	30	PHE	Sidechain
1	A	300	GLU	Mainchain
1	A	301	VAL	Mainchain
1	A	310	GLU	Mainchain
1	A	312	ASN	Mainchain
1	A	323	SER	Mainchain
1	A	325	LEU	Mainchain
1	A	49	VAL	Mainchain
1	A	62	ALA	Mainchain
1	A	77	ASP	Mainchain
1	A	94	ILE	Mainchain
1	B	111	ASP	Mainchain
1	B	134	LEU	Mainchain
1	B	147	THR	Mainchain
1	B	152	GLY	Mainchain
1	B	154	PRO	Mainchain
1	B	167	THR	Mainchain
1	B	170	PHE	Sidechain
1	B	171	ARG	Sidechain
1	B	184	ASN	Mainchain
1	B	188	TYR	Mainchain
1	B	191	GLY	Mainchain
1	B	206	ILE	Mainchain
1	B	207	GLY	Mainchain
1	B	229	ILE	Mainchain
1	B	23	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	B	275	TYR	Sidechain
1	B	281	GLY	Mainchain
1	B	285	VAL	Mainchain
1	B	286	TYR	Sidechain
1	B	295	ARG	Mainchain
1	B	30	PHE	Sidechain
1	B	300	GLU	Mainchain
1	B	301	VAL	Mainchain
1	B	310	GLU	Mainchain
1	B	312	ASN	Mainchain
1	B	323	SER	Mainchain
1	B	325	LEU	Mainchain
1	B	326	ALA	Mainchain
1	B	49	VAL	Mainchain
1	B	62	ALA	Mainchain
1	B	77	ASP	Mainchain
1	B	94	ILE	Mainchain
1	C	111	ASP	Mainchain
1	C	134	LEU	Mainchain
1	C	147	THR	Mainchain
1	C	152	GLY	Mainchain
1	C	154	PRO	Mainchain
1	C	167	THR	Mainchain
1	C	170	PHE	Sidechain
1	C	171	ARG	Sidechain
1	C	184	ASN	Mainchain
1	C	188	TYR	Mainchain
1	C	191	GLY	Mainchain
1	C	206	ILE	Mainchain
1	C	207	GLY	Mainchain
1	C	229	ILE	Mainchain
1	C	23	VAL	Mainchain
1	C	275	TYR	Sidechain
1	C	281	GLY	Mainchain
1	C	285	VAL	Mainchain
1	C	286	TYR	Sidechain
1	C	295	ARG	Mainchain
1	C	30	PHE	Sidechain
1	C	300	GLU	Mainchain
1	C	301	VAL	Mainchain
1	C	310	GLU	Mainchain
1	C	312	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	C	323	SER	Mainchain
1	C	325	LEU	Mainchain
1	C	49	VAL	Mainchain
1	C	62	ALA	Mainchain
1	C	77	ASP	Mainchain
1	C	94	ILE	Mainchain
1	D	111	ASP	Mainchain
1	D	134	LEU	Mainchain
1	D	147	THR	Mainchain
1	D	152	GLY	Mainchain
1	D	154	PRO	Mainchain
1	D	167	THR	Mainchain
1	D	170	PHE	Sidechain
1	D	171	ARG	Sidechain
1	D	184	ASN	Mainchain
1	D	188	TYR	Mainchain
1	D	191	GLY	Mainchain
1	D	206	ILE	Mainchain
1	D	207	GLY	Mainchain
1	D	229	ILE	Mainchain
1	D	23	VAL	Mainchain
1	D	275	TYR	Sidechain
1	D	281	GLY	Mainchain
1	D	285	VAL	Mainchain
1	D	286	TYR	Sidechain
1	D	295	ARG	Mainchain
1	D	30	PHE	Sidechain
1	D	300	GLU	Mainchain
1	D	301	VAL	Mainchain
1	D	310	GLU	Mainchain
1	D	312	ASN	Mainchain
1	D	323	SER	Mainchain
1	D	325	LEU	Mainchain
1	D	49	VAL	Mainchain
1	D	62	ALA	Mainchain
1	D	77	ASP	Mainchain
1	D	94	ILE	Mainchain

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2277	0	2251	201	46
1	B	2277	0	2251	199	0
1	C	2277	0	2251	206	11
1	D	2277	0	2251	197	57
2	A	10	0	0	2	0
3	A	1	0	0	1	0
All	All	9119	0	9004	750	57

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 41.

All (750) 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:D:87:ARG:HG3	1:D:88:ASP:H	1.12	1.13
1:B:87:ARG:HG3	1:B:88:ASP:H	1.11	1.12
1:D:142:ILE:HD13	1:D:324:VAL:HG11	1.31	1.11
1:C:142:ILE:HD13	1:C:324:VAL:HG11	1.31	1.10
1:B:142:ILE:HD13	1:B:324:VAL:HG11	1.32	1.09
1:B:265:ASN:HD22	1:B:295:ARG:HB2	1.18	1.09
1:C:265:ASN:HD22	1:C:295:ARG:HB2	1.18	1.08
1:A:87:ARG:HG3	1:A:88:ASP:H	1.11	1.08
1:C:87:ARG:HG3	1:C:88:ASP:H	1.11	1.07
1:A:265:ASN:HD22	1:A:295:ARG:HB2	1.18	1.06
1:D:265:ASN:HD22	1:D:295:ARG:HB2	1.18	1.06
1:A:142:ILE:HD13	1:A:324:VAL:HG11	1.32	1.06
1:B:311:LYS:HA	1:B:315:HIS:HB2	1.40	1.03
1:A:311:LYS:HA	1:A:315:HIS:HB2	1.40	1.03
1:A:310:GLU:O	1:A:312:ASN:N	1.93	1.02
1:B:18:ASN:HD22	1:B:18:ASN:N	1.50	1.02
1:D:18:ASN:N	1:D:18:ASN:HD22	1.50	1.02
1:C:311:LYS:HA	1:C:315:HIS:HB2	1.41	1.02
1:D:18:ASN:H	1:D:18:ASN:ND2	1.53	1.02
1:B:310:GLU:O	1:B:312:ASN:N	1.93	1.01
1:C:310:GLU:O	1:C:312:ASN:N	1.93	1.00
1:D:310:GLU:O	1:D:312:ASN:N	1.93	1.00
1:B:18:ASN:ND2	1:B:18:ASN:H	1.53	1.00
1:A:18:ASN:H	1:A:18:ASN:ND2	1.53	1.00
1:C:18:ASN:N	1:C:18:ASN:HD22	1.49	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:LYS:HA	1:D:315:HIS:HB2	1.40	0.99
1:C:18:ASN:H	1:C:18:ASN:ND2	1.52	0.97
1:A:18:ASN:N	1:A:18:ASN:HD22	1.50	0.94
1:A:87:ARG:CG	1:A:88:ASP:H	1.77	0.94
1:B:87:ARG:CG	1:B:88:ASP:H	1.77	0.93
1:A:265:ASN:ND2	1:A:295:ARG:HB2	1.84	0.93
1:D:265:ASN:ND2	1:D:295:ARG:HB2	1.84	0.93
1:C:265:ASN:ND2	1:C:295:ARG:HB2	1.84	0.92
1:B:265:ASN:ND2	1:B:295:ARG:HB2	1.84	0.92
1:C:87:ARG:CG	1:C:88:ASP:H	1.77	0.92
1:C:87:ARG:HG3	1:C:88:ASP:N	1.86	0.91
1:D:87:ARG:HG3	1:D:88:ASP:N	1.86	0.90
1:A:87:ARG:HG3	1:A:88:ASP:N	1.86	0.90
1:B:87:ARG:HG3	1:B:88:ASP:N	1.86	0.90
1:A:142:ILE:CD1	1:A:324:VAL:HG11	2.04	0.88
1:C:87:ARG:NH1	1:C:87:ARG:HB2	1.89	0.88
1:B:87:ARG:HB2	1:B:87:ARG:NH1	1.89	0.88
1:C:200:VAL:HG11	1:C:304:ILE:HD12	1.56	0.87
1:D:87:ARG:CG	1:D:88:ASP:H	1.77	0.87
1:D:200:VAL:HG11	1:D:304:ILE:HD12	1.56	0.87
1:D:142:ILE:CD1	1:D:324:VAL:HG11	2.04	0.87
1:B:142:ILE:CD1	1:B:324:VAL:HG11	2.04	0.87
1:C:142:ILE:CD1	1:C:324:VAL:HG11	2.04	0.87
1:A:182:PRO:HB2	1:C:70:VAL:HG22	1.57	0.86
1:B:182:PRO:HB2	1:D:70:VAL:HG22	1.57	0.86
1:A:87:ARG:NH1	1:A:87:ARG:HB2	1.89	0.86
1:B:70:VAL:HG22	1:D:182:PRO:HB2	1.57	0.86
1:D:295:ARG:HG3	1:D:295:ARG:HH11	1.40	0.86
1:B:200:VAL:HG11	1:B:304:ILE:HD12	1.56	0.85
1:D:87:ARG:HB2	1:D:87:ARG:NH1	1.89	0.85
1:A:295:ARG:HG3	1:A:295:ARG:HH11	1.40	0.85
1:B:244:LYS:HG2	1:B:244:LYS:O	1.77	0.85
1:C:295:ARG:HG3	1:C:295:ARG:HH11	1.40	0.85
1:A:200:VAL:HG11	1:A:304:ILE:HD12	1.57	0.85
1:A:311:LYS:HA	1:A:315:HIS:CB	2.07	0.85
1:A:70:VAL:HG22	1:C:182:PRO:HB2	1.58	0.85
1:B:295:ARG:HG3	1:B:295:ARG:HH11	1.40	0.84
1:A:244:LYS:O	1:A:244:LYS:HG2	1.77	0.84
1:C:109:LEU:O	1:C:113:ASN:HB2	1.78	0.84
1:B:55:GLU:O	1:B:59:ILE:HD12	1.78	0.84
1:B:311:LYS:HA	1:B:315:HIS:CB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:LYS:HA	1:D:315:HIS:CB	2.07	0.83
1:D:109:LEU:O	1:D:113:ASN:HB2	1.78	0.83
1:B:109:LEU:O	1:B:113:ASN:HB2	1.78	0.83
1:D:55:GLU:O	1:D:59:ILE:HD12	1.78	0.83
1:A:55:GLU:O	1:A:59:ILE:HD12	1.78	0.83
1:A:109:LEU:O	1:A:113:ASN:HB2	1.78	0.83
1:C:311:LYS:HA	1:C:315:HIS:CB	2.07	0.83
1:C:55:GLU:O	1:C:59:ILE:HD12	1.78	0.82
1:C:200:VAL:HG11	1:C:304:ILE:CD1	2.10	0.82
1:D:328:ALA:O	1:D:329:PHE:HB2	1.80	0.82
1:C:244:LYS:O	1:C:244:LYS:HG2	1.77	0.81
1:D:200:VAL:HG11	1:D:304:ILE:CD1	2.11	0.81
1:B:200:VAL:HG11	1:B:304:ILE:CD1	2.10	0.81
1:D:244:LYS:O	1:D:244:LYS:HG2	1.77	0.81
1:A:328:ALA:O	1:A:329:PHE:HB2	1.81	0.80
1:C:328:ALA:O	1:C:329:PHE:HB2	1.80	0.80
1:C:240:ILE:CG1	1:C:247:THR:HG22	2.12	0.80
1:B:328:ALA:O	1:B:329:PHE:HB2	1.80	0.80
1:B:270:LEU:HD12	1:B:293:ILE:HD12	1.64	0.80
1:A:15:MET:HE2	1:A:18:ASN:HA	1.62	0.80
1:A:130:GLN:O	1:A:157:ARG:NH1	2.15	0.80
1:A:270:LEU:HD12	1:A:293:ILE:HD12	1.64	0.80
1:B:163:THR:O	1:B:167:THR:HG23	1.82	0.80
1:B:240:ILE:CG1	1:B:247:THR:HG22	2.12	0.80
1:D:15:MET:HE2	1:D:18:ASN:HA	1.61	0.80
1:D:240:ILE:CG1	1:D:247:THR:HG22	2.12	0.80
1:A:200:VAL:HG11	1:A:304:ILE:CD1	2.11	0.79
1:A:163:THR:O	1:A:167:THR:HG23	1.82	0.79
1:B:178:PHE:CE1	1:B:206:ILE:CD1	2.66	0.79
1:A:240:ILE:CG1	1:A:247:THR:HG22	2.12	0.79
1:B:130:GLN:O	1:B:157:ARG:NH1	2.15	0.79
1:B:244:LYS:HE3	1:D:61:ASP:OD1	1.83	0.79
1:D:130:GLN:O	1:D:157:ARG:NH1	2.15	0.79
1:C:130:GLN:O	1:C:157:ARG:NH1	2.15	0.79
1:D:178:PHE:CE1	1:D:206:ILE:CD1	2.66	0.79
1:A:61:ASP:OD1	1:C:244:LYS:HE3	1.83	0.78
1:B:15:MET:HE2	1:B:18:ASN:HA	1.65	0.78
1:D:163:THR:O	1:D:167:THR:HG23	1.83	0.78
1:A:178:PHE:CE1	1:A:206:ILE:CD1	2.66	0.78
1:A:244:LYS:HE3	1:C:61:ASP:OD1	1.83	0.78
1:B:61:ASP:OD1	1:D:244:LYS:HE3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:MET:HE2	1:C:18:ASN:HA	1.62	0.78
1:C:178:PHE:CE1	1:C:206:ILE:CD1	2.66	0.78
1:C:270:LEU:HD12	1:C:293:ILE:HD12	1.64	0.78
1:C:163:THR:O	1:C:167:THR:HG23	1.83	0.78
1:D:270:LEU:HD12	1:D:293:ILE:HD12	1.64	0.77
1:D:310:GLU:C	1:D:312:ASN:H	1.89	0.76
1:C:310:GLU:C	1:C:312:ASN:H	1.89	0.76
1:A:310:GLU:C	1:A:312:ASN:H	1.89	0.75
1:B:257:ARG:NH2	1:B:266:GLU:OE2	2.18	0.75
1:B:310:GLU:C	1:B:312:ASN:H	1.89	0.75
1:A:178:PHE:CE1	1:A:206:ILE:HD11	2.22	0.74
1:B:178:PHE:CE1	1:B:206:ILE:HD11	2.22	0.74
1:C:178:PHE:CE1	1:C:206:ILE:HD11	2.22	0.74
1:B:18:ASN:HD22	1:B:18:ASN:H	0.77	0.74
1:D:178:PHE:CE1	1:D:206:ILE:HD11	2.22	0.74
1:B:15:MET:CE	1:B:18:ASN:HA	2.18	0.74
1:C:257:ARG:NH2	1:C:266:GLU:OE2	2.18	0.73
1:D:306:LEU:O	1:D:307:ASN:O	2.06	0.73
1:C:306:LEU:O	1:C:307:ASN:O	2.06	0.73
1:D:257:ARG:NH2	1:D:266:GLU:OE2	2.18	0.73
1:C:15:MET:CE	1:C:18:ASN:HA	2.18	0.73
1:B:306:LEU:O	1:B:307:ASN:O	2.06	0.73
1:A:306:LEU:O	1:A:307:ASN:O	2.06	0.73
1:C:55:GLU:HG3	1:C:59:ILE:HD11	1.71	0.73
1:A:15:MET:CE	1:A:18:ASN:HA	2.19	0.73
1:D:15:MET:CE	1:D:18:ASN:HA	2.18	0.72
1:C:87:ARG:HB2	1:C:87:ARG:CZ	2.20	0.72
1:D:87:ARG:HB2	1:D:87:ARG:CZ	2.20	0.72
1:A:118:ARG:O	1:A:122:GLU:HG2	1.90	0.72
1:C:310:GLU:C	1:C:312:ASN:N	2.41	0.71
1:B:87:ARG:HB2	1:B:87:ARG:CZ	2.20	0.71
1:A:55:GLU:HG3	1:A:59:ILE:HD11	1.71	0.71
1:C:24:VAL:HG22	1:C:49:VAL:HB	1.73	0.71
1:D:55:GLU:HG3	1:D:59:ILE:HD11	1.71	0.71
1:A:86:CYS:HA	1:A:89:ALA:CB	2.21	0.71
1:B:24:VAL:HG22	1:B:49:VAL:HB	1.73	0.71
1:B:118:ARG:O	1:B:122:GLU:HG2	1.90	0.71
1:D:18:ASN:HD22	1:D:18:ASN:H	0.77	0.71
1:D:118:ARG:O	1:D:122:GLU:HG2	1.90	0.71
1:C:86:CYS:HA	1:C:89:ALA:CB	2.21	0.70
1:B:55:GLU:HG3	1:B:59:ILE:HD11	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:CYS:HA	1:B:89:ALA:CB	2.21	0.70
1:B:167:THR:HG22	1:B:189:ILE:H	1.56	0.70
1:C:118:ARG:O	1:C:122:GLU:HG2	1.90	0.70
1:B:283:ARG:H	1:B:322:LYS:NZ	1.90	0.70
1:D:68:GLY:O	1:D:71:PHE:HB2	1.91	0.70
1:A:68:GLY:O	1:A:71:PHE:HB2	1.91	0.70
1:C:68:GLY:O	1:C:71:PHE:HB2	1.92	0.70
1:D:283:ARG:H	1:D:322:LYS:NZ	1.90	0.70
1:A:283:ARG:H	1:A:322:LYS:NZ	1.90	0.70
1:D:86:CYS:HA	1:D:89:ALA:CB	2.21	0.70
1:A:167:THR:HG22	1:A:189:ILE:H	1.56	0.69
1:A:257:ARG:NH2	1:A:266:GLU:OE2	2.18	0.69
1:B:68:GLY:O	1:B:71:PHE:HB2	1.91	0.69
1:D:125:MET:HE3	1:D:129:PHE:HB3	1.75	0.69
1:A:24:VAL:HG22	1:A:49:VAL:HB	1.73	0.69
1:C:167:THR:HG22	1:C:189:ILE:H	1.57	0.69
1:C:283:ARG:H	1:C:322:LYS:NZ	1.90	0.69
1:D:167:THR:HG22	1:D:189:ILE:H	1.56	0.69
1:A:87:ARG:HB2	1:A:87:ARG:CZ	2.20	0.69
1:A:279:LEU:HD23	1:A:301:VAL:CG1	2.22	0.69
1:B:279:LEU:HD23	1:B:301:VAL:CG1	2.22	0.69
1:C:279:LEU:HD23	1:C:301:VAL:CG1	2.22	0.69
1:D:24:VAL:HG22	1:D:49:VAL:HB	1.73	0.69
1:D:279:LEU:HD23	1:D:301:VAL:CG1	2.22	0.69
1:B:189:ILE:CD1	1:B:233:VAL:HG11	2.23	0.69
1:C:189:ILE:CD1	1:C:233:VAL:HG11	2.23	0.69
1:B:310:GLU:C	1:B:312:ASN:N	2.42	0.68
1:C:83:TYR:C	1:C:85:ASP:H	1.96	0.68
1:A:189:ILE:CD1	1:A:233:VAL:HG11	2.23	0.68
1:D:83:TYR:C	1:D:85:ASP:H	1.96	0.68
1:D:189:ILE:CG2	1:D:197:GLU:HG3	2.24	0.68
1:A:310:GLU:C	1:A:312:ASN:N	2.41	0.68
1:D:189:ILE:CD1	1:D:233:VAL:HG11	2.24	0.68
1:A:83:TYR:C	1:A:85:ASP:H	1.96	0.68
1:C:18:ASN:HD22	1:C:18:ASN:H	0.77	0.67
1:A:189:ILE:CG2	1:A:197:GLU:HG3	2.24	0.67
1:C:189:ILE:CG2	1:C:197:GLU:HG3	2.24	0.67
1:B:83:TYR:C	1:B:85:ASP:H	1.97	0.67
1:B:189:ILE:CG2	1:B:197:GLU:HG3	2.24	0.67
1:D:257:ARG:NH1	1:D:257:ARG:HG3	2.10	0.67
1:A:125:MET:HE3	1:A:129:PHE:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:H	1:A:18:ASN:HD22	0.77	0.66
1:D:18:ASN:N	1:D:18:ASN:ND2	2.24	0.66
1:D:310:GLU:C	1:D:312:ASN:N	2.41	0.66
1:C:257:ARG:HG3	1:C:257:ARG:HH11	1.61	0.66
1:C:257:ARG:HG3	1:C:257:ARG:NH1	2.10	0.66
1:D:265:ASN:ND2	1:D:295:ARG:CB	2.60	0.65
1:A:142:ILE:HD13	1:A:324:VAL:CG1	2.20	0.65
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.62	0.65
1:B:257:ARG:NH1	1:B:257:ARG:HG3	2.10	0.65
1:A:18:ASN:ND2	1:A:18:ASN:N	2.24	0.65
1:B:257:ARG:HG3	1:B:257:ARG:HH11	1.61	0.65
1:D:110:VAL:O	1:D:114:ILE:HG13	1.97	0.65
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.10	0.65
1:C:265:ASN:ND2	1:C:295:ARG:CB	2.60	0.65
1:B:42:GLN:OE1	1:B:44:ILE:HD11	1.97	0.65
1:B:125:MET:HE3	1:B:129:PHE:HB3	1.79	0.65
1:A:42:GLN:OE1	1:A:44:ILE:HD11	1.97	0.64
1:B:110:VAL:O	1:B:114:ILE:HG13	1.97	0.64
1:B:87:ARG:CG	1:B:88:ASP:N	2.51	0.64
1:A:110:VAL:O	1:A:114:ILE:HG13	1.97	0.64
1:B:49:VAL:HG22	1:B:78:ILE:HD12	1.79	0.64
1:C:125:MET:HE3	1:C:129:PHE:HB3	1.80	0.64
1:A:49:VAL:HG22	1:A:78:ILE:HD12	1.79	0.64
1:A:192:GLU:HB2	1:A:321:LEU:HD11	1.80	0.64
1:C:110:VAL:O	1:C:114:ILE:HG13	1.97	0.64
1:D:42:GLN:OE1	1:D:44:ILE:HD11	1.97	0.64
1:C:42:GLN:OE1	1:C:44:ILE:HD11	1.97	0.64
1:B:192:GLU:HB2	1:B:321:LEU:HD11	1.80	0.64
1:C:192:GLU:HB2	1:C:321:LEU:HD11	1.80	0.64
1:B:18:ASN:N	1:B:18:ASN:ND2	2.24	0.63
1:C:15:MET:HE2	1:C:18:ASN:CA	2.28	0.63
1:C:49:VAL:HG22	1:C:78:ILE:HD12	1.79	0.63
1:D:49:VAL:HG22	1:D:78:ILE:HD12	1.79	0.63
1:D:15:MET:HE2	1:D:18:ASN:CA	2.28	0.63
1:D:257:ARG:HG3	1:D:257:ARG:HH11	1.61	0.63
1:A:265:ASN:ND2	1:A:295:ARG:CB	2.59	0.63
1:D:192:GLU:HB2	1:D:321:LEU:HD11	1.80	0.63
1:B:15:MET:HE2	1:B:18:ASN:CA	2.29	0.63
1:B:35:TYR:O	1:B:38:ALA:HB3	1.98	0.63
1:C:35:TYR:O	1:C:38:ALA:HB3	1.99	0.63
1:D:35:TYR:O	1:D:38:ALA:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:O	1:A:38:ALA:HB3	1.98	0.62
1:A:70:VAL:HG22	1:C:182:PRO:CB	2.29	0.62
1:B:182:PRO:CB	1:D:70:VAL:HG22	2.29	0.62
1:A:182:PRO:CB	1:C:70:VAL:HG22	2.29	0.62
1:D:324:VAL:O	1:D:328:ALA:HB3	2.00	0.62
1:B:129:PHE:CZ	1:B:131:GLY:HA3	2.35	0.62
1:C:324:VAL:O	1:C:328:ALA:HB3	2.00	0.62
1:A:243:LYS:HD3	1:C:59:ILE:HG22	1.82	0.62
1:B:324:VAL:O	1:B:328:ALA:HB3	1.99	0.62
1:C:129:PHE:CZ	1:C:131:GLY:HA3	2.35	0.62
1:A:15:MET:HE2	1:A:18:ASN:CA	2.29	0.62
1:B:70:VAL:HG22	1:D:182:PRO:CB	2.29	0.62
1:D:132:LEU:HD12	1:D:262:ILE:HG21	1.82	0.61
1:A:132:LEU:HD12	1:A:262:ILE:HG21	1.82	0.61
1:A:324:VAL:O	1:A:328:ALA:HB3	1.99	0.61
1:D:28:ALA:HB2	1:D:50:LEU:CD1	2.30	0.61
1:B:265:ASN:ND2	1:B:295:ARG:CB	2.60	0.61
1:B:59:ILE:HG22	1:D:243:LYS:HD3	1.82	0.61
1:A:59:ILE:HG22	1:C:243:LYS:HD3	1.82	0.61
1:B:28:ALA:HB2	1:B:50:LEU:CD1	2.31	0.61
1:B:73:PRO:O	1:B:74:LYS:HB2	2.01	0.61
1:D:129:PHE:CZ	1:D:131:GLY:HA3	2.35	0.61
1:B:295:ARG:HG3	1:B:295:ARG:NH1	2.15	0.61
1:A:28:ALA:HB2	1:A:50:LEU:CD1	2.30	0.61
1:A:129:PHE:CZ	1:A:131:GLY:HA3	2.35	0.61
1:C:132:LEU:HD12	1:C:262:ILE:HG21	1.82	0.61
1:D:73:PRO:O	1:D:74:LYS:HB2	2.00	0.61
1:B:178:PHE:CD1	1:B:206:ILE:HD13	2.36	0.61
1:A:178:PHE:CD1	1:A:206:ILE:HD13	2.36	0.61
1:C:28:ALA:HB2	1:C:50:LEU:CD1	2.30	0.61
1:C:87:ARG:CG	1:C:88:ASP:N	2.51	0.61
1:B:243:LYS:HD3	1:D:59:ILE:HG22	1.82	0.60
1:D:178:PHE:CD1	1:D:206:ILE:HD13	2.36	0.60
1:C:73:PRO:O	1:C:74:LYS:HB2	2.01	0.60
1:C:178:PHE:CD1	1:C:206:ILE:HD13	2.36	0.60
1:D:189:ILE:HD11	1:D:233:VAL:HG11	1.84	0.60
1:A:324:VAL:O	1:A:324:VAL:HG12	2.02	0.60
1:B:132:LEU:HD12	1:B:262:ILE:HG21	1.82	0.60
1:A:189:ILE:HD11	1:A:233:VAL:HG11	1.83	0.60
1:B:306:LEU:C	1:B:307:ASN:O	2.40	0.60
1:D:87:ARG:CG	1:D:88:ASP:N	2.52	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:LEU:C	1:C:307:ASN:O	2.40	0.59
1:A:73:PRO:O	1:A:74:LYS:HB2	2.01	0.59
1:C:190:ILE:HD13	1:C:200:VAL:HG21	1.83	0.59
1:D:190:ILE:HD13	1:D:200:VAL:HG21	1.83	0.59
1:A:87:ARG:HB2	1:A:87:ARG:HH11	1.66	0.59
1:C:189:ILE:HD11	1:C:233:VAL:HG11	1.83	0.59
1:D:192:GLU:O	1:D:197:GLU:HB3	2.02	0.59
1:B:189:ILE:HD11	1:B:233:VAL:HG11	1.83	0.59
1:C:272:VAL:O	1:C:288:GLY:HA2	2.03	0.59
1:A:190:ILE:HD13	1:A:200:VAL:HG21	1.83	0.59
1:B:190:ILE:HD13	1:B:200:VAL:HG21	1.83	0.59
1:C:142:ILE:HD13	1:C:324:VAL:CG1	2.20	0.59
1:B:324:VAL:O	1:B:324:VAL:HG12	2.02	0.59
1:C:324:VAL:O	1:C:324:VAL:CG1	2.51	0.59
1:A:324:VAL:CG1	1:A:324:VAL:O	2.51	0.59
1:C:87:ARG:HB2	1:C:87:ARG:HH11	1.65	0.59
1:D:324:VAL:O	1:D:324:VAL:CG1	2.51	0.59
1:B:324:VAL:O	1:B:324:VAL:CG1	2.51	0.59
1:A:15:MET:CG	1:A:16:LYS:N	2.66	0.58
1:C:192:GLU:O	1:C:197:GLU:HB3	2.03	0.58
1:D:55:GLU:HG3	1:D:59:ILE:CD1	2.33	0.58
1:A:55:GLU:HG3	1:A:59:ILE:CD1	2.33	0.58
1:A:192:GLU:O	1:A:197:GLU:HB3	2.02	0.58
1:D:15:MET:CG	1:D:16:LYS:N	2.67	0.58
1:B:272:VAL:O	1:B:288:GLY:HA2	2.03	0.58
1:C:15:MET:CG	1:C:16:LYS:H	2.17	0.58
1:B:55:GLU:HG3	1:B:59:ILE:CD1	2.33	0.58
1:B:189:ILE:HG23	1:B:197:GLU:HG3	1.86	0.58
1:C:55:GLU:HG3	1:C:59:ILE:CD1	2.33	0.58
1:D:15:MET:HG3	1:D:16:LYS:N	2.18	0.58
1:A:83:TYR:C	1:A:85:ASP:N	2.57	0.58
1:A:189:ILE:HG23	1:A:197:GLU:HG3	1.86	0.58
1:D:83:TYR:C	1:D:85:ASP:N	2.57	0.58
1:A:272:VAL:O	1:A:288:GLY:HA2	2.03	0.58
1:C:15:MET:HG3	1:C:16:LYS:N	2.19	0.58
1:C:83:TYR:C	1:C:85:ASP:N	2.57	0.58
1:C:295:ARG:HG3	1:C:295:ARG:NH1	2.15	0.58
1:D:87:ARG:HB2	1:D:87:ARG:HH11	1.66	0.58
1:A:15:MET:CG	1:A:16:LYS:H	2.16	0.58
1:D:132:LEU:HD12	1:D:262:ILE:CG2	2.34	0.58
1:D:324:VAL:O	1:D:324:VAL:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ILE:HG13	1:B:247:THR:HG22	1.86	0.58
1:A:15:MET:HG3	1:A:16:LYS:N	2.18	0.58
1:C:132:LEU:HD12	1:C:262:ILE:CG2	2.34	0.58
1:B:87:ARG:HB2	1:B:87:ARG:HH11	1.66	0.57
1:B:192:GLU:O	1:B:197:GLU:HB3	2.03	0.57
1:D:272:VAL:O	1:D:288:GLY:HA2	2.03	0.57
1:D:306:LEU:C	1:D:307:ASN:O	2.40	0.57
1:A:32:GLY:O	1:A:36:VAL:HG23	2.05	0.57
1:B:15:MET:HG3	1:B:16:LYS:N	2.18	0.57
1:C:324:VAL:O	1:C:324:VAL:HG12	2.02	0.57
1:D:32:GLY:O	1:D:36:VAL:HG23	2.04	0.57
1:A:240:ILE:HG13	1:A:247:THR:HG22	1.86	0.57
1:C:189:ILE:HG23	1:C:197:GLU:HG3	1.86	0.57
1:B:83:TYR:C	1:B:85:ASP:N	2.57	0.57
1:B:132:LEU:HD12	1:B:262:ILE:CG2	2.34	0.57
1:C:240:ILE:HG13	1:C:247:THR:HG22	1.86	0.57
1:A:132:LEU:HD12	1:A:262:ILE:CG2	2.34	0.57
1:A:28:ALA:HB2	1:A:50:LEU:HD11	1.87	0.56
1:B:15:MET:CG	1:B:16:LYS:N	2.67	0.56
1:A:169:ARG:NH1	2:A:1:SO4:O2	2.35	0.56
1:A:279:LEU:HG	1:A:303:GLU:HG3	1.88	0.56
1:C:32:GLY:O	1:C:36:VAL:HG23	2.04	0.56
1:C:170:PHE:HB2	1:C:189:ILE:HD12	1.88	0.56
1:C:331:ARG:C	1:C:331:ARG:HD3	2.26	0.56
1:D:15:MET:CG	1:D:16:LYS:H	2.16	0.56
1:D:142:ILE:HD13	1:D:324:VAL:CG1	2.20	0.56
1:D:189:ILE:HG23	1:D:197:GLU:HG3	1.86	0.56
1:A:306:LEU:C	1:A:307:ASN:O	2.40	0.56
1:D:279:LEU:HG	1:D:303:GLU:HG3	1.87	0.56
1:B:15:MET:CG	1:B:16:LYS:H	2.17	0.56
1:B:28:ALA:HB2	1:B:50:LEU:HD11	1.88	0.56
1:B:275:TYR:O	1:B:277:ASP:OD1	2.24	0.56
1:C:279:LEU:HG	1:C:303:GLU:HG3	1.88	0.56
1:D:170:PHE:HB2	1:D:189:ILE:HD12	1.87	0.56
1:D:240:ILE:HG13	1:D:247:THR:HG22	1.86	0.56
1:B:142:ILE:HD13	1:B:324:VAL:CG1	2.21	0.56
1:D:331:ARG:HD3	1:D:331:ARG:C	2.26	0.56
1:D:295:ARG:HG3	1:D:295:ARG:NH1	2.15	0.56
1:A:206:ILE:HD11	1:A:211:ILE:HD11	1.88	0.56
1:A:299:ARG:NH1	1:D:179:SER:O	2.36	0.56
1:B:179:SER:O	1:C:299:ARG:NH1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ILE:HD11	1:D:211:ILE:HD11	1.88	0.56
1:D:275:TYR:O	1:D:277:ASP:OD1	2.24	0.56
1:A:64:ASP:OD2	1:C:244:LYS:NZ	2.39	0.55
1:A:179:SER:O	1:D:299:ARG:NH1	2.36	0.55
1:A:244:LYS:NZ	1:C:64:ASP:OD2	2.39	0.55
1:A:170:PHE:HB2	1:A:189:ILE:HD12	1.87	0.55
1:A:331:ARG:HD3	1:A:331:ARG:C	2.26	0.55
1:B:64:ASP:OD2	1:D:244:LYS:NZ	2.40	0.55
1:B:331:ARG:HD3	1:B:331:ARG:C	2.26	0.55
1:C:275:TYR:O	1:C:277:ASP:OD1	2.24	0.55
1:B:32:GLY:O	1:B:36:VAL:HG23	2.05	0.55
1:B:113:ASN:ND2	1:B:116:ILE:HD12	2.22	0.55
1:B:244:LYS:NZ	1:D:64:ASP:OD2	2.39	0.55
1:D:28:ALA:HB2	1:D:50:LEU:HD11	1.87	0.55
1:D:113:ASN:ND2	1:D:116:ILE:HD12	2.22	0.55
1:B:112:LYS:CB	1:B:112:LYS:NZ	2.70	0.55
1:D:112:LYS:CB	1:D:112:LYS:NZ	2.70	0.55
1:B:206:ILE:HD11	1:B:211:ILE:HD11	1.89	0.55
1:B:279:LEU:HG	1:B:303:GLU:HG3	1.88	0.55
1:C:15:MET:CG	1:C:16:LYS:N	2.67	0.55
1:C:279:LEU:HD23	1:C:301:VAL:HG12	1.89	0.55
1:A:113:ASN:ND2	1:A:116:ILE:HD12	2.22	0.55
1:A:275:TYR:O	1:A:277:ASP:OD1	2.24	0.55
1:A:112:LYS:NZ	1:A:112:LYS:CB	2.70	0.55
1:C:266:GLU:HG2	1:D:74:LYS:HE2	1.89	0.55
1:D:279:LEU:HD23	1:D:301:VAL:HG12	1.89	0.55
1:C:113:ASN:ND2	1:C:116:ILE:HD12	2.22	0.54
1:B:170:PHE:HB2	1:B:189:ILE:HD12	1.88	0.54
1:C:28:ALA:HB2	1:C:50:LEU:HD11	1.88	0.54
1:C:283:ARG:H	1:C:322:LYS:HZ2	1.54	0.54
1:C:74:LYS:HE2	1:D:266:GLU:HG2	1.89	0.54
1:D:206:ILE:HD11	1:D:211:ILE:CD1	2.38	0.54
1:D:229:ILE:O	1:D:233:VAL:HG23	2.08	0.54
1:A:266:GLU:HG2	1:B:74:LYS:HE2	1.89	0.54
1:C:112:LYS:NZ	1:C:112:LYS:CB	2.70	0.54
1:C:206:ILE:HD11	1:C:211:ILE:HD11	1.89	0.54
1:A:229:ILE:O	1:A:233:VAL:HG23	2.08	0.54
1:A:253:MET:CE	1:C:72:ALA:HB2	2.38	0.54
1:C:229:ILE:O	1:C:233:VAL:HG23	2.08	0.54
1:A:22:ARG:NH2	1:A:47:GLU:OE1	2.36	0.54
1:A:279:LEU:HD23	1:A:301:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ILE:HD13	1:C:233:VAL:HG11	1.90	0.54
1:A:206:ILE:HD11	1:A:211:ILE:CD1	2.38	0.54
1:B:206:ILE:HD11	1:B:211:ILE:CD1	2.38	0.54
1:A:87:ARG:CG	1:A:88:ASP:N	2.51	0.53
1:B:86:CYS:HA	1:B:89:ALA:HB2	1.90	0.53
1:B:229:ILE:O	1:B:233:VAL:HG23	2.08	0.53
1:A:26:ILE:HD12	1:A:92:VAL:CG1	2.39	0.53
1:A:178:PHE:CD1	1:A:206:ILE:CD1	2.92	0.53
1:A:74:LYS:HE2	1:B:266:GLU:HG2	1.89	0.53
1:A:189:ILE:HD13	1:A:233:VAL:HG11	1.91	0.53
1:B:279:LEU:HD23	1:B:301:VAL:HG12	1.89	0.53
1:C:206:ILE:HD11	1:C:211:ILE:CD1	2.38	0.53
1:A:249:TYR:O	1:A:250:GLY:C	2.47	0.53
1:B:299:ARG:NH1	1:C:179:SER:O	2.36	0.53
1:C:167:THR:CG2	1:C:189:ILE:H	2.22	0.53
1:D:26:ILE:HD12	1:D:92:VAL:CG1	2.39	0.53
1:D:86:CYS:HA	1:D:89:ALA:HB2	1.90	0.53
1:B:26:ILE:HD12	1:B:92:VAL:CG1	2.38	0.53
1:C:249:TYR:O	1:C:250:GLY:C	2.47	0.53
1:A:113:ASN:HB3	1:A:143:LEU:HD21	1.90	0.53
1:B:167:THR:CG2	1:B:189:ILE:H	2.22	0.53
1:B:249:TYR:O	1:B:250:GLY:C	2.47	0.53
1:C:178:PHE:CD1	1:C:206:ILE:CD1	2.92	0.53
1:D:178:PHE:CD1	1:D:206:ILE:CD1	2.92	0.53
1:D:189:ILE:HD13	1:D:233:VAL:HG11	1.91	0.53
1:A:72:ALA:HB2	1:C:253:MET:CE	2.38	0.53
1:A:86:CYS:HA	1:A:89:ALA:HB2	1.90	0.53
1:A:283:ARG:H	1:A:322:LYS:HZ2	1.56	0.53
1:B:72:ALA:HB2	1:D:253:MET:CE	2.38	0.53
1:D:113:ASN:HB3	1:D:143:LEU:HD21	1.91	0.53
1:A:307:ASN:C	1:A:309:ASP:H	2.12	0.52
1:B:253:MET:CE	1:D:72:ALA:HB2	2.38	0.52
1:C:113:ASN:HB3	1:C:143:LEU:HD21	1.90	0.52
1:D:15:MET:CE	1:D:18:ASN:CA	2.86	0.52
1:D:22:ARG:NH2	1:D:47:GLU:OE1	2.36	0.52
1:B:93:VAL:HG22	1:B:134:LEU:HD23	1.91	0.52
1:B:113:ASN:HB3	1:B:143:LEU:HD21	1.90	0.52
1:B:178:PHE:CD1	1:B:206:ILE:CD1	2.91	0.52
1:B:307:ASN:C	1:B:309:ASP:H	2.12	0.52
1:C:15:MET:HG2	1:D:296:ASN:OD1	2.10	0.52
1:D:167:THR:CG2	1:D:189:ILE:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MET:HG2	1:B:296:ASN:OD1	2.09	0.52
1:A:167:THR:CG2	1:A:189:ILE:H	2.22	0.52
1:B:189:ILE:HD13	1:B:233:VAL:HG11	1.90	0.52
1:B:15:MET:CE	1:B:18:ASN:CA	2.86	0.52
1:C:93:VAL:HG22	1:C:134:LEU:HD23	1.92	0.52
1:C:296:ASN:OD1	1:D:15:MET:HG2	2.09	0.52
1:C:26:ILE:HD12	1:C:92:VAL:CG1	2.39	0.52
1:A:200:VAL:HG11	1:A:304:ILE:HD11	1.92	0.52
1:C:15:MET:CE	1:C:18:ASN:CA	2.86	0.52
1:A:93:VAL:HG22	1:A:134:LEU:HD23	1.91	0.52
1:C:28:ALA:CB	1:C:50:LEU:HD11	2.40	0.52
1:C:86:CYS:HA	1:C:89:ALA:HB2	1.90	0.52
1:D:26:ILE:HG21	1:D:120:ILE:HD13	1.92	0.52
1:D:307:ASN:C	1:D:309:ASP:H	2.12	0.52
1:B:28:ALA:CB	1:B:50:LEU:HD11	2.40	0.51
1:D:93:VAL:HG22	1:D:134:LEU:HD23	1.91	0.51
1:C:26:ILE:HG21	1:C:120:ILE:HD13	1.92	0.51
1:C:307:ASN:C	1:C:309:ASP:H	2.12	0.51
1:D:249:TYR:O	1:D:250:GLY:C	2.47	0.51
1:D:283:ARG:H	1:D:322:LYS:HZ2	1.56	0.51
1:A:15:MET:CE	1:A:18:ASN:N	2.74	0.51
1:A:296:ASN:OD1	1:B:15:MET:HG2	2.09	0.51
1:A:26:ILE:HD12	1:A:92:VAL:HG13	1.93	0.51
1:B:26:ILE:HG21	1:B:120:ILE:HD13	1.92	0.51
1:D:15:MET:CE	1:D:18:ASN:N	2.74	0.51
1:B:200:VAL:HG11	1:B:304:ILE:HD11	1.92	0.51
1:C:15:MET:CE	1:C:18:ASN:N	2.74	0.51
1:A:28:ALA:CB	1:A:50:LEU:HD11	2.40	0.51
1:C:267:ASN:ND2	1:C:299:ARG:CZ	2.74	0.51
1:D:28:ALA:CB	1:D:50:LEU:HD11	2.40	0.51
1:A:267:ASN:ND2	1:A:294:ASN:OD1	2.44	0.51
1:A:267:ASN:ND2	1:A:299:ARG:CZ	2.74	0.51
1:B:267:ASN:ND2	1:B:294:ASN:OD1	2.44	0.51
1:B:26:ILE:HD12	1:B:92:VAL:HG13	1.93	0.50
1:B:22:ARG:NH2	1:B:47:GLU:OE1	2.37	0.50
1:A:15:MET:CE	1:A:18:ASN:CA	2.86	0.50
1:A:26:ILE:HG21	1:A:120:ILE:HD13	1.92	0.50
1:B:267:ASN:ND2	1:B:299:ARG:CZ	2.74	0.50
1:D:26:ILE:HD12	1:D:92:VAL:HG13	1.93	0.50
1:D:125:MET:O	1:D:128:GLY:N	2.45	0.50
1:D:267:ASN:ND2	1:D:294:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ASN:ND2	1:D:299:ARG:CZ	2.74	0.50
1:B:15:MET:CE	1:B:18:ASN:N	2.74	0.50
1:A:280:TYR:HB2	1:A:314:PHE:CE2	2.47	0.50
1:C:18:ASN:N	1:C:18:ASN:ND2	2.24	0.50
1:B:280:TYR:HB2	1:B:314:PHE:CE2	2.47	0.50
1:C:267:ASN:ND2	1:C:294:ASN:OD1	2.45	0.49
1:A:270:LEU:CD1	1:A:293:ILE:HD12	2.40	0.49
1:D:200:VAL:HG11	1:D:304:ILE:HD11	1.92	0.49
1:A:125:MET:O	1:A:128:GLY:N	2.45	0.49
1:C:26:ILE:HD12	1:C:92:VAL:HG13	1.93	0.49
1:C:280:TYR:HB2	1:C:314:PHE:CE2	2.47	0.49
1:A:279:LEU:CD2	1:A:301:VAL:HB	2.43	0.49
1:B:279:LEU:CD2	1:B:301:VAL:HB	2.43	0.49
1:D:280:TYR:HB2	1:D:314:PHE:CE2	2.47	0.49
1:B:283:ARG:H	1:B:322:LYS:HZ2	1.59	0.48
1:C:279:LEU:CD2	1:C:301:VAL:HB	2.43	0.48
1:D:170:PHE:HB2	1:D:189:ILE:CD1	2.43	0.48
1:A:26:ILE:CG2	1:A:120:ILE:HD13	2.44	0.48
1:D:279:LEU:CD2	1:D:301:VAL:HB	2.43	0.48
1:C:170:PHE:HB2	1:C:189:ILE:CD1	2.43	0.48
1:B:125:MET:O	1:B:128:GLY:N	2.45	0.48
1:D:26:ILE:CG2	1:D:120:ILE:HD13	2.43	0.48
1:D:112:LYS:O	1:D:116:ILE:HG13	2.14	0.48
1:D:164:ILE:HG21	1:D:164:ILE:HD13	1.53	0.48
1:D:206:ILE:CD1	1:D:211:ILE:HD11	2.44	0.47
1:B:26:ILE:CG2	1:B:120:ILE:HD13	2.44	0.47
1:A:324:VAL:O	1:A:328:ALA:CB	2.62	0.47
1:B:170:PHE:HB2	1:B:189:ILE:CD1	2.44	0.47
1:C:112:LYS:O	1:C:116:ILE:HG13	2.14	0.47
1:A:170:PHE:HB2	1:A:189:ILE:CD1	2.43	0.47
1:B:59:ILE:HG13	1:B:79:TRP:CD1	2.50	0.47
1:B:112:LYS:O	1:B:116:ILE:HG13	2.14	0.47
1:A:206:ILE:CD1	1:A:211:ILE:HD11	2.44	0.47
1:C:125:MET:O	1:C:128:GLY:N	2.45	0.47
1:C:324:VAL:O	1:C:328:ALA:CB	2.62	0.47
1:D:270:LEU:CD1	1:D:293:ILE:HD12	2.40	0.47
1:A:112:LYS:O	1:A:116:ILE:HG13	2.14	0.47
1:B:42:GLN:OE1	1:B:44:ILE:CD1	2.63	0.47
1:C:26:ILE:CG2	1:C:120:ILE:HD13	2.43	0.47
1:C:59:ILE:HG13	1:C:79:TRP:CD1	2.50	0.47
1:C:302:ILE:HG21	1:C:302:ILE:HD13	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:OE1	1:A:44:ILE:CD1	2.63	0.47
1:A:59:ILE:HG13	1:A:79:TRP:CD1	2.50	0.47
1:B:22:ARG:O	1:B:90:ASP:HB2	2.15	0.47
1:B:96:ALA:O	1:B:137:THR:HG21	2.15	0.47
1:C:206:ILE:CD1	1:C:211:ILE:HD11	2.44	0.47
1:D:24:VAL:HA	1:D:49:VAL:O	2.15	0.47
1:D:228:ARG:HD2	1:D:228:ARG:HA	1.56	0.47
1:A:228:ARG:HD2	1:A:228:ARG:HA	1.55	0.47
1:B:270:LEU:CD1	1:B:293:ILE:HD12	2.40	0.47
1:C:200:VAL:HG11	1:C:304:ILE:HD11	1.92	0.47
1:D:96:ALA:O	1:D:137:THR:HG21	2.15	0.47
1:D:324:VAL:O	1:D:328:ALA:CB	2.62	0.47
1:A:160:GLY:HA3	1:A:273:SER:HB2	1.97	0.46
1:B:206:ILE:CD1	1:B:211:ILE:HD11	2.44	0.46
1:C:129:PHE:CZ	1:C:131:GLY:CA	2.98	0.46
1:D:160:GLY:HA3	1:D:273:SER:HB2	1.97	0.46
1:C:160:GLY:HA3	1:C:273:SER:HB2	1.97	0.46
1:D:129:PHE:CZ	1:D:131:GLY:CA	2.99	0.46
1:A:24:VAL:HA	1:A:49:VAL:O	2.15	0.46
1:B:293:ILE:O	1:B:294:ASN:HB3	2.15	0.46
1:C:24:VAL:HA	1:C:49:VAL:O	2.15	0.46
1:C:112:LYS:HZ3	1:C:112:LYS:HB3	1.80	0.46
1:C:138:ASN:HA	1:C:140:VAL:N	2.31	0.46
1:D:22:ARG:O	1:D:90:ASP:HB2	2.15	0.46
1:A:96:ALA:O	1:A:137:THR:HG21	2.15	0.46
1:A:295:ARG:HG3	1:A:295:ARG:NH1	2.15	0.46
1:B:164:ILE:HD13	1:B:164:ILE:HG21	1.52	0.46
1:C:96:ALA:O	1:C:137:THR:HG21	2.15	0.46
1:B:129:PHE:CZ	1:B:131:GLY:CA	2.98	0.46
1:D:167:THR:HG22	1:D:189:ILE:HB	1.98	0.46
1:A:22:ARG:O	1:A:90:ASP:HB2	2.15	0.46
1:D:59:ILE:HG13	1:D:79:TRP:CD1	2.50	0.46
1:B:24:VAL:HA	1:B:49:VAL:O	2.15	0.46
1:B:160:GLY:HA3	1:B:273:SER:HB2	1.97	0.46
1:B:321:LEU:C	1:B:323:SER:H	2.19	0.46
1:B:324:VAL:O	1:B:328:ALA:CB	2.62	0.46
1:D:138:ASN:HA	1:D:140:VAL:N	2.31	0.46
1:B:240:ILE:CD1	1:B:247:THR:HG22	2.45	0.46
1:C:167:THR:HG22	1:C:189:ILE:HB	1.98	0.46
1:D:293:ILE:O	1:D:294:ASN:HB3	2.15	0.46
1:B:118:ARG:CZ	1:B:122:GLU:OE2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:O	1:A:234:ARG:HG2	2.17	0.45
1:B:138:ASN:HA	1:B:140:VAL:N	2.31	0.45
1:C:22:ARG:NH2	1:C:47:GLU:OE1	2.37	0.45
1:D:118:ARG:CZ	1:D:122:GLU:OE2	2.64	0.45
1:D:328:ALA:O	1:D:329:PHE:CB	2.59	0.45
1:A:138:ASN:HA	1:A:140:VAL:N	2.31	0.45
1:A:240:ILE:CD1	1:A:247:THR:HG22	2.45	0.45
1:B:240:ILE:HG12	1:B:247:THR:HG22	1.97	0.45
1:C:22:ARG:O	1:C:90:ASP:HB2	2.15	0.45
1:C:42:GLN:OE1	1:C:44:ILE:CD1	2.63	0.45
1:C:164:ILE:HG21	1:C:164:ILE:HD13	1.52	0.45
1:D:149:LYS:HA	1:D:149:LYS:HD3	1.73	0.45
1:D:240:ILE:CD1	1:D:247:THR:HG22	2.45	0.45
1:A:129:PHE:CZ	1:A:131:GLY:CA	2.98	0.45
1:A:167:THR:HG22	1:A:189:ILE:HB	1.98	0.45
1:B:243:LYS:HD3	1:D:59:ILE:CG2	2.45	0.45
1:C:118:ARG:CZ	1:C:122:GLU:OE2	2.64	0.45
2:A:2:SO4:O2	1:D:186:HIS:NE2	2.42	0.45
1:B:167:THR:HG22	1:B:189:ILE:HB	1.98	0.45
1:C:293:ILE:O	1:C:294:ASN:HB3	2.15	0.45
1:A:258:VAL:HG13	1:A:293:ILE:HD13	1.98	0.45
1:A:293:ILE:O	1:A:294:ASN:HB3	2.15	0.45
1:C:232:ASN:HD22	1:C:232:ASN:HA	1.40	0.45
1:A:232:ASN:HD22	1:A:232:ASN:HA	1.41	0.45
1:C:240:ILE:CD1	1:C:247:THR:HG22	2.46	0.45
1:A:149:LYS:HA	1:A:149:LYS:HD3	1.73	0.45
1:C:270:LEU:CD1	1:C:293:ILE:HD12	2.40	0.45
1:D:240:ILE:HD11	1:D:247:THR:HG22	1.99	0.45
1:A:260:ARG:HH11	1:A:260:ARG:HD3	1.04	0.45
1:C:234:ARG:HG2	1:C:234:ARG:O	2.17	0.45
1:A:118:ARG:CZ	1:A:122:GLU:OE2	2.64	0.45
1:A:304:ILE:HG21	1:A:304:ILE:HD13	1.74	0.45
1:B:258:VAL:HG13	1:B:293:ILE:HD13	1.98	0.45
1:D:15:MET:HE3	1:D:18:ASN:ND2	2.32	0.45
1:D:42:GLN:OE1	1:D:44:ILE:CD1	2.63	0.45
1:A:59:ILE:CG2	1:C:243:LYS:HD3	2.45	0.44
1:A:243:LYS:HD3	1:C:59:ILE:CG2	2.45	0.44
1:C:136:ALA:HB2	1:C:255:LEU:HD21	1.99	0.44
1:B:161:SER:OG	1:B:251:ILE:HD11	2.17	0.44
1:C:55:GLU:C	1:C:59:ILE:HD12	2.37	0.44
1:B:59:ILE:CG2	1:D:243:LYS:HD3	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ILE:HD11	1:C:247:THR:HG22	2.00	0.44
1:A:15:MET:HE3	1:A:18:ASN:ND2	2.32	0.44
1:B:228:ARG:HA	1:B:228:ARG:HD2	1.55	0.44
1:B:260:ARG:HH11	1:B:260:ARG:HD3	1.04	0.44
1:D:258:VAL:HG13	1:D:293:ILE:HD13	1.99	0.44
1:A:48:ILE:HD13	1:A:48:ILE:HG21	1.74	0.44
1:A:136:ALA:HB2	1:A:255:LEU:HD21	1.99	0.44
1:B:327:ARG:HH11	1:B:327:ARG:HD3	1.59	0.44
1:C:161:SER:OG	1:C:251:ILE:HD11	2.18	0.44
1:A:161:SER:OG	1:A:251:ILE:HD11	2.18	0.44
1:A:164:ILE:HG21	1:A:164:ILE:HD13	1.53	0.44
1:C:258:VAL:HG13	1:C:293:ILE:HD13	1.99	0.44
1:B:229:ILE:O	1:B:229:ILE:HG22	2.18	0.44
1:B:328:ALA:O	1:B:329:PHE:CB	2.59	0.44
1:D:161:SER:OG	1:D:251:ILE:HD11	2.18	0.44
1:D:322:LYS:HA	1:D:325:LEU:HD12	2.00	0.44
1:A:243:LYS:HE3	1:A:243:LYS:HB3	1.88	0.44
1:B:190:ILE:HD13	1:B:200:VAL:CG2	2.48	0.44
1:D:321:LEU:C	1:D:323:SER:H	2.19	0.44
1:A:184:ASN:HB3	1:D:269:ILE:HD12	2.00	0.43
1:B:304:ILE:HD13	1:B:304:ILE:HG21	1.74	0.43
1:D:229:ILE:O	1:D:229:ILE:HG22	2.17	0.43
1:A:112:LYS:HZ3	1:A:112:LYS:HB3	1.83	0.43
1:A:322:LYS:HA	1:A:325:LEU:HD12	2.00	0.43
1:B:55:GLU:C	1:B:59:ILE:HD12	2.38	0.43
1:C:244:LYS:HE2	1:C:248:TYR:CZ	2.54	0.43
1:C:279:LEU:C	1:C:281:GLY:H	2.22	0.43
1:A:161:SER:CB	3:A:332:HOH:O	2.67	0.43
1:A:244:LYS:HE2	1:A:248:TYR:CZ	2.53	0.43
1:C:229:ILE:O	1:C:229:ILE:HG22	2.18	0.43
1:C:240:ILE:HG12	1:C:247:THR:HG22	1.98	0.43
1:D:136:ALA:HB2	1:D:255:LEU:HD21	1.99	0.43
1:D:167:THR:HG22	1:D:189:ILE:N	2.30	0.43
1:A:229:ILE:O	1:A:229:ILE:HG22	2.18	0.43
1:A:279:LEU:C	1:A:281:GLY:H	2.22	0.43
1:B:234:ARG:O	1:B:234:ARG:HG2	2.17	0.43
1:B:244:LYS:HE2	1:B:248:TYR:CZ	2.53	0.43
1:C:138:ASN:HA	1:C:140:VAL:H	1.84	0.43
1:C:321:LEU:C	1:C:323:SER:H	2.19	0.43
1:A:240:ILE:HD11	1:A:247:THR:HG22	1.99	0.43
1:A:279:LEU:HD23	1:A:301:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ASP:HB3	1:D:83:TYR:H	1.64	0.43
1:D:234:ARG:O	1:D:234:ARG:HG2	2.17	0.43
1:A:55:GLU:C	1:A:59:ILE:HD12	2.38	0.43
1:B:136:ALA:HB2	1:B:255:LEU:HD21	2.00	0.43
1:C:15:MET:HE3	1:C:18:ASN:ND2	2.34	0.43
1:C:167:THR:HG22	1:C:189:ILE:N	2.30	0.43
1:D:311:LYS:CA	1:D:315:HIS:CB	2.90	0.43
1:B:75:PRO:CD	1:B:75:PRO:O	2.67	0.43
1:B:232:ASN:HD22	1:B:232:ASN:HA	1.40	0.43
1:D:55:GLU:C	1:D:59:ILE:HD12	2.37	0.43
1:D:138:ASN:HA	1:D:140:VAL:H	1.84	0.43
1:A:190:ILE:HD13	1:A:200:VAL:CG2	2.48	0.43
1:C:327:ARG:HH11	1:C:327:ARG:HD3	1.60	0.43
1:D:321:LEU:C	1:D:323:SER:N	2.72	0.43
1:A:138:ASN:HA	1:A:140:VAL:H	1.84	0.42
1:A:327:ARG:HH11	1:A:327:ARG:HD3	1.59	0.42
1:B:304:ILE:HA	1:C:209:MET:SD	2.59	0.42
1:D:75:PRO:CD	1:D:75:PRO:O	2.67	0.42
1:B:269:ILE:HD12	1:C:184:ASN:HB3	2.01	0.42
1:C:322:LYS:HA	1:C:325:LEU:HD12	2.00	0.42
1:A:75:PRO:CD	1:A:75:PRO:O	2.67	0.42
1:A:304:ILE:HA	1:D:209:MET:SD	2.59	0.42
1:B:184:ASN:HB3	1:C:269:ILE:HD12	2.01	0.42
1:B:270:LEU:HA	1:B:270:LEU:HD23	1.78	0.42
1:B:322:LYS:HA	1:B:325:LEU:HD12	2.00	0.42
1:B:279:LEU:HD23	1:B:301:VAL:HG11	1.99	0.42
1:D:302:ILE:HD13	1:D:302:ILE:HG21	1.60	0.42
1:B:138:ASN:HA	1:B:140:VAL:H	1.83	0.42
1:B:240:ILE:HD11	1:B:247:THR:HG22	1.99	0.42
1:D:244:LYS:HE2	1:D:248:TYR:CZ	2.53	0.42
1:A:167:THR:O	1:A:171:ARG:HG3	2.20	0.42
1:C:75:PRO:O	1:C:75:PRO:CD	2.67	0.42
1:C:293:ILE:HD13	1:C:293:ILE:HG21	1.83	0.42
1:A:321:LEU:C	1:A:323:SER:N	2.72	0.42
1:B:165:LEU:O	1:B:169:ARG:HG3	2.20	0.42
1:C:279:LEU:HD23	1:C:301:VAL:HG11	1.99	0.42
1:D:190:ILE:HD13	1:D:200:VAL:CG2	2.48	0.42
1:A:132:LEU:CD1	1:A:262:ILE:CG2	2.98	0.42
1:C:132:LEU:CD1	1:C:262:ILE:CG2	2.98	0.42
1:D:279:LEU:C	1:D:281:GLY:H	2.22	0.42
1:A:136:ALA:HA	1:A:161:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:O	1:A:169:ARG:HG3	2.20	0.42
1:A:269:ILE:HD12	1:D:184:ASN:HB3	2.01	0.42
1:A:280:TYR:CE2	1:A:289:VAL:CG2	3.03	0.42
1:B:209:MET:SD	1:C:304:ILE:HA	2.60	0.42
1:D:167:THR:O	1:D:171:ARG:HG3	2.20	0.42
1:B:167:THR:O	1:B:171:ARG:HG3	2.20	0.42
1:C:149:LYS:HD3	1:C:149:LYS:HA	1.73	0.42
1:C:165:LEU:O	1:C:169:ARG:HG3	2.20	0.42
1:D:165:LEU:O	1:D:169:ARG:HG3	2.20	0.42
1:D:181:ALA:HA	1:D:182:PRO:HD3	1.82	0.42
1:D:279:LEU:HD23	1:D:301:VAL:HG11	1.99	0.42
1:C:181:ALA:HA	1:C:182:PRO:HD3	1.82	0.41
1:C:206:ILE:CD1	1:C:211:ILE:CD1	2.98	0.41
1:C:311:LYS:CA	1:C:315:HIS:CB	2.90	0.41
1:B:279:LEU:C	1:B:281:GLY:H	2.22	0.41
1:B:280:TYR:CE2	1:B:289:VAL:CG2	3.03	0.41
1:D:132:LEU:CD1	1:D:262:ILE:CG2	2.98	0.41
1:A:209:MET:SD	1:D:304:ILE:HA	2.60	0.41
1:D:280:TYR:CE2	1:D:289:VAL:CG2	3.04	0.41
1:A:321:LEU:C	1:A:323:SER:H	2.19	0.41
1:B:71:PHE:CE1	1:D:168:ALA:HB2	2.56	0.41
1:C:280:TYR:CE2	1:C:289:VAL:CG2	3.03	0.41
1:C:287:ILE:HD13	1:C:287:ILE:HG21	1.85	0.41
1:C:328:ALA:O	1:C:329:PHE:CB	2.59	0.41
1:B:132:LEU:CD1	1:B:262:ILE:CG2	2.98	0.41
1:B:321:LEU:C	1:B:323:SER:N	2.73	0.41
1:C:112:LYS:CB	1:C:112:LYS:HZ3	2.33	0.41
1:C:167:THR:O	1:C:171:ARG:HG3	2.20	0.41
1:A:27:GLY:O	1:A:32:GLY:HA3	2.21	0.41
1:A:114:ILE:O	1:A:114:ILE:HG22	2.21	0.41
1:A:168:ALA:HB2	1:C:71:PHE:CE1	2.56	0.41
1:A:199:PRO:O	1:A:199:PRO:HG2	2.21	0.41
1:B:203:GLN:O	1:C:208:VAL:HB	2.21	0.41
1:C:120:ILE:HD13	1:C:120:ILE:HG21	1.80	0.41
1:C:136:ALA:HA	1:C:161:SER:HB2	2.03	0.41
1:C:243:LYS:HE3	1:C:243:LYS:HB3	1.89	0.41
1:C:304:ILE:HD13	1:C:304:ILE:HG21	1.74	0.41
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.82	0.41
1:C:199:PRO:O	1:C:199:PRO:HG2	2.21	0.41
1:D:136:ALA:HA	1:D:161:SER:HB2	2.02	0.41
1:B:114:ILE:O	1:B:114:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ALA:HA	1:B:161:SER:HB2	2.02	0.40
1:B:149:LYS:HA	1:B:149:LYS:HD3	1.73	0.40
1:B:199:PRO:O	1:B:199:PRO:HG2	2.21	0.40
1:B:208:VAL:HB	1:C:203:GLN:O	2.21	0.40
1:C:27:GLY:O	1:C:32:GLY:HA3	2.21	0.40
1:C:118:ARG:NH2	1:C:122:GLU:OE2	2.54	0.40
1:C:228:ARG:HA	1:C:228:ARG:HD2	1.56	0.40
1:A:42:GLN:HB2	1:A:44:ILE:HD12	2.03	0.40
1:A:206:ILE:CD1	1:A:211:ILE:CD1	2.98	0.40
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.86	0.40
1:C:42:GLN:HB2	1:C:44:ILE:HD12	2.03	0.40
1:C:209:MET:C	1:C:210:PRO:O	2.59	0.40
1:D:112:LYS:NZ	1:D:112:LYS:HB3	2.36	0.40
1:D:118:ARG:NH2	1:D:122:GLU:OE2	2.54	0.40
1:A:71:PHE:CE1	1:C:168:ALA:HB2	2.56	0.40
1:A:118:ARG:NH2	1:A:122:GLU:OE2	2.55	0.40
1:B:27:GLY:O	1:B:32:GLY:HA3	2.21	0.40
1:B:112:LYS:CB	1:B:112:LYS:HZ2	2.33	0.40
1:B:118:ARG:NH2	1:B:122:GLU:OE2	2.55	0.40
1:B:251:ILE:O	1:B:254:GLY:N	2.55	0.40
1:C:112:LYS:NZ	1:C:112:LYS:HB3	2.36	0.40
1:D:48:ILE:HD13	1:D:48:ILE:HG21	1.74	0.40
1:D:206:ILE:CD1	1:D:211:ILE:CD1	2.98	0.40
1:D:313:ARG:HH11	1:D:313:ARG:HG2	1.87	0.40
1:D:327:ARG:HH11	1:D:327:ARG:HD3	1.59	0.40
1:A:70:VAL:O	1:A:70:VAL:CG1	2.70	0.40
1:A:167:THR:HG22	1:A:189:ILE:N	2.30	0.40
1:D:27:GLY:O	1:D:32:GLY:HA3	2.21	0.40

All (57) 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:A:326:ALA:N	1:D:331:ARG:CB[6_665]	0.71	1.49
1:A:326:ALA:C	1:D:331:ARG:C[6_665]	0.78	1.42
1:A:325:LEU:C	1:D:331:ARG:CB[6_665]	0.88	1.32
1:C:316:HIS:CE1	1:D:316:HIS:CE1[6_655]	1.07	1.13
1:C:316:HIS:NE2	1:D:316:HIS:CE1[6_655]	1.09	1.11
1:A:326:ALA:N	1:D:331:ARG:CA[6_665]	1.12	1.08
1:A:326:ALA:CA	1:D:331:ARG:C[6_665]	1.23	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:C	1:D:330:THR:CB[6_665]	1.24	0.96
1:C:316:HIS:NE2	1:D:316:HIS:NE2[6_655]	1.24	0.96
1:A:325:LEU:O	1:D:331:ARG:CG[6_665]	1.28	0.92
1:A:327:ARG:CB	1:D:330:THR:O[6_665]	1.32	0.88
1:C:235:ASP:OD2	1:D:235:ASP:OD2[6_655]	1.34	0.86
1:A:323:SER:O	1:D:330:THR:CA[6_665]	1.42	0.78
1:A:323:SER:O	1:D:330:THR:CB[6_665]	1.42	0.78
1:A:327:ARG:N	1:D:331:ARG:C[6_665]	1.42	0.78
1:C:316:HIS:CE1	1:D:316:HIS:NE2[6_655]	1.48	0.72
1:A:326:ALA:CA	1:D:331:ARG:CA[6_665]	1.54	0.66
1:A:325:LEU:O	1:D:331:ARG:CB[6_665]	1.55	0.65
1:A:326:ALA:C	1:D:331:ARG:CA[6_665]	1.57	0.63
1:A:327:ARG:CA	1:D:330:THR:O[6_665]	1.59	0.61
1:A:327:ARG:N	1:D:331:ARG:CA[6_665]	1.59	0.61
1:A:323:SER:O	1:D:330:THR:C[6_665]	1.60	0.60
1:A:326:ALA:CA	1:D:331:ARG:CB[6_665]	1.60	0.60
1:A:324:VAL:N	1:D:330:THR:CB[6_665]	1.67	0.53
1:A:323:SER:O	1:D:330:THR:OG1[6_665]	1.68	0.52
1:A:323:SER:O	1:D:331:ARG:N[6_665]	1.70	0.50
1:A:326:ALA:CB	1:D:331:ARG:O[6_665]	1.70	0.50
1:A:323:SER:CB	1:D:330:THR:OG1[6_665]	1.72	0.48
1:A:326:ALA:CA	1:D:331:ARG:CG[6_665]	1.85	0.35
1:C:316:HIS:CD2	1:D:316:HIS:NE2[6_655]	1.88	0.32
1:A:323:SER:C	1:D:330:THR:OG1[6_665]	1.89	0.31
1:A:326:ALA:N	1:D:331:ARG:N[6_665]	1.89	0.31
1:A:326:ALA:CA	1:D:331:ARG:CD[6_665]	1.90	0.30
1:A:325:LEU:C	1:D:331:ARG:CG[6_665]	1.91	0.29
1:A:323:SER:OG	1:D:330:THR:CG2[6_665]	1.93	0.27
1:A:323:SER:CA	1:D:330:THR:OG1[6_665]	1.93	0.27
1:A:326:ALA:O	1:D:331:ARG:C[6_665]	1.95	0.25
1:A:327:ARG:N	1:D:331:ARG:N[6_665]	1.95	0.25
1:A:326:ALA:CA	1:D:331:ARG:O[6_665]	1.97	0.23
1:C:316:HIS:NE2	1:D:316:HIS:ND1[6_655]	1.97	0.23
1:A:326:ALA:CB	1:D:331:ARG:C[6_665]	2.00	0.20
1:A:327:ARG:CB	1:D:330:THR:C[6_665]	2.01	0.19
1:A:326:ALA:C	1:D:331:ARG:O[6_665]	2.02	0.18
1:A:327:ARG:N	1:D:330:THR:O[6_665]	2.02	0.18
1:C:327:ARG:NH1	1:D:312:ASN:CG[6_655]	2.05	0.15
1:A:327:ARG:N	1:D:330:THR:C[6_665]	2.07	0.13
1:A:325:LEU:C	1:D:331:ARG:CA[6_665]	2.11	0.09
1:C:316:HIS:ND1	1:D:316:HIS:NE2[6_655]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:C	1:D:330:THR:O[6_665]	2.12	0.08
1:A:327:ARG:N	1:D:331:ARG:O[6_665]	2.13	0.07
1:A:323:SER:CA	1:D:330:THR:CB[6_665]	2.14	0.06
1:A:327:ARG:CB	1:D:329:PHE:O[6_665]	2.14	0.06
1:C:316:HIS:NE2	1:D:316:HIS:CD2[6_655]	2.14	0.06
1:A:326:ALA:N	1:D:331:ARG:CG[6_665]	2.16	0.04
1:C:228:ARG:NE	1:D:242:GLU:OE2[6_655]	2.17	0.03
1:A:323:SER:C	1:D:330:THR:CA[6_665]	2.18	0.02
1:A:326:ALA:CB	1:D:331:ARG:CD[6_665]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	2	5
1	B	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	2	5
1	C	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	2	5
1	D	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	2	5
All	All	1144/1268 (90%)	928 (81%)	152 (13%)	64 (6%)	2	5

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	98	ALA
1	A	307	ASN
1	A	311	LYS
1	A	329	PHE
1	B	18	ASN
1	B	98	ALA
1	B	307	ASN

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Mol	Chain	Res	Type
1	B	311	LYS
1	B	329	PHE
1	C	18	ASN
1	C	98	ALA
1	C	307	ASN
1	C	311	LYS
1	C	329	PHE
1	D	18	ASN
1	D	98	ALA
1	D	307	ASN
1	D	311	LYS
1	D	329	PHE
1	A	75	PRO
1	A	330	THR
1	B	75	PRO
1	B	330	THR
1	C	75	PRO
1	C	330	THR
1	D	75	PRO
1	D	330	THR
1	A	284	ASP
1	B	284	ASP
1	C	284	ASP
1	D	284	ASP
1	A	250	GLY
1	B	250	GLY
1	C	250	GLY
1	D	250	GLY
1	A	248	TYR
1	B	248	TYR
1	C	248	TYR
1	D	248	TYR
1	A	210	PRO
1	A	267	ASN
1	B	210	PRO
1	B	267	ASN
1	C	210	PRO
1	C	267	ASN
1	D	210	PRO
1	D	267	ASN
1	A	74	LYS
1	B	74	LYS

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Mol	Chain	Res	Type
1	C	74	LYS
1	D	74	LYS
1	A	73	PRO
1	B	73	PRO
1	C	73	PRO
1	D	73	PRO
1	A	180	VAL
1	B	180	VAL
1	C	180	VAL
1	D	180	VAL
1	A	139	PRO
1	B	139	PRO
1	C	139	PRO
1	D	139	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/255 (92%)	206 (87%)	30 (13%)	4	14
1	B	236/255 (92%)	207 (88%)	29 (12%)	4	15
1	C	236/255 (92%)	207 (88%)	29 (12%)	4	15
1	D	236/255 (92%)	207 (88%)	29 (12%)	4	15
All	All	944/1020 (92%)	827 (88%)	117 (12%)	4	14

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	18	ASN
1	A	74	LYS
1	A	77	ASP
1	A	87	ARG
1	A	90	ASP
1	A	99	ASN

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Mol	Chain	Res	Type
1	A	112	LYS
1	A	113	ASN
1	A	119	SER
1	A	134	LEU
1	A	179	SER
1	A	183	GLN
1	A	192	GLU
1	A	197	GLU
1	A	198	LEU
1	A	203	GLN
1	A	227	GLU
1	A	228	ARG
1	A	243	LYS
1	A	257	ARG
1	A	265	ASN
1	A	266	GLU
1	A	277	ASP
1	A	283	ARG
1	A	289	VAL
1	A	294	ASN
1	A	295	ARG
1	A	329	PHE
1	A	331	ARG
1	B	15	MET
1	B	18	ASN
1	B	74	LYS
1	B	77	ASP
1	B	87	ARG
1	B	90	ASP
1	B	99	ASN
1	B	112	LYS
1	B	113	ASN
1	B	119	SER
1	B	134	LEU
1	B	179	SER
1	B	183	GLN
1	B	192	GLU
1	B	197	GLU
1	B	198	LEU
1	B	203	GLN
1	B	227	GLU
1	B	228	ARG

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Mol	Chain	Res	Type
1	B	243	LYS
1	B	257	ARG
1	B	265	ASN
1	B	266	GLU
1	B	277	ASP
1	B	283	ARG
1	B	289	VAL
1	B	294	ASN
1	B	295	ARG
1	B	331	ARG
1	C	15	MET
1	C	18	ASN
1	C	74	LYS
1	C	77	ASP
1	C	87	ARG
1	C	90	ASP
1	C	99	ASN
1	C	112	LYS
1	C	113	ASN
1	C	119	SER
1	C	134	LEU
1	C	179	SER
1	C	183	GLN
1	C	192	GLU
1	C	197	GLU
1	C	198	LEU
1	C	203	GLN
1	C	227	GLU
1	C	228	ARG
1	C	243	LYS
1	C	257	ARG
1	C	265	ASN
1	C	266	GLU
1	C	277	ASP
1	C	283	ARG
1	C	289	VAL
1	C	294	ASN
1	C	295	ARG
1	C	331	ARG
1	D	15	MET
1	D	18	ASN
1	D	74	LYS

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Mol	Chain	Res	Type
1	D	77	ASP
1	D	87	ARG
1	D	90	ASP
1	D	99	ASN
1	D	112	LYS
1	D	113	ASN
1	D	119	SER
1	D	134	LEU
1	D	179	SER
1	D	183	GLN
1	D	192	GLU
1	D	197	GLU
1	D	198	LEU
1	D	203	GLN
1	D	227	GLU
1	D	228	ARG
1	D	243	LYS
1	D	257	ARG
1	D	265	ASN
1	D	266	GLU
1	D	277	ASP
1	D	283	ARG
1	D	289	VAL
1	D	294	ASN
1	D	295	ARG
1	D	331	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	99	ASN
1	A	113	ASN
1	A	138	ASN
1	A	232	ASN
1	A	239	GLN
1	A	265	ASN
1	A	267	ASN
1	A	294	ASN
1	A	307	ASN
1	B	18	ASN
1	B	99	ASN

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Mol	Chain	Res	Type
1	B	113	ASN
1	B	138	ASN
1	B	193	HIS
1	B	232	ASN
1	B	239	GLN
1	B	265	ASN
1	B	267	ASN
1	B	294	ASN
1	B	307	ASN
1	C	18	ASN
1	C	99	ASN
1	C	113	ASN
1	C	138	ASN
1	C	193	HIS
1	C	232	ASN
1	C	239	GLN
1	C	265	ASN
1	C	267	ASN
1	C	294	ASN
1	C	307	ASN
1	D	18	ASN
1	D	99	ASN
1	D	113	ASN
1	D	138	ASN
1	D	193	HIS
1	D	232	ASN
1	D	239	GLN
1	D	265	ASN
1	D	267	ASN
1	D	294	ASN
1	D	307	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	1	-	4,4,4	0.92	0	6,6,6	0.78	0
2	SO4	A	2	-	4,4,4	1.20	1 (25%)	6,6,6	1.03	1 (16%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	SO4	O2-S	2.11	1.57	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	SO4	O4-S-O1	2.17	120.65	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SO4	1	0
2	A	2	SO4	1	0

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.