Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2021 – 08:00 AM EST

PDB ID	:	9RUB
Title	:	CRYSTAL STRUCTURE OF ACTIVATED RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE COMPLEXED WITH ITS SUBSTRATE, RIBULOSE-1,5-BISPHOSPHATE
Authors	:	Lundqvist, T.; Schneider, G.
Deposited on	:	1990-11-28
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

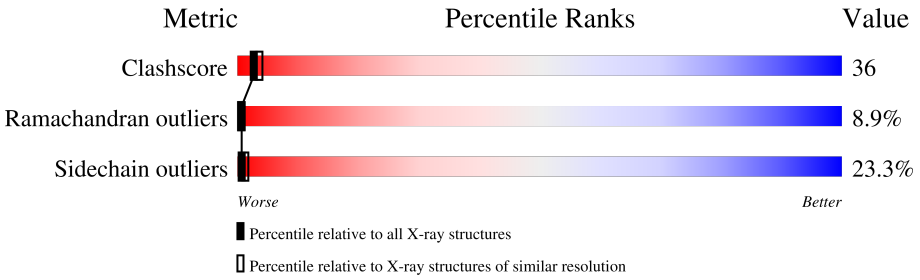
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	466	19% 44% 24% 12% .
1	B	466	29% 35% 27% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMT	A	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7044 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.

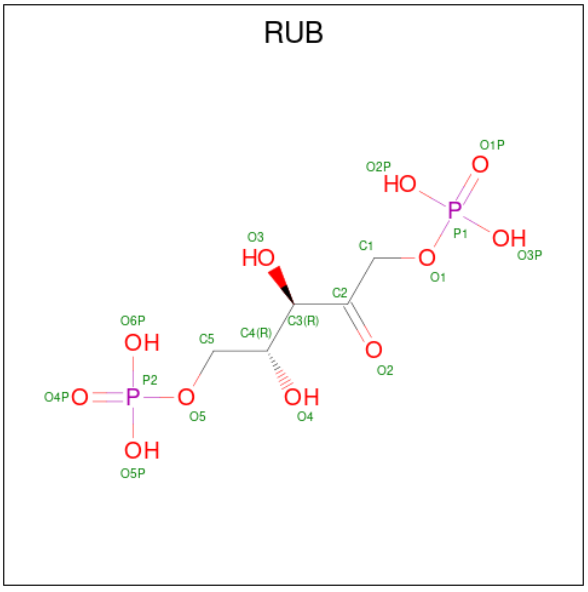
- Molecule 1 is a protein called RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	8	0	0
			3502	2213	613	658	18			
1	B	458	Total	C	N	O	S	1	0	0
			3498	2211	612	657	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	conflict	UNP P04718
B	91	ASP	HIS	conflict	UNP P04718

- Molecule 2 is RIBULOSE-1,5-DIPHOSPHATE (three-letter code: RUB) (formula: $C_5H_{12}O_{11}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			18	5	11	2		

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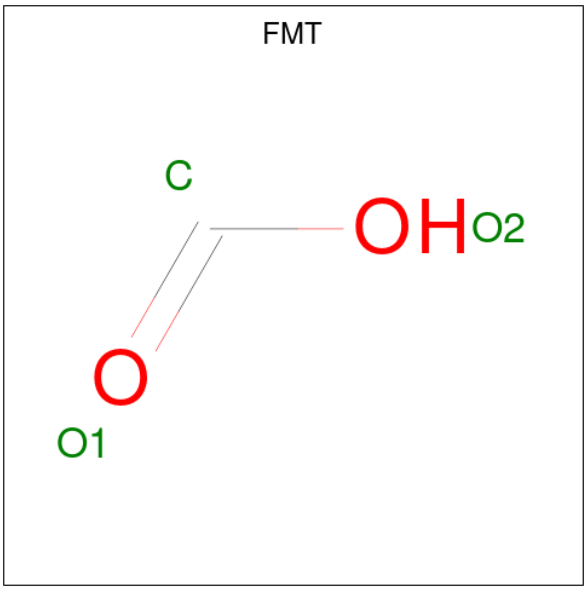
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O P 18 5 11 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0

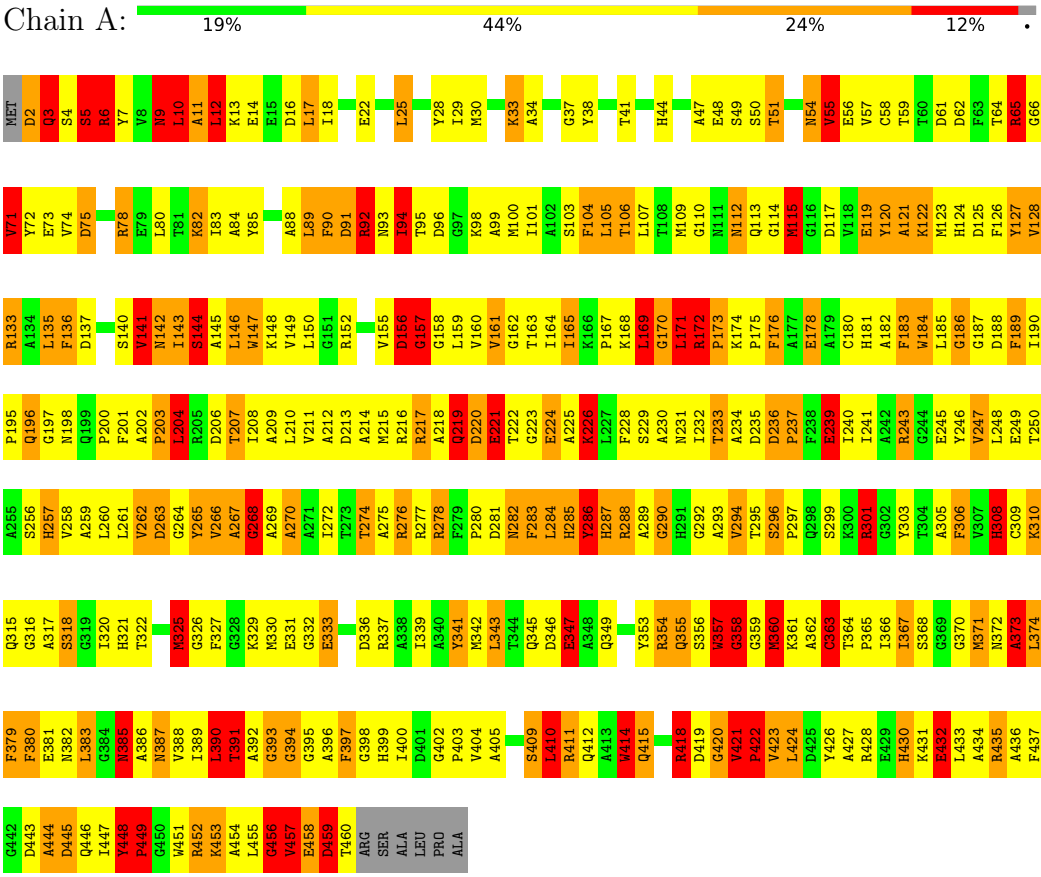
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

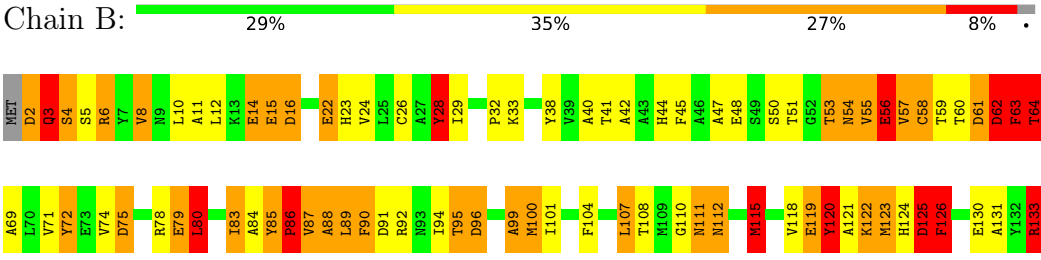
• Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE

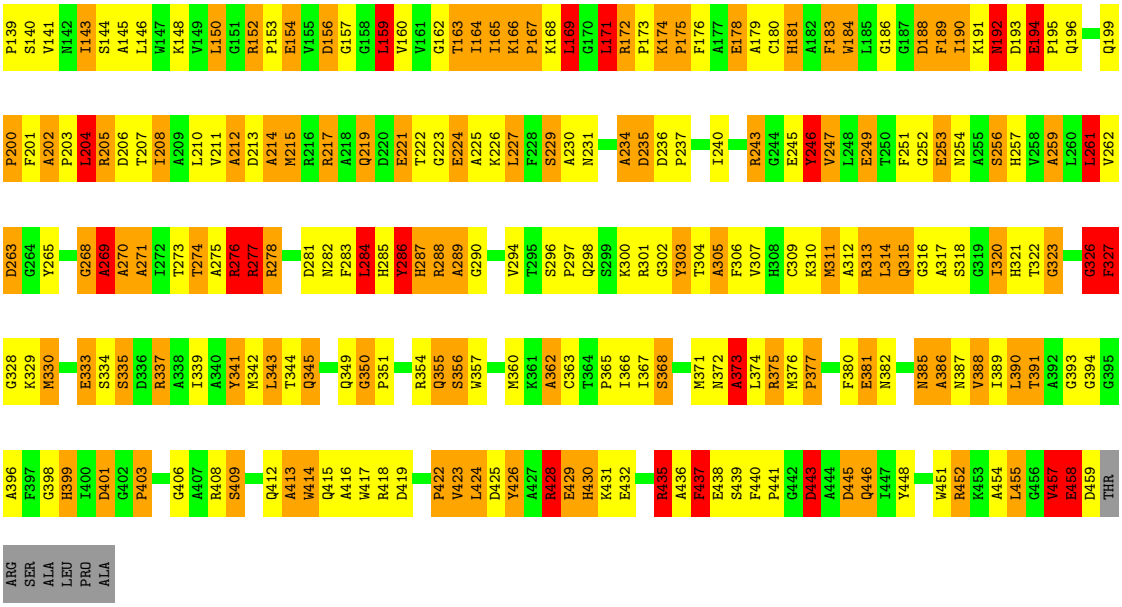
Chain A:



• Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE

Chain B:




P139 S140 V141 N142 I143 S144 A145 L146 W147 K148 V149 L150 G151 R152 P153 E154 V155 D156 G157 G158 L159 V160 V161 G162 T163 I164 I165 K166 P167 K168 L169 G170 L171 R172 P173 K174 P175 F176 A177 E178 A179 C180 H181 A182 F183 W184 L185 G186 G187 D188 F189 I190 K191 N192 D193 E194 P195 Q196 Q199
P200 F201 A202 P203 L204 R205 D206 T207 I208 A209 L210 V211 A212 D213 A214 M215 R216 R217 A218 Q219 D220 E221 T222 G223 E224 A225 K226 L227 F228 S229 A230 N231 A234 D235 D236 P237 I240 R243 G244 E245 Y246 V247 L248 E249 T250 F251 G252 E253 N254 A255 S256 H257 V258 A259 L260 L261 V262
D263 G264 Y265 G268 A269 A270 A271 I272 T273 T274 A275 R276 R277 R278 D281 N282 F283 L284 H285 Y286 H287 R288 A289 G290 V294 T295 S296 P297 Q298 S299 K300 R301 G302 Y303 T304 A305 F306 V307 H308 C309 K310 M311 A312 R313 L314 Q315 G316 A317 S318 G319 I320 H321 T322 G323 G326 F327
G328 K329 M330 E333 S334 S335 D336 R337 A338 I339 A340 Y341 M342 L343 T344 Q345 Q349 G350 P351 R354 Q355 S356 W357 M360 K361 A362 C363 T364 P365 I366 I367 S368 M371 N372 A373 L374 R375 M376 P377 F380 E381 N382 N385 A386 N387 V388 I389 L390 T391 A392 G393 G394 G395
A396 F397 G398 H399 I400 D401 G402 P403 G406 A407 R408 S409 Q412 A413 W414 Q415 A416 W417 R418 D419 P422 V423 L424 D425 Y426 A427 R428 E429 H430 K431 E432 R435 A436 F437 E438 S439 F440 P441 G442 D443 A444 D445 Q446 I447 Y448 W451 R452 K453 A454 L455 G456 V457 E458 D459 THR
ARG SER ALA LEU PRO ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.50Å 70.60Å 104.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7044	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: MG, RUB, FMT

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	1.14	4/3586 (0.1%)	2.90	360/4859 (7.4%)
1	B	1.02	1/3582 (0.0%)	2.84	300/4854 (6.2%)
All	All	1.08	5/7168 (0.1%)	2.87	660/9713 (6.8%)

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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	GLU	CG-CD	21.57	1.84	1.51
1	A	459	ASP	CG-OD2	13.53	1.56	1.25
1	A	460	THR	N-CA	-10.23	1.25	1.46
1	B	457	VAL	C-O	-9.22	1.05	1.23
1	A	459	ASP	CB-CG	-5.24	1.40	1.51

All (660) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	428	ARG	CD-NE-CZ	38.62	177.67	123.60
1	B	65	ARG	CD-NE-CZ	26.96	161.35	123.60
1	A	78	ARG	CD-NE-CZ	23.14	156.00	123.60
1	A	96	ASP	CB-CG-OD1	20.82	137.03	118.30
1	A	459	ASP	C-N-CA	20.41	172.74	121.70
1	B	428	ARG	NE-CZ-NH1	18.43	129.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	TYR	CB-CG-CD1	18.26	131.96	121.00
1	B	277	ARG	NE-CZ-NH2	18.26	129.43	120.30
1	B	435	ARG	NE-CZ-NH1	17.74	129.17	120.30
1	B	172	ARG	CD-NE-CZ	16.82	147.15	123.60
1	B	418	ARG	NE-CZ-NH1	-16.65	111.97	120.30
1	B	286	TYR	CB-CG-CD1	16.45	130.87	121.00
1	A	125	ASP	CB-CG-OD1	15.78	132.50	118.30
1	B	92	ARG	CD-NE-CZ	15.62	145.47	123.60
1	A	286	TYR	CB-CG-CD2	-15.52	111.69	121.00
1	B	6	ARG	NE-CZ-NH1	15.42	128.01	120.30
1	A	313	ARG	NE-CZ-NH1	-15.23	112.68	120.30
1	B	172	ARG	NE-CZ-NH1	15.20	127.90	120.30
1	B	276	ARG	NE-CZ-NH1	-15.14	112.73	120.30
1	A	313	ARG	NE-CZ-NH2	14.88	127.74	120.30
1	A	337	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	A	277	ARG	NE-CZ-NH2	14.53	127.56	120.30
1	A	56	GLU	C-N-CA	14.41	157.73	121.70
1	A	243	ARG	CD-NE-CZ	14.14	143.40	123.60
1	A	411	ARG	NE-CZ-NH2	14.13	127.37	120.30
1	A	333	GLU	CB-CG-CD	14.06	152.17	114.20
1	B	6	ARG	CD-NE-CZ	13.71	142.80	123.60
1	B	100	MET	CG-SD-CE	13.51	121.81	100.20
1	B	278	ARG	CD-NE-CZ	13.50	142.50	123.60
1	B	334	SER	C-N-CA	13.37	155.12	121.70
1	A	96	ASP	CB-CG-OD2	-13.32	106.31	118.30
1	A	410	LEU	CB-CA-C	13.29	135.45	110.20
1	A	127	TYR	CB-CG-CD2	13.23	128.94	121.00
1	B	356	SER	N-CA-CB	13.16	130.25	110.50
1	B	337	ARG	NE-CZ-NH2	-13.09	113.75	120.30
1	A	460	THR	N-CA-C	13.07	146.28	111.00
1	A	277	ARG	NE-CZ-NH1	-12.93	113.83	120.30
1	A	301	ARG	NE-CZ-NH2	12.78	126.69	120.30
1	A	288	ARG	NE-CZ-NH1	12.77	126.69	120.30
1	B	445	ASP	CA-CB-CG	12.72	141.39	113.40
1	B	115	MET	CA-CB-CG	12.65	134.81	113.30
1	A	375	ARG	NE-CZ-NH2	12.39	126.50	120.30
1	B	286	TYR	CB-CG-CD2	-12.39	113.57	121.00
1	B	418	ARG	NE-CZ-NH2	12.36	126.48	120.30
1	A	92	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	B	92	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	B	277	ARG	NE-CZ-NH1	-12.08	114.26	120.30
1	B	408	ARG	CB-CG-CD	12.01	142.83	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	ASP	CB-CG-OD2	-11.85	107.64	118.30
1	A	6	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	A	156	ASP	C-N-CA	11.78	147.04	122.30
1	A	133	ARG	NE-CZ-NH1	-11.71	114.44	120.30
1	B	91	ASP	CB-CG-OD2	11.65	128.78	118.30
1	A	422	PRO	CB-CA-C	11.64	141.10	112.00
1	B	120	TYR	CB-CG-CD1	11.60	127.96	121.00
1	A	249	GLU	CA-CB-CG	11.54	138.79	113.40
1	B	159	LEU	CA-CB-CG	11.47	141.68	115.30
1	B	375	ARG	NE-CZ-NH1	11.43	126.02	120.30
1	A	310	LYS	CB-CG-CD	11.38	141.19	111.60
1	A	106	THR	N-CA-CB	11.14	131.47	110.30
1	A	243	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	A	62	ASP	CB-CG-OD2	-11.02	108.39	118.30
1	A	394	GLY	C-N-CA	10.98	145.37	122.30
1	A	337	ARG	CD-NE-CZ	10.96	138.95	123.60
1	A	183	PHE	N-CA-CB	10.93	130.27	110.60
1	B	133	ARG	NE-CZ-NH2	10.88	125.74	120.30
1	B	278	ARG	CG-CD-NE	10.88	134.64	111.80
1	B	92	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	172	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	A	156	ASP	CB-CG-OD1	10.59	127.83	118.30
1	A	373	ALA	N-CA-CB	-10.59	95.27	110.10
1	B	375	ARG	NE-CZ-NH2	-10.55	115.02	120.30
1	B	65	ARG	NE-CZ-NH1	10.43	125.51	120.30
1	A	127	TYR	CB-CG-CD1	-10.42	114.75	121.00
1	B	413	ALA	N-CA-CB	10.22	124.40	110.10
1	A	158	GLY	N-CA-C	10.14	138.46	113.10
1	B	435	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	188	ASP	CB-CG-OD2	10.13	127.42	118.30
1	A	194	GLU	CA-CB-CG	10.11	135.64	113.40
1	B	205	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	457	VAL	CA-CB-CG1	9.96	125.84	110.90
1	A	336	ASP	CB-CG-OD1	9.95	127.26	118.30
1	A	145	ALA	C-N-CA	9.94	146.55	121.70
1	B	61	ASP	CB-CG-OD1	9.91	127.22	118.30
1	B	125	ASP	CB-CG-OD2	9.90	127.21	118.30
1	A	382	ASN	CA-CB-CG	9.89	135.15	113.40
1	A	137	ASP	CB-CG-OD2	-9.88	109.41	118.30
1	B	259	ALA	CB-CA-C	9.85	124.88	110.10
1	B	62	ASP	CA-CB-CG	9.79	134.93	113.40
1	A	236	ASP	CB-CG-OD1	9.78	127.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	343	LEU	CA-CB-CG	9.73	137.68	115.30
1	A	422	PRO	CA-N-CD	-9.63	98.02	111.50
1	B	418	ARG	CG-CD-NE	9.62	132.01	111.80
1	B	313	ARG	NE-CZ-NH1	-9.50	115.55	120.30
1	B	253	GLU	CA-CB-CG	9.50	134.29	113.40
1	A	263	ASP	C-N-CA	9.45	142.14	122.30
1	A	336	ASP	CB-CG-OD2	-9.41	109.83	118.30
1	B	419	ASP	CB-CG-OD1	9.40	126.76	118.30
1	A	54	ASN	CA-CB-CG	9.38	134.03	113.40
1	A	71	VAL	N-CA-CB	9.35	132.06	111.50
1	A	268	GLY	CA-C-O	9.35	137.42	120.60
1	A	270	ALA	CB-CA-C	9.34	124.11	110.10
1	A	347	GLU	OE1-CD-OE2	9.29	134.45	123.30
1	B	282	ASN	CA-CB-CG	-9.28	92.98	113.40
1	A	220	ASP	CB-CG-OD1	9.24	126.61	118.30
1	A	278	ARG	CB-CG-CD	9.22	135.57	111.60
1	B	388	VAL	N-CA-CB	-9.21	91.23	111.50
1	A	245	GLU	CA-CB-CG	9.21	133.66	113.40
1	B	212	ALA	O-C-N	9.18	137.38	122.70
1	B	206	ASP	CA-CB-CG	9.16	133.56	113.40
1	B	236	ASP	CB-CG-OD2	9.12	126.50	118.30
1	B	56	GLU	N-CA-C	9.10	135.56	111.00
1	B	68	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	A	127	TYR	CA-C-N	9.08	137.19	117.20
1	A	193	ASP	CB-CG-OD2	9.05	126.45	118.30
1	B	171	LEU	O-C-N	9.05	137.17	122.70
1	B	88	ALA	N-CA-CB	9.02	122.72	110.10
1	A	207	THR	CA-CB-CG2	9.01	125.01	112.40
1	B	337	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	B	438	GLU	OE1-CD-OE2	8.92	134.00	123.30
1	A	64	THR	C-N-CA	8.85	143.83	121.70
1	A	284	LEU	N-CA-CB	8.75	127.90	110.40
1	A	127	TYR	CA-C-O	-8.74	101.74	120.10
1	B	278	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	B	152	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	B	65	ARG	NE-CZ-NH2	8.71	124.65	120.30
1	B	65	ARG	NH1-CZ-NH2	-8.70	109.83	119.40
1	A	381	GLU	OE1-CD-OE2	8.69	133.73	123.30
1	B	154	GLU	CG-CD-OE1	-8.69	100.93	118.30
1	A	66	GLY	C-N-CA	8.66	143.35	121.70
1	A	56	GLU	CA-C-O	8.64	138.25	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	ARG	CD-NE-CZ	8.64	135.70	123.60
1	B	343	LEU	CA-CB-CG	8.60	135.07	115.30
1	B	246	TYR	CB-CG-CD2	8.59	126.15	121.00
1	A	233	THR	CA-CB-CG2	8.50	124.30	112.40
1	A	333	GLU	OE1-CD-OE2	-8.46	113.14	123.30
1	A	239	GLU	CA-CB-CG	-8.46	94.79	113.40
1	B	243	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	A	3	GLN	C-N-CA	8.41	142.73	121.70
1	A	64	THR	CA-C-O	8.35	137.63	120.10
1	B	243	ARG	CD-NE-CZ	8.35	135.28	123.60
1	A	147	TRP	N-CA-CB	8.34	125.61	110.60
1	B	375	ARG	CD-NE-CZ	8.33	135.27	123.60
1	B	303	TYR	CB-CG-CD2	8.30	125.98	121.00
1	B	2	ASP	C-N-CA	8.26	142.34	121.70
1	A	449	PRO	CA-N-CD	-8.25	99.95	111.50
1	B	90	PHE	CA-C-N	8.24	135.33	117.20
1	A	156	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	B	120	TYR	CB-CG-CD2	-8.21	116.07	121.00
1	A	236	ASP	OD1-CG-OD2	-8.19	107.73	123.30
1	A	449	PRO	N-CA-C	8.15	133.30	112.10
1	B	140	SER	C-N-CA	8.15	142.09	121.70
1	B	188	ASP	CB-CG-OD2	8.15	125.63	118.30
1	A	146	LEU	CB-CA-C	8.13	125.64	110.20
1	A	250	THR	CA-CB-CG2	8.12	123.78	112.40
1	B	152	ARG	CA-CB-CG	8.12	131.27	113.40
1	A	119	GLU	CA-CB-CG	8.10	131.22	113.40
1	A	68	ASP	CB-CG-OD2	8.07	125.57	118.30
1	A	130	GLU	OE1-CD-OE2	-8.07	113.61	123.30
1	B	356	SER	CB-CA-C	-8.05	94.80	110.10
1	A	56	GLU	O-C-N	-8.04	109.83	122.70
1	B	145	ALA	C-N-CA	8.04	141.80	121.70
1	B	57	VAL	C-N-CA	8.03	141.76	121.70
1	A	325	MET	CA-CB-CG	8.01	126.92	113.30
1	B	286	TYR	CA-CB-CG	8.01	128.62	113.40
1	A	58	CYS	C-N-CA	7.97	141.63	121.70
1	A	411	ARG	CD-NE-CZ	-7.95	112.47	123.60
1	A	420	GLY	N-CA-C	7.95	132.98	113.10
1	A	152	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	A	172	ARG	CD-NE-CZ	7.88	134.64	123.60
1	B	418	ARG	CA-CB-CG	7.82	130.59	113.40
1	B	122	LYS	CA-CB-CG	7.78	130.52	113.40
1	B	217	ARG	NE-CZ-NH2	7.77	124.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	ASP	CB-CG-OD2	7.76	125.29	118.30
1	B	422	PRO	N-CA-C	7.76	132.27	112.10
1	A	104	PHE	CB-CG-CD1	-7.75	115.38	120.80
1	B	72	TYR	CB-CG-CD2	7.72	125.63	121.00
1	A	421	VAL	CA-CB-CG2	7.69	122.44	110.90
1	B	133	ARG	CA-CB-CG	7.69	130.31	113.40
1	B	90	PHE	CA-C-O	-7.67	103.99	120.10
1	A	182	ALA	N-CA-CB	7.67	120.83	110.10
1	A	414	TRP	N-CA-CB	7.66	124.39	110.60
1	B	224	GLU	OE1-CD-OE2	7.66	132.49	123.30
1	B	337	ARG	CD-NE-CZ	7.65	134.31	123.60
1	A	105	LEU	CA-C-N	7.64	134.01	117.20
1	A	313	ARG	CG-CD-NE	7.64	127.85	111.80
1	B	334	SER	O-C-N	-7.64	110.47	122.70
1	A	333	GLU	C-N-CA	7.63	140.78	121.70
1	B	253	GLU	CB-CG-CD	7.62	134.78	114.20
1	B	428	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	112	ASN	N-CA-CB	-7.62	96.89	110.60
1	B	135	LEU	CB-CA-C	7.60	124.65	110.20
1	A	236	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	6	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	456	GLY	N-CA-C	7.56	132.00	113.10
1	B	192	ASN	N-CA-CB	7.52	124.14	110.60
1	A	202	ALA	N-CA-CB	-7.52	99.58	110.10
1	A	410	LEU	O-C-N	-7.48	110.73	122.70
1	B	246	TYR	CB-CG-CD1	-7.46	116.52	121.00
1	A	220	ASP	CB-CA-C	7.45	125.31	110.40
1	A	310	LYS	CA-CB-CG	7.45	129.78	113.40
1	B	68	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	189	PHE	N-CA-C	7.43	131.07	111.00
1	A	105	LEU	CA-C-O	-7.42	104.51	120.10
1	A	156	ASP	CA-CB-CG	7.42	129.73	113.40
1	A	285	HIS	CA-CB-CG	7.37	126.12	113.60
1	A	363	CYS	CB-CA-C	7.37	125.14	110.40
1	B	437	PHE	CA-CB-CG	7.36	131.55	113.90
1	B	443	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	225	ALA	CA-C-O	7.33	135.49	120.10
1	A	59	THR	C-N-CA	7.31	139.98	121.70
1	A	357	TRP	CA-C-N	7.30	130.81	116.20
1	A	172	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	61	ASP	C-N-CA	7.27	139.87	121.70
1	B	256	SER	CB-CA-C	-7.22	96.38	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	PRO	C-N-CA	7.21	139.72	121.70
1	B	152	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	75	ASP	N-CA-CB	7.19	123.55	110.60
1	B	388	VAL	CA-CB-CG2	7.19	121.69	110.90
1	B	305	ALA	CB-CA-C	7.18	120.87	110.10
1	B	386	ALA	C-N-CA	7.15	139.58	121.70
1	B	245	GLU	N-CA-CB	7.14	123.46	110.60
1	A	22	GLU	CA-CB-CG	7.14	129.11	113.40
1	B	277	ARG	O-C-N	-7.14	111.28	122.70
1	A	420	GLY	C-N-CA	7.10	139.45	121.70
1	B	457	VAL	CA-C-N	-7.10	101.58	117.20
1	A	65	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	150	LEU	CA-CB-CG	7.09	131.62	115.30
1	A	221	GLU	CG-CD-OE1	7.09	132.48	118.30
1	B	111	ASN	C-N-CA	7.08	139.41	121.70
1	A	296	SER	N-CA-CB	7.06	121.09	110.50
1	B	111	ASN	CB-CG-OD1	-7.05	107.50	121.60
1	B	144	SER	CB-CA-C	-7.04	96.72	110.10
1	B	262	VAL	CB-CA-C	7.04	124.78	111.40
1	A	448	TYR	CB-CG-CD1	-7.04	116.78	121.00
1	A	448	TYR	CB-CG-CD2	7.04	125.22	121.00
1	B	458	GLU	CG-CD-OE1	7.03	132.35	118.30
1	A	72	TYR	CB-CG-CD2	7.02	125.21	121.00
1	B	362	ALA	CB-CA-C	7.02	120.63	110.10
1	A	173	PRO	N-CA-C	7.01	130.32	112.10
1	B	390	LEU	C-N-CA	7.00	139.19	121.70
1	B	200	PRO	C-N-CA	6.99	139.18	121.70
1	A	286	TYR	CA-CB-CG	6.97	126.64	113.40
1	B	345	GLN	CA-CB-CG	6.95	128.69	113.40
1	B	87	VAL	CA-CB-CG1	6.93	121.30	110.90
1	B	277	ARG	CA-C-N	6.92	132.42	117.20
1	B	157	GLY	CA-C-O	-6.90	108.19	120.60
1	B	94	ILE	CA-C-O	6.89	134.57	120.10
1	A	276	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	184	TRP	C-N-CA	6.88	138.90	121.70
1	B	133	ARG	NH1-CZ-NH2	-6.88	111.83	119.40
1	A	37	GLY	C-N-CA	6.87	138.87	121.70
1	A	337	ARG	CA-CB-CG	6.86	128.49	113.40
1	A	443	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	189	PHE	N-CA-CB	-6.85	98.26	110.60
1	A	10	LEU	N-CA-C	-6.84	92.53	111.00
1	B	90	PHE	CB-CG-CD2	6.83	125.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	LEU	CB-CA-C	6.83	123.18	110.20
1	B	445	ASP	CB-CG-OD1	6.83	124.44	118.30
1	B	166	LYS	CB-CA-C	6.82	124.05	110.40
1	A	170	GLY	N-CA-C	-6.80	96.09	113.10
1	A	223	GLY	C-N-CA	6.80	138.71	121.70
1	B	23	HIS	N-CA-CB	-6.80	98.35	110.60
1	B	284	LEU	CA-CB-CG	6.80	130.95	115.30
1	A	361	LYS	CB-CA-C	6.80	124.00	110.40
1	B	157	GLY	CA-C-N	6.76	129.72	116.20
1	B	143	ILE	CB-CA-C	6.76	125.12	111.60
1	B	88	ALA	CA-C-O	-6.75	105.94	120.10
1	A	203	PRO	N-CA-C	6.74	129.62	112.10
1	B	134	ALA	CB-CA-C	-6.72	100.02	110.10
1	B	314	LEU	CA-CB-CG	6.72	130.75	115.30
1	B	172	ARG	NH1-CZ-NH2	-6.71	112.02	119.40
1	A	98	LYS	O-C-N	6.71	133.43	122.70
1	B	315	GLN	OE1-CD-NE2	6.69	137.29	121.90
1	A	269	ALA	N-CA-CB	-6.69	100.73	110.10
1	B	156	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	192	ASN	CB-CA-C	6.68	123.76	110.40
1	A	120	TYR	N-CA-CB	6.67	122.61	110.60
1	A	25	LEU	O-C-N	6.66	133.36	122.70
1	B	6	ARG	CA-CB-CG	6.66	128.06	113.40
1	B	270	ALA	CB-CA-C	6.66	120.09	110.10
1	A	209	ALA	CB-CA-C	-6.66	100.11	110.10
1	A	235	ASP	CB-CA-C	-6.64	97.12	110.40
1	A	418	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	A	61	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	355	GLN	N-CA-CB	-6.63	98.67	110.60
1	A	143	ILE	CA-C-N	6.62	131.76	117.20
1	A	361	LYS	CA-CB-CG	6.62	127.95	113.40
1	B	304	THR	CA-CB-OG1	-6.61	95.11	109.00
1	A	393	GLY	N-CA-C	-6.61	96.57	113.10
1	A	263	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	432	GLU	CG-CD-OE1	-6.60	105.10	118.30
1	B	354	ARG	CD-NE-CZ	6.60	132.84	123.60
1	A	115	MET	CB-CA-C	6.57	123.54	110.40
1	B	119	GLU	OE1-CD-OE2	6.57	131.18	123.30
1	A	247	VAL	CA-CB-CG1	6.57	120.75	110.90
1	B	28	TYR	CA-CB-CG	6.55	125.86	113.40
1	A	22	GLU	OE1-CD-OE2	-6.54	115.45	123.30
1	B	144	SER	CA-C-O	-6.53	106.38	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	132	TYR	CB-CG-CD1	6.53	124.92	121.00
1	B	261	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	335	SER	N-CA-C	6.52	128.60	111.00
1	A	257	HIS	CA-CB-CG	6.51	124.67	113.60
1	B	262	VAL	CA-C-O	6.50	133.74	120.10
1	A	55	VAL	CA-CB-CG2	6.49	120.63	110.90
1	A	117	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	443	ASP	CB-CG-OD1	6.46	124.12	118.30
1	B	16	ASP	CB-CG-OD2	6.46	124.11	118.30
1	B	188	ASP	CB-CA-C	-6.46	97.48	110.40
1	A	95	THR	CA-CB-CG2	6.46	121.44	112.40
1	A	130	GLU	CB-CG-CD	6.45	131.62	114.20
1	A	64	THR	N-CA-CB	6.45	122.56	110.30
1	B	72	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	A	265	TYR	CB-CA-C	6.43	123.26	110.40
1	A	293	ALA	CB-CA-C	6.43	119.74	110.10
1	A	147	TRP	CB-CA-C	-6.42	97.56	110.40
1	A	380	PHE	CA-CB-CG	6.41	129.29	113.90
1	A	363	CYS	CA-CB-SG	6.39	125.51	114.00
1	A	418	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	A	332	GLY	C-N-CA	6.38	137.66	121.70
1	B	89	LEU	CB-CA-C	-6.38	98.08	110.20
1	A	148	LYS	CA-C-N	6.38	131.24	117.20
1	A	169	LEU	CA-CB-CG	6.37	129.96	115.30
1	A	414	TRP	CA-C-O	-6.37	106.72	120.10
1	B	120	TYR	CA-CB-CG	6.37	125.50	113.40
1	A	78	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	A	306	PHE	CB-CG-CD1	-6.36	116.35	120.80
1	B	214	ALA	CA-C-N	6.36	131.19	117.20
1	A	135	LEU	N-CA-C	-6.35	93.86	111.00
1	B	111	ASN	OD1-CG-ND2	6.33	136.46	121.90
1	A	337	ARG	NH1-CZ-NH2	-6.32	112.45	119.40
1	B	354	ARG	CG-CD-NE	6.32	125.06	111.80
1	A	277	ARG	CG-CD-NE	6.30	125.03	111.80
1	A	4	SER	N-CA-CB	6.30	119.95	110.50
1	B	223	GLY	C-N-CA	6.30	137.45	121.70
1	A	171	LEU	N-CA-CB	-6.30	97.81	110.40
1	A	135	LEU	CA-C-O	-6.28	106.91	120.10
1	A	64	THR	CA-C-N	-6.28	103.39	117.20
1	B	381	GLU	CG-CD-OE1	6.27	130.84	118.30
1	B	363	CYS	N-CA-C	-6.27	94.08	111.00
1	A	59	THR	N-CA-C	-6.26	94.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	62	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	131	ALA	CB-CA-C	6.26	119.49	110.10
1	B	287	HIS	C-N-CA	6.26	137.34	121.70
1	B	412	GLN	CA-C-N	6.25	130.96	117.20
1	A	146	LEU	C-N-CA	6.24	137.30	121.70
1	A	390	LEU	CA-C-O	6.23	133.18	120.10
1	B	261	LEU	CB-CG-CD1	6.21	121.57	111.00
1	A	217	ARG	CG-CD-NE	6.21	124.85	111.80
1	B	303	TYR	CA-CB-CG	6.20	125.18	113.40
1	B	179	ALA	N-CA-CB	6.20	118.78	110.10
1	A	226	LYS	C-N-CA	6.19	137.19	121.70
1	B	354	ARG	CB-CG-CD	6.19	127.70	111.60
1	A	371	MET	N-CA-C	-6.19	94.29	111.00
1	A	284	LEU	CB-CG-CD2	6.18	121.51	111.00
1	B	28	TYR	CB-CG-CD2	6.18	124.71	121.00
1	B	78	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	A	160	VAL	CA-CB-CG1	6.17	120.16	110.90
1	A	243	ARG	NH1-CZ-NH2	-6.17	112.61	119.40
1	B	268	GLY	CA-C-O	6.16	131.69	120.60
1	A	220	ASP	N-CA-C	-6.16	94.37	111.00
1	A	432	GLU	CG-CD-OE2	6.16	130.62	118.30
1	B	303	TYR	CB-CA-C	-6.16	98.08	110.40
1	B	265	TYR	CB-CG-CD2	6.16	124.69	121.00
1	B	75	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	115	MET	CA-CB-CG	6.15	123.75	113.30
1	A	135	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	16	ASP	CA-CB-CG	6.14	126.92	113.40
1	A	361	LYS	N-CA-C	-6.14	94.42	111.00
1	A	176	PHE	CB-CG-CD2	6.13	125.09	120.80
1	A	458	GLU	N-CA-CB	-6.12	99.58	110.60
1	B	268	GLY	N-CA-C	6.12	128.40	113.10
1	A	458	GLU	CB-CG-CD	-6.12	97.69	114.20
1	B	428	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
1	A	173	PRO	CA-C-N	6.09	130.60	117.20
1	A	91	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	260	LEU	CB-CG-CD1	6.08	121.34	111.00
1	A	418	ARG	CD-NE-CZ	-6.07	115.10	123.60
1	A	386	ALA	N-CA-CB	-6.07	101.60	110.10
1	A	452	ARG	CD-NE-CZ	6.07	132.10	123.60
1	B	234	ALA	CB-CA-C	6.07	119.20	110.10
1	B	24	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	A	90	PHE	CB-CG-CD2	6.06	125.04	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	188	ASP	CA-CB-CG	6.06	126.72	113.40
1	A	278	ARG	CG-CD-NE	6.06	124.52	111.80
1	A	112	ASN	CA-CB-CG	6.05	126.71	113.40
1	A	198	ASN	CA-C-O	-6.04	107.41	120.10
1	A	75	ASP	N-CA-C	-6.04	94.69	111.00
1	B	22	GLU	N-CA-CB	6.04	121.47	110.60
1	A	130	GLU	CG-CD-OE2	6.03	130.35	118.30
1	B	221	GLU	CB-CG-CD	6.03	130.48	114.20
1	A	157	GLY	N-CA-C	6.02	128.14	113.10
1	B	99	ALA	CB-CA-C	6.00	119.10	110.10
1	A	85	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	B	24	VAL	CA-C-N	6.00	130.39	117.20
1	A	381	GLU	CB-CA-C	-5.99	98.43	110.40
1	A	2	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	278	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	165	ILE	CA-C-O	-5.98	107.55	120.10
1	B	133	ARG	O-C-N	-5.98	113.14	122.70
1	B	144	SER	CA-C-N	5.97	130.34	117.20
1	B	333	GLU	CA-CB-CG	5.97	126.53	113.40
1	A	142	ASN	CB-CG-OD1	5.96	133.53	121.60
1	B	2	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	263	ASP	N-CA-C	5.95	127.07	111.00
1	B	14	GLU	CB-CG-CD	5.94	130.25	114.20
1	A	341	TYR	CB-CA-C	5.94	122.28	110.40
1	B	61	ASP	N-CA-CB	-5.94	99.90	110.60
1	A	141	VAL	CA-CB-CG2	5.94	119.81	110.90
1	B	315	GLN	O-C-N	5.94	133.30	123.20
1	B	69	ALA	CB-CA-C	5.93	118.99	110.10
1	A	411	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	254	ASN	N-CA-CB	5.92	121.25	110.60
1	A	389	ILE	O-C-N	5.91	132.16	122.70
1	B	282	ASN	N-CA-CB	-5.91	99.97	110.60
1	B	303	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	A	183	PHE	N-CA-C	-5.89	95.10	111.00
1	A	230	ALA	C-N-CA	5.88	136.40	121.70
1	A	58	CYS	CA-C-N	-5.88	104.27	117.20
1	A	3	GLN	CA-CB-CG	5.88	126.33	113.40
1	B	6	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	413	ALA	CA-C-O	-5.87	107.78	120.10
1	A	33	LYS	CB-CG-CD	5.86	126.84	111.60
1	A	414	TRP	O-C-N	5.86	132.08	122.70
1	B	181	HIS	CA-C-O	5.86	132.41	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	152	ARG	CG-CD-NE	5.85	124.08	111.80
1	A	71	VAL	N-CA-C	-5.84	95.23	111.00
1	B	15	GLU	OE1-CD-OE2	5.83	130.30	123.30
1	B	135	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	353	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	B	432	GLU	OE1-CD-OE2	-5.81	116.32	123.30
1	A	149	VAL	N-CA-CB	5.81	124.28	111.50
1	A	125	ASP	N-CA-CB	-5.81	100.15	110.60
1	B	277	ARG	CB-CA-C	5.80	122.00	110.40
1	B	362	ALA	C-N-CA	5.79	136.18	121.70
1	A	390	LEU	CB-CA-C	5.79	121.20	110.20
1	B	326	GLY	C-N-CA	5.79	136.17	121.70
1	A	288	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	389	ILE	O-C-N	5.77	131.94	122.70
1	A	34	ALA	CA-C-O	5.76	132.20	120.10
1	B	235	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	268	GLY	CA-C-N	-5.76	104.54	117.20
1	B	159	LEU	N-CA-C	5.76	126.54	111.00
1	A	246	TYR	CG-CD1-CE1	5.75	125.90	121.30
1	A	358	GLY	N-CA-C	5.75	127.47	113.10
1	A	385	ASN	CA-CB-CG	5.75	126.04	113.40
1	A	89	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	357	TRP	C-N-CA	5.73	134.34	122.30
1	A	215	MET	CA-CB-CG	-5.73	103.55	113.30
1	B	3	GLN	N-CA-CB	5.73	120.91	110.60
1	B	207	THR	CA-CB-OG1	-5.73	96.97	109.00
1	A	213	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	B	265	TYR	N-CA-CB	5.72	120.89	110.60
1	B	455	LEU	CB-CA-C	5.71	121.05	110.20
1	B	214	ALA	C-N-CA	5.71	135.98	121.70
1	A	438	GLU	CB-CG-CD	5.70	129.58	114.20
1	B	414	TRP	CB-CA-C	5.68	121.76	110.40
1	B	219	GLN	CB-CG-CD	5.68	126.36	111.60
1	B	8	VAL	N-CA-CB	5.67	123.98	111.50
1	B	122	LYS	CB-CG-CD	5.67	126.36	111.60
1	A	198	ASN	CA-C-N	5.67	129.68	117.20
1	A	92	ARG	O-C-N	-5.67	113.64	122.70
1	B	12	LEU	CB-CA-C	5.66	120.95	110.20
1	A	430	HIS	CB-CA-C	5.66	121.72	110.40
1	A	398	GLY	N-CA-C	-5.65	98.98	113.10
1	A	2	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	123	MET	CA-CB-CG	-5.64	103.72	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	265	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	B	154	GLU	CG-CD-OE2	5.63	129.57	118.30
1	A	221	GLU	CG-CD-OE2	-5.62	107.06	118.30
1	A	239	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	A	282	ASN	CB-CG-OD1	5.61	132.82	121.60
1	A	51	THR	CA-CB-CG2	5.61	120.25	112.40
1	B	53	THR	CA-CB-CG2	5.60	120.24	112.40
1	B	356	SER	O-C-N	5.60	131.66	122.70
1	B	409	SER	CA-C-O	-5.60	108.33	120.10
1	B	178	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	B	355	GLN	C-N-CA	5.59	135.68	121.70
1	B	372	ASN	N-CA-CB	-5.58	100.55	110.60
1	A	207	THR	CA-CB-OG1	-5.58	97.28	109.00
1	B	79	GLU	CG-CD-OE1	5.58	129.45	118.30
1	A	141	VAL	N-CA-CB	-5.57	99.24	111.50
1	A	382	ASN	CB-CA-C	5.57	121.54	110.40
1	A	311	MET	CB-CG-SD	-5.57	95.70	112.40
1	B	412	GLN	CA-C-O	-5.56	108.42	120.10
1	A	247	VAL	CG1-CB-CG2	-5.56	102.00	110.90
1	A	274	THR	CA-CB-CG2	5.56	120.19	112.40
1	B	287	HIS	CA-CB-CG	-5.56	104.15	113.60
1	A	285	HIS	N-CA-CB	-5.55	100.60	110.60
1	A	37	GLY	N-CA-C	5.55	126.97	113.10
1	B	316	GLY	O-C-N	5.55	131.58	122.70
1	A	359	GLY	O-C-N	5.55	131.58	122.70
1	A	197	GLY	O-C-N	5.54	131.56	122.70
1	B	215	MET	O-C-N	5.54	131.56	122.70
1	A	68	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	353	TYR	CA-C-O	5.53	131.72	120.10
1	B	401	ASP	C-N-CA	5.53	133.91	122.30
1	A	305	ALA	N-CA-CB	5.53	117.84	110.10
1	A	204	LEU	CB-CG-CD2	-5.53	101.61	111.00
1	A	25	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	A	362	ALA	O-C-N	5.51	131.52	122.70
1	A	245	GLU	N-CA-CB	-5.50	100.70	110.60
1	B	304	THR	CA-CB-CG2	5.50	120.10	112.40
1	B	399	HIS	CA-CB-CG	5.49	122.94	113.60
1	B	373	ALA	CA-C-N	5.49	129.28	117.20
1	B	371	MET	N-CA-C	-5.49	96.19	111.00
1	A	183	PHE	CA-C-O	-5.48	108.59	120.10
1	A	11	ALA	N-CA-CB	5.47	117.77	110.10
1	A	165	ILE	CA-C-N	5.47	129.23	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	354	ARG	CB-CA-C	5.47	121.34	110.40
1	B	38	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	B	72	TYR	O-C-N	5.47	131.45	122.70
1	A	65	ARG	CD-NE-CZ	5.46	131.25	123.60
1	B	204	LEU	CA-CB-CG	5.46	127.87	115.30
1	B	87	VAL	CG1-CB-CG2	-5.46	102.16	110.90
1	B	22	GLU	OE1-CD-OE2	5.46	129.85	123.30
1	B	262	VAL	O-C-N	-5.45	113.97	122.70
1	A	44	HIS	CB-CA-C	5.45	121.30	110.40
1	B	183	PHE	CB-CG-CD2	-5.45	116.99	120.80
1	A	287	HIS	C-N-CA	5.44	135.30	121.70
1	B	311	MET	O-C-N	5.44	131.41	122.70
1	A	197	GLY	N-CA-C	-5.44	99.50	113.10
1	A	121	ALA	CB-CA-C	5.44	118.26	110.10
1	A	259	ALA	N-CA-C	-5.44	96.32	111.00
1	B	316	GLY	N-CA-C	5.44	126.69	113.10
1	B	88	ALA	CB-CA-C	-5.42	101.96	110.10
1	A	354	ARG	N-CA-C	-5.42	96.38	111.00
1	B	243	ARG	NH1-CZ-NH2	-5.41	113.44	119.40
1	B	245	GLU	CA-CB-CG	5.41	125.31	113.40
1	B	194	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	B	91	ASP	CA-C-O	5.40	131.45	120.10
1	A	219	GLN	CA-CB-CG	5.40	125.28	113.40
1	A	283	PHE	CB-CA-C	5.40	121.20	110.40
1	B	426	TYR	CB-CA-C	5.40	121.20	110.40
1	B	126	PHE	CA-CB-CG	5.39	126.84	113.90
1	B	414	TRP	CB-CG-CD1	5.39	134.01	127.00
1	A	129	PRO	CA-N-CD	-5.39	103.96	111.50
1	A	212	ALA	CB-CA-C	-5.38	102.03	110.10
1	A	198	ASN	CB-CG-OD1	5.37	132.34	121.60
1	B	8	VAL	CA-C-N	-5.37	105.39	117.20
1	A	58	CYS	O-C-N	5.37	131.29	122.70
1	A	383	LEU	CB-CA-C	5.37	120.40	110.20
1	A	392	ALA	CA-C-N	-5.37	105.47	116.20
1	A	444	ALA	CA-C-O	5.36	131.35	120.10
1	B	282	ASN	CB-CA-C	5.36	121.12	110.40
1	A	418	ARG	CG-CD-NE	5.36	123.05	111.80
1	B	11	ALA	CB-CA-C	-5.36	102.07	110.10
1	B	409	SER	O-C-N	5.35	131.27	122.70
1	A	94	ILE	C-N-CA	5.35	135.06	121.70
1	A	410	LEU	N-CA-CB	-5.34	99.71	110.40
1	B	61	ASP	CA-CB-CG	5.34	125.16	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	330	MET	N-CA-CB	5.34	120.22	110.60
1	B	57	VAL	CA-C-O	5.34	131.31	120.10
1	B	243	ARG	O-C-N	-5.33	114.13	123.20
1	A	284	LEU	CB-CA-C	-5.33	100.07	110.20
1	B	167	PRO	C-N-CA	5.33	135.03	121.70
1	A	234	ALA	N-CA-CB	-5.33	102.64	110.10
1	A	289	ALA	CB-CA-C	-5.33	102.11	110.10
1	A	357	TRP	O-C-N	-5.32	114.15	123.20
1	B	313	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	A	58	CYS	N-CA-CB	5.30	120.15	110.60
1	A	391	THR	N-CA-C	-5.30	96.68	111.00
1	B	341	TYR	CB-CG-CD1	5.30	124.18	121.00
1	B	48	GLU	N-CA-CB	5.29	120.12	110.60
1	A	331	GLU	CA-CB-CG	5.29	125.03	113.40
1	B	274	THR	C-N-CA	5.28	134.91	121.70
1	B	256	SER	N-CA-CB	5.28	118.42	110.50
1	B	57	VAL	O-C-N	-5.28	114.26	122.70
1	B	350	GLY	N-CA-C	-5.26	99.94	113.10
1	A	260	LEU	CB-CA-C	5.26	120.20	110.20
1	A	422	PRO	CA-C-O	5.26	132.83	120.20
1	A	146	LEU	N-CA-CB	-5.26	99.89	110.40
1	B	326	GLY	CA-C-O	5.26	130.06	120.60
1	B	269	ALA	CA-C-N	5.25	128.76	117.20
1	A	331	GLU	CG-CD-OE2	5.25	128.79	118.30
1	B	83	ILE	C-N-CA	5.25	134.81	121.70
1	B	327	PHE	N-CA-C	-5.24	96.86	111.00
1	B	189	PHE	O-C-N	5.23	131.07	122.70
1	A	133	ARG	NH1-CZ-NH2	5.23	125.16	119.40
1	A	367	ILE	CB-CA-C	5.22	122.04	111.60
1	A	225	ALA	CA-C-N	-5.22	105.72	117.20
1	B	139	PRO	CB-CA-C	5.21	125.04	112.00
1	B	164	ILE	N-CA-CB	5.21	122.78	110.80
1	B	249	GLU	CA-CB-CG	5.21	124.85	113.40
1	A	288	ARG	N-CA-C	5.21	125.05	111.00
1	A	135	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	B	90	PHE	N-CA-C	5.20	125.03	111.00
1	A	186	GLY	CA-C-N	-5.20	105.81	116.20
1	A	189	PHE	O-C-N	5.20	131.01	122.70
1	A	431	LYS	N-CA-C	5.19	125.02	111.00
1	B	150	LEU	C-N-CA	5.19	133.20	122.30
1	B	451	TRP	C-N-CA	5.19	134.68	121.70
1	A	410	LEU	CA-C-N	5.18	128.60	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	419	ASP	C-N-CA	5.18	133.18	122.30
1	A	336	ASP	CA-CB-CG	-5.18	102.00	113.40
1	A	73	GLU	CB-CA-C	-5.18	100.04	110.40
1	B	192	ASN	O-C-N	5.18	130.98	122.70
1	A	353	TYR	CA-C-N	-5.17	105.82	117.20
1	B	271	ALA	CB-CA-C	5.17	117.86	110.10
1	B	192	ASN	CB-CA-C	-5.17	100.06	110.40
1	B	211	VAL	C-N-CA	5.17	134.62	121.70
1	B	341	TYR	CA-CB-CG	5.16	123.21	113.40
1	A	144	SER	CB-CA-C	-5.16	100.30	110.10
1	B	154	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	B	269	ALA	CB-CA-C	5.16	117.83	110.10
1	A	290	GLY	C-N-CA	5.15	134.59	121.70
1	A	441	PRO	C-N-CA	5.15	133.11	122.30
1	B	85	TYR	CB-CG-CD1	5.14	124.08	121.00
1	B	96	ASP	CA-C-O	-5.14	109.31	120.10
1	B	3	GLN	CB-CA-C	-5.14	100.12	110.40
1	B	408	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	181	HIS	C-N-CA	5.13	134.53	121.70
1	A	262	VAL	CA-C-O	-5.13	109.34	120.10
1	B	389	ILE	CA-C-O	-5.12	109.34	120.10
1	A	226	LYS	N-CA-CB	-5.12	101.38	110.60
1	A	252	GLY	N-CA-C	5.12	125.90	113.10
1	B	183	PHE	CA-CB-CG	5.12	126.19	113.90
1	B	284	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	457	VAL	CG1-CB-CG2	-5.12	102.72	110.90
1	B	121	ALA	CB-CA-C	5.12	117.77	110.10
1	A	219	GLN	N-CA-CB	5.11	119.80	110.60
1	A	106	THR	CB-CA-C	-5.11	97.80	111.60
1	A	275	ALA	O-C-N	5.11	130.88	122.70
1	A	226	LYS	CA-CB-CG	5.11	124.64	113.40
1	A	257	HIS	CB-CA-C	-5.11	100.19	110.40
1	A	127	TYR	CG-CD1-CE1	5.10	125.38	121.30
1	A	203	PRO	O-C-N	-5.10	114.53	122.70
1	B	261	LEU	CA-C-O	5.10	130.82	120.10
1	B	80	LEU	N-CA-C	5.10	124.77	111.00
1	B	192	ASN	N-CA-C	-5.10	97.23	111.00
1	B	64	THR	C-N-CA	5.09	134.43	121.70
1	A	137	ASP	CB-CA-C	5.09	120.57	110.40
1	A	233	THR	CA-CB-OG1	-5.09	98.32	109.00
1	A	316	GLY	CA-C-O	-5.08	111.45	120.60
1	B	252	GLY	C-N-CA	5.08	134.41	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	152	ARG	CA-CB-CG	5.08	124.58	113.40
1	A	308	HIS	CA-CB-CG	5.08	122.23	113.60
1	B	446	GLN	N-CA-CB	5.07	119.73	110.60
1	A	306	PHE	CB-CA-C	5.07	120.54	110.40
1	A	9	ASN	N-CA-CB	5.07	119.72	110.60
1	A	136	PHE	N-CA-CB	5.06	119.72	110.60
1	B	175	PRO	N-CA-CB	5.06	109.38	103.30
1	A	355	GLN	C-N-CA	5.06	134.35	121.70
1	A	54	ASN	N-CA-CB	5.05	119.69	110.60
1	A	159	LEU	N-CA-C	5.05	124.63	111.00
1	A	84	ALA	CB-CA-C	-5.05	102.53	110.10
1	A	62	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	379	PHE	N-CA-C	-5.03	97.41	111.00
1	B	57	VAL	CA-CB-CG2	5.03	118.45	110.90
1	A	136	PHE	O-C-N	5.03	130.74	122.70
1	B	414	TRP	CB-CG-CD2	-5.03	120.06	126.60
1	A	232	ILE	C-N-CA	5.02	134.26	121.70
1	B	148	LYS	CA-C-O	-5.02	109.56	120.10
1	A	457	VAL	C-N-CA	5.01	134.24	121.70
1	A	12	LEU	CB-CA-C	5.01	119.72	110.20
1	A	171	LEU	CB-CA-C	-5.01	100.68	110.20
1	A	10	LEU	O-C-N	5.00	130.71	122.70
1	B	120	TYR	CA-C-O	5.00	130.61	120.10
1	A	122	LYS	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	457	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	3502	0	3368	276	0
1	B	3498	0	3371	244	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	18	0	8	3	0
2	B	18	0	7	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	2	0
4	B	3	0	0	1	0
All	All	7044	0	6754	496	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (496) 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:B:234:ALA:HB3	1:B:240:ILE:HG13	1.25	1.11
1:B:321:HIS:HB3	2:B:700:RUB:O6P	1.56	1.05
1:A:167:PRO:HD3	1:B:59:THR:HG21	1.41	1.01
1:A:285:HIS:HE2	1:A:321:HIS:HE2	1.05	0.94
1:B:322:THR:HG22	1:B:323:GLY:H	1.34	0.92
1:A:457:VAL:CG1	1:A:458:GLU:H	1.81	0.92
1:B:165:ILE:HG12	1:B:176:PHE:HE1	1.32	0.90
1:A:456:GLY:O	1:A:457:VAL:HB	1.70	0.89
1:B:124:HIS:O	1:B:125:ASP:HB2	1.70	0.87
1:A:306:PHE:HZ	1:A:342:MET:HE3	1.39	0.87
1:A:99:ALA:HB1	1:A:132:TYR:HE1	1.40	0.86
1:B:208:ILE:HD12	1:B:247:VAL:HG22	1.57	0.85
1:B:222:THR:HG22	1:B:224:GLU:HB2	1.57	0.85
1:A:321:HIS:HB3	2:A:600:RUB:O6P	1.75	0.85
1:A:356:SER:O	1:A:358:GLY:N	2.12	0.83
1:B:286:TYR:HB3	1:B:320:ILE:HG12	1.63	0.81
1:A:239:GLU:HG3	1:B:95:THR:HB	1.64	0.79
1:A:170:GLY:HA3	1:B:64:THR:HG23	1.63	0.79
1:A:415:GLN:HG2	1:A:418:ARG:HH21	1.49	0.78
1:B:33:LYS:HG2	1:B:119:GLU:HB2	1.66	0.78
2:B:700:RUB:O3	4:B:701:FMT:O2	2.03	0.77
1:A:129:PRO:O	1:A:133:ARG:HB2	1.83	0.77
1:B:374:LEU:HD11	1:B:437:PHE:HA	1.68	0.76
1:B:74:VAL:HA	1:B:80:LEU:O	1.86	0.76
1:A:67:VAL:HG13	1:A:89:LEU:HD12	1.65	0.76
1:B:169:LEU:HD11	1:B:195:PRO:HB2	1.66	0.76
1:B:296:SER:HB3	1:B:298:GLN:OE1	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD13	1:A:17:LEU:HD11	1.69	0.75
1:A:400:ILE:HD11	1:A:435:ARG:HG2	1.70	0.74
1:B:181:HIS:CD2	1:B:217:ARG:HH21	2.05	0.73
1:A:437:PHE:HD1	1:A:444:ALA:HB1	1.51	0.73
1:A:89:LEU:HD23	1:A:107:LEU:HD22	1.70	0.73
1:A:194:GLU:OE1	1:A:195:PRO:HD3	1.89	0.72
1:B:341:TYR:HB3	1:B:345:GLN:HG2	1.72	0.72
1:A:75:ASP:HB3	1:A:78:ARG:HG2	1.71	0.72
1:B:276:ARG:HG3	1:B:277:ARG:H	1.54	0.71
1:B:309:CYS:O	1:B:312:ALA:HB3	1.89	0.71
1:A:161:VAL:HG11	1:A:410:LEU:HD11	1.73	0.70
1:A:370:GLY:HA3	1:A:396:ALA:HB2	1.74	0.70
1:A:94:ILE:HG21	1:B:204:LEU:HD12	1.73	0.70
1:B:231:ASN:HB2	1:B:261:LEU:HD23	1.74	0.70
1:B:263:ASP:HA	1:B:287:HIS:O	1.92	0.70
1:A:183:PHE:CE1	1:A:187:GLY:HA3	2.26	0.70
1:A:233:THR:OG1	1:A:262:VAL:HA	1.92	0.69
1:A:285:HIS:CD2	1:A:321:HIS:HE2	2.09	0.69
1:B:3:GLN:O	1:B:4:SER:HB2	1.91	0.69
1:B:164:ILE:CD1	2:B:700:RUB:O3P	2.40	0.69
1:A:168:LYS:O	1:A:196:GLN:NE2	2.26	0.69
1:A:28:TYR:CE2	1:A:83:ILE:HD12	2.28	0.69
1:A:286:TYR:OH	1:A:308:HIS:HE1	1.75	0.69
1:A:373:ALA:HB3	1:A:374:LEU:HD22	1.76	0.68
1:A:74:VAL:HA	1:A:80:LEU:O	1.92	0.68
1:A:311:MET:O	1:A:315:GLN:HG3	1.93	0.68
1:B:3:GLN:HE21	1:B:40:ALA:HB1	1.59	0.68
1:A:176:PHE:HE2	1:A:211:VAL:HG21	1.59	0.68
1:A:200:PRO:HD2	1:B:88:ALA:O	1.94	0.68
1:A:313:ARG:CG	1:A:313:ARG:HH11	2.07	0.68
1:A:313:ARG:HH11	1:A:313:ARG:HG3	1.59	0.67
1:A:214:ALA:HA	1:A:217:ARG:HH11	1.59	0.67
1:B:344:THR:HA	1:B:362:ALA:CB	2.25	0.67
1:A:165:ILE:HG21	1:A:176:PHE:CD1	2.30	0.66
1:B:165:ILE:HG12	1:B:176:PHE:CE1	2.23	0.66
1:A:217:ARG:O	1:A:221:GLU:HG3	1.95	0.66
1:B:115:MET:O	1:B:118:VAL:HG22	1.95	0.66
1:A:214:ALA:HA	1:A:217:ARG:NH1	2.11	0.66
1:B:276:ARG:O	1:B:278:ARG:N	2.29	0.66
1:A:219:GLN:HE22	1:A:257:HIS:CE1	2.14	0.66
1:A:99:ALA:HB1	1:A:132:TYR:CE1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ASN:ND2	1:B:387:ASN:HB2	2.11	0.65
1:B:251:PHE:O	1:B:254:ASN:HB2	1.95	0.65
1:B:194:GLU:HB2	1:B:195:PRO:HD3	1.78	0.65
1:B:344:THR:HA	1:B:362:ALA:HB1	1.76	0.65
1:A:276:ARG:HD2	1:A:276:ARG:O	1.96	0.65
1:A:310:LYS:O	1:A:313:ARG:HB3	1.96	0.65
1:B:143:ILE:HD11	1:B:160:VAL:HG23	1.78	0.65
1:A:321:HIS:CB	2:A:600:RUB:O6P	2.43	0.65
1:B:45:PHE:HD2	1:B:118:VAL:HG11	1.62	0.65
1:A:165:ILE:HD11	1:A:180:CYS:SG	2.37	0.65
1:A:310:LYS:HD3	1:A:357:TRP:CZ2	2.32	0.65
1:B:399:HIS:HD2	1:B:401:ASP:H	1.45	0.65
1:A:14:GLU:HG2	1:A:18:ILE:HD12	1.78	0.64
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.78	0.64
1:B:194:GLU:HG2	1:B:287:HIS:CE1	2.31	0.64
1:A:167:PRO:HG2	1:A:171:LEU:HD13	1.79	0.64
1:A:376:MET:HB3	1:A:377:PRO:HD3	1.79	0.64
1:B:268:GLY:O	1:B:270:ALA:N	2.30	0.64
1:B:55:VAL:O	1:B:56:GLU:HB2	1.97	0.64
1:B:44:HIS:O	1:B:47:ALA:HB3	1.98	0.64
1:B:152:ARG:NH2	1:B:159:LEU:O	2.31	0.64
1:A:28:TYR:HE2	1:A:83:ILE:HD12	1.62	0.64
1:B:150:LEU:HD13	1:B:152:ARG:NH1	2.12	0.64
1:A:457:VAL:HG12	1:A:458:GLU:H	1.62	0.63
1:B:167:PRO:HD2	1:B:171:LEU:HG	1.79	0.63
1:A:437:PHE:CD1	1:A:444:ALA:HB1	2.34	0.63
1:A:262:VAL:HG11	1:A:272:ILE:HD13	1.80	0.63
1:A:7:TYR:HE2	1:A:47:ALA:HA	1.62	0.62
1:A:80:LEU:HD21	1:A:82:LYS:HD2	1.80	0.62
1:A:310:LYS:HD3	1:A:357:TRP:HZ2	1.63	0.62
1:A:49:SER:HB3	1:A:107:LEU:O	1.99	0.62
1:A:165:ILE:HG13	1:A:176:PHE:CE1	2.35	0.62
1:A:310:LYS:NZ	1:A:355:GLN:HG2	2.15	0.62
1:A:9:ASN:ND2	1:A:12:LEU:HG	2.15	0.62
1:B:202:ALA:H	1:B:203:PRO:HD3	1.64	0.62
1:A:75:ASP:HB3	1:A:78:ARG:CG	2.30	0.62
1:A:219:GLN:HE22	1:A:257:HIS:HE1	1.48	0.62
1:B:62:ASP:O	1:B:63:PHE:HB2	1.99	0.62
1:A:286:TYR:OH	1:A:308:HIS:CE1	2.52	0.62
1:A:432:GLU:O	1:A:436:ALA:HB2	2.00	0.62
1:A:175:PRO:HB3	1:B:60:THR:HG21	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:HD23	1:B:391:THR:N	2.14	0.61
1:A:33:LYS:HG2	1:A:119:GLU:OE1	2.00	0.61
1:A:193:ASP:HA	4:A:601:FMT:O2	1.99	0.61
1:A:266:VAL:O	1:A:267:ALA:HB2	2.00	0.61
1:A:374:LEU:HD21	1:A:436:ALA:O	2.01	0.61
1:A:421:VAL:HG23	1:A:421:VAL:O	2.01	0.61
1:B:63:PHE:HA	1:B:65:ARG:HH11	1.65	0.61
1:A:143:ILE:HB	1:A:364:THR:OG1	2.01	0.60
1:B:288:ARG:O	1:B:289:ALA:HB3	2.00	0.60
1:A:147:TRP:CZ2	1:A:387:ASN:HB3	2.36	0.60
1:B:202:ALA:N	1:B:203:PRO:HD3	2.15	0.60
1:B:215:MET:O	1:B:219:GLN:HG3	2.02	0.60
1:B:285:HIS:CD2	1:B:366:ILE:HD12	2.36	0.60
1:B:217:ARG:O	1:B:221:GLU:HG3	2.02	0.60
1:A:310:LYS:HZ3	1:A:355:GLN:HG2	1.65	0.60
1:B:401:ASP:OD2	1:B:435:ARG:HD3	2.02	0.60
1:A:173:PRO:HB3	1:A:207:THR:OG1	2.02	0.60
1:B:294:VAL:HG13	1:B:302:GLY:HA3	1.82	0.59
1:A:458:GLU:O	1:A:459:ASP:HB2	2.02	0.59
1:B:385:ASN:HD22	1:B:386:ALA:N	1.99	0.59
1:A:29:ILE:HG13	1:A:124:HIS:CD2	2.37	0.59
1:B:181:HIS:CG	1:B:217:ARG:HH21	2.20	0.59
1:B:234:ALA:CB	1:B:240:ILE:HG13	2.16	0.59
1:A:14:GLU:HG2	1:A:18:ILE:CD1	2.32	0.59
1:A:55:VAL:O	1:A:57:VAL:HG22	2.03	0.59
1:A:113:GLN:HB2	1:B:290:GLY:HA2	1.83	0.59
1:B:152:ARG:HG3	1:B:153:PRO:HD2	1.84	0.59
1:A:457:VAL:HG13	1:A:458:GLU:H	1.67	0.59
1:B:126:PHE:CZ	1:B:310:LYS:HG2	2.37	0.59
1:A:309:CYS:HB3	1:A:343:LEU:HD21	1.84	0.59
1:B:131:ALA:O	1:B:135:LEU:HD22	2.01	0.59
1:A:427:ALA:HB3	1:A:455:LEU:HD21	1.84	0.59
1:A:347:GLU:O	1:A:347:GLU:HG3	2.03	0.59
1:B:274:THR:O	1:B:278:ARG:HB3	2.03	0.58
1:A:453:LYS:HD2	1:A:454:ALA:N	2.18	0.58
1:A:162:GLY:N	1:A:390:LEU:O	2.32	0.58
1:B:329:LYS:HG2	1:B:333:GLU:OE1	2.04	0.58
1:A:14:GLU:OE1	1:A:82:LYS:NZ	2.37	0.58
1:A:169:LEU:O	1:B:51:THR:HG22	2.03	0.58
1:A:301:ARG:HB2	1:A:301:ARG:NH1	2.19	0.58
1:A:237:PRO:O	1:A:241:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:TRP:CE2	1:B:190:ILE:HG13	2.38	0.58
1:B:428:ARG:O	1:B:429:GLU:HB2	2.04	0.58
1:A:183:PHE:CZ	1:A:187:GLY:HA3	2.38	0.57
1:A:195:PRO:HB3	1:B:107:LEU:CD1	2.34	0.57
1:A:376:MET:CB	1:A:377:PRO:HD3	2.34	0.57
1:B:133:ARG:HD3	1:B:356:SER:O	2.04	0.57
1:A:7:TYR:OH	1:A:51:THR:HB	2.03	0.57
1:A:191:LYS:CB	1:A:229:SER:HB3	2.35	0.57
1:A:6:ARG:HD3	1:A:7:TYR:CE1	2.39	0.57
1:B:276:ARG:HG3	1:B:277:ARG:N	2.20	0.57
1:B:428:ARG:NH2	1:B:454:ALA:HB1	2.19	0.57
1:B:398:GLY:HA3	1:B:440:PHE:CZ	2.40	0.57
1:A:311:MET:HA	1:A:314:LEU:HD12	1.87	0.57
1:A:457:VAL:CG1	1:A:458:GLU:N	2.63	0.57
1:B:415:GLN:O	1:B:416:ALA:C	2.42	0.57
1:A:167:PRO:HD3	1:B:59:THR:CG2	2.27	0.57
1:B:42:ALA:HB1	1:B:71:VAL:HG21	1.87	0.57
1:A:421:VAL:O	1:A:422:PRO:O	2.22	0.56
1:A:409:SER:HB2	1:A:436:ALA:HB2	1.88	0.56
1:B:62:ASP:H	1:B:65:ARG:HD2	1.69	0.56
1:A:349:GLN:OE1	1:A:354:ARG:HB2	2.04	0.56
1:B:192:ASN:ND2	1:B:196:GLN:OE1	2.38	0.56
1:B:171:LEU:CD1	1:B:176:PHE:HA	2.35	0.56
1:A:285:HIS:HE2	1:A:321:HIS:CE1	2.24	0.56
1:B:191:LYS:O	1:B:229:SER:O	2.24	0.55
1:A:6:ARG:HD3	1:A:7:TYR:HE1	1.71	0.55
1:A:294:VAL:O	1:A:299:SER:HB3	2.06	0.55
1:A:320:ILE:HG22	1:A:363:CYS:SG	2.46	0.55
1:B:67:VAL:O	1:B:89:LEU:HD11	2.06	0.55
1:A:437:PHE:HD1	1:A:444:ALA:CB	2.20	0.55
1:B:368:SER:OG	2:B:700:RUB:O1P	2.24	0.55
1:A:423:VAL:HG11	1:A:448:TYR:CD2	2.41	0.55
1:A:127:TYR:CE2	1:A:129:PRO:HD3	2.42	0.55
1:A:130:GLU:CD	1:A:133:ARG:HH12	2.09	0.55
1:B:309:CYS:HB3	1:B:343:LEU:HD21	1.89	0.55
1:A:224:GLU:OE1	1:A:411:ARG:NH2	2.39	0.54
1:A:364:THR:HG22	1:A:365:PRO:O	2.06	0.54
1:A:380:PHE:CZ	1:A:414:TRP:HB2	2.42	0.54
1:A:427:ALA:CB	1:A:455:LEU:HD21	2.36	0.54
1:B:288:ARG:O	1:B:289:ALA:CB	2.56	0.54
1:A:373:ALA:CB	1:A:436:ALA:HB1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ARG:HG3	1:A:435:ARG:HH11	1.72	0.54
1:A:385:ASN:HB2	1:A:387:ASN:ND2	2.21	0.54
1:A:400:ILE:HD11	1:A:435:ARG:CG	2.38	0.54
1:B:231:ASN:HB2	1:B:261:LEU:CD2	2.37	0.54
1:B:396:ALA:HA	1:B:406:GLY:HA3	1.88	0.54
1:B:399:HIS:CD2	1:B:401:ASP:H	2.23	0.54
1:A:5:SER:O	1:A:6:ARG:HB3	2.07	0.54
1:A:147:TRP:HZ2	1:A:387:ASN:HB3	1.73	0.54
1:A:374:LEU:HG	1:A:444:ALA:HB2	1.89	0.54
1:A:3:GLN:HE22	1:A:6:ARG:HD2	1.74	0.53
1:A:192:ASN:ND2	1:A:228:PHE:HZ	2.06	0.53
1:B:202:ALA:N	1:B:203:PRO:CD	2.72	0.53
1:A:88:ALA:O	1:B:200:PRO:HD2	2.07	0.53
1:B:376:MET:HG2	1:B:380:PHE:CE2	2.43	0.53
1:B:399:HIS:HA	1:B:439:SER:OG	2.09	0.53
1:B:3:GLN:O	1:B:4:SER:CB	2.55	0.53
1:B:341:TYR:HB3	1:B:345:GLN:CG	2.39	0.53
1:A:262:VAL:CG1	1:A:272:ILE:HD13	2.38	0.53
1:B:72:TYR:HD2	1:B:84:ALA:HB2	1.73	0.53
1:A:109:MET:HA	1:A:109:MET:CE	2.38	0.53
1:A:341:TYR:O	1:A:345:GLN:HB3	2.09	0.53
1:A:261:LEU:HD11	1:A:287:HIS:HB3	1.90	0.52
1:A:405:ALA:HB1	1:A:432:GLU:HB3	1.92	0.52
1:B:96:ASP:OD2	1:B:277:ARG:NH1	2.42	0.52
1:B:152:ARG:CG	1:B:153:PRO:HD2	2.40	0.52
1:A:6:ARG:HD3	1:A:68:ASP:OD2	2.09	0.52
1:A:25:LEU:HB2	1:A:127:TYR:HB3	1.91	0.52
1:A:325:MET:HB3	1:A:379:PHE:HE1	1.74	0.52
1:A:146:LEU:HD22	1:A:283:PHE:CD2	2.44	0.52
1:A:445:ASP:OD2	1:A:452:ARG:NH2	2.42	0.52
1:B:164:ILE:HD11	2:B:700:RUB:O3P	2.10	0.52
1:A:123:MET:CE	1:A:126:PHE:HB3	2.39	0.52
1:A:427:ALA:O	1:A:434:ALA:HB2	2.09	0.52
1:A:376:MET:CE	1:A:390:LEU:HD22	2.40	0.51
1:B:184:TRP:NE1	1:B:190:ILE:HG12	2.24	0.51
1:B:311:MET:O	1:B:315:GLN:HG3	2.10	0.51
1:B:341:TYR:O	1:B:345:GLN:HB2	2.10	0.51
1:A:440:PHE:O	1:A:444:ALA:HB3	2.09	0.51
1:B:339:ILE:O	1:B:343:LEU:HG	2.10	0.51
1:A:428:ARG:HG2	1:A:455:LEU:HD12	1.91	0.51
1:A:168:LYS:HE3	1:A:195:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:OD1	4:A:601:FMT:O2	2.29	0.51
1:B:284:LEU:HD13	1:B:317:ALA:HA	1.92	0.51
1:A:140:SER:O	1:A:141:VAL:HG23	2.11	0.51
1:B:322:THR:HG22	1:B:323:GLY:N	2.15	0.51
1:B:428:ARG:O	1:B:429:GLU:CB	2.58	0.51
1:B:374:LEU:HD21	1:B:437:PHE:CD1	2.46	0.51
1:B:6:ARG:NH1	1:B:65:ARG:HA	2.26	0.51
1:B:191:LYS:O	1:B:192:ASN:HB2	2.11	0.51
1:A:168:LYS:HG3	1:A:193:ASP:HB3	1.93	0.50
1:A:456:GLY:O	1:A:457:VAL:CB	2.51	0.50
1:B:213:ASP:O	1:B:215:MET:N	2.44	0.50
1:B:439:SER:O	1:B:441:PRO:HD3	2.11	0.50
1:A:50:SER:OG	1:A:69:ALA:HB3	2.12	0.50
1:B:349:GLN:NE2	1:B:350:GLY:O	2.44	0.50
1:A:10:LEU:HD21	1:A:71:VAL:HG23	1.93	0.50
1:B:321:HIS:HA	1:B:366:ILE:HB	1.92	0.50
1:A:228:PHE:O	1:A:258:VAL:HA	2.12	0.50
1:B:436:ALA:O	1:B:439:SER:HB2	2.11	0.50
1:A:284:LEU:N	1:A:318:SER:HB2	2.27	0.50
1:B:29:ILE:HA	1:B:79:GLU:O	2.11	0.50
1:B:165:ILE:N	1:B:165:ILE:HD12	2.26	0.50
1:B:86:PRO:HB2	1:B:89:LEU:HD13	1.94	0.50
1:A:7:TYR:CE2	1:A:47:ALA:HB2	2.47	0.49
1:A:57:VAL:HB	1:B:166:LYS:HB3	1.94	0.49
1:B:377:PRO:HG2	1:B:448:TYR:OH	2.12	0.49
1:B:22:GLU:O	1:B:87:VAL:HG23	2.11	0.49
1:B:322:THR:CG2	1:B:323:GLY:H	2.08	0.49
1:A:200:PRO:HG2	1:B:88:ALA:HB1	1.94	0.49
1:A:161:VAL:HG11	1:A:410:LEU:CD1	2.41	0.49
1:A:174:LYS:N	1:A:175:PRO:HD2	2.28	0.49
1:A:123:MET:HE1	1:A:126:PHE:HB3	1.93	0.49
1:A:196:GLN:O	1:A:231:ASN:ND2	2.46	0.49
1:B:171:LEU:HD13	1:B:176:PHE:HA	1.94	0.49
1:A:399:HIS:ND1	1:A:405:ALA:HB3	2.28	0.49
1:B:150:LEU:HD21	1:B:227:LEU:HD22	1.94	0.49
1:A:88:ALA:HB1	1:B:200:PRO:HG2	1.94	0.49
1:A:29:ILE:HG13	1:A:124:HIS:NE2	2.27	0.48
1:A:184:TRP:CE2	1:A:190:ILE:HD12	2.48	0.48
1:A:409:SER:HB2	1:A:432:GLU:O	2.13	0.48
1:B:313:ARG:NH2	1:B:360:MET:O	2.37	0.48
1:A:12:LEU:HD13	1:A:17:LEU:CD1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:HE2	1:A:211:VAL:CG2	2.24	0.48
1:B:399:HIS:HD2	1:B:401:ASP:N	2.10	0.48
1:A:173:PRO:O	1:A:210:LEU:HD23	2.13	0.48
1:A:184:TRP:CD1	1:A:226:LYS:HG3	2.49	0.48
1:A:299:SER:HB2	1:B:301:ARG:HD3	1.95	0.48
1:A:210:LEU:O	1:A:211:VAL:C	2.52	0.48
1:B:95:THR:HG22	1:B:96:ASP:N	2.29	0.48
1:B:254:ASN:O	1:B:257:HIS:HB2	2.14	0.48
1:A:101:ILE:O	1:A:105:LEU:HB2	2.14	0.48
1:A:357:TRP:HE3	1:A:360:MET:HE2	1.78	0.48
1:B:184:TRP:CE2	1:B:190:ILE:CG1	2.97	0.48
1:B:174:LYS:HB3	1:B:175:PRO:HD3	1.95	0.48
1:B:326:GLY:O	1:B:327:PHE:HB2	2.14	0.48
1:B:165:ILE:HD12	1:B:165:ILE:H	1.79	0.47
1:B:194:GLU:HG2	1:B:287:HIS:HE1	1.79	0.47
1:A:67:VAL:HG12	1:A:67:VAL:O	2.13	0.47
1:A:290:GLY:HA2	1:B:110:GLY:O	2.14	0.47
1:B:414:TRP:O	1:B:417:TRP:N	2.47	0.47
1:A:377:PRO:HA	1:A:380:PHE:CD2	2.49	0.47
1:A:284:LEU:H	1:A:318:SER:HB2	1.78	0.47
1:A:411:ARG:O	1:A:411:ARG:HG2	2.14	0.47
1:B:452:ARG:HB2	1:B:458:GLU:O	2.15	0.47
1:B:231:ASN:CB	1:B:261:LEU:HD23	2.44	0.47
1:B:415:GLN:NE2	1:B:426:TYR:OH	2.47	0.47
1:A:247:VAL:HG23	1:A:251:PHE:CD1	2.50	0.47
1:A:346:ASP:O	1:A:347:GLU:HB2	2.15	0.47
1:A:424:LEU:H	1:A:424:LEU:HG	1.42	0.47
1:B:90:PHE:HE1	1:B:104:PHE:HA	1.79	0.47
1:A:427:ALA:CB	1:A:437:PHE:HE2	2.28	0.47
1:B:141:VAL:O	1:B:318:SER:HB3	2.14	0.47
1:A:294:VAL:HG23	1:A:295:THR:H	1.79	0.47
1:A:373:ALA:HB2	1:A:409:SER:OG	2.15	0.47
1:B:174:LYS:HB3	1:B:175:PRO:CD	2.45	0.47
1:A:171:LEU:C	1:A:172:ARG:O	2.53	0.47
1:A:306:PHE:CZ	1:A:342:MET:HE3	2.31	0.47
1:A:194:GLU:N	1:A:195:PRO:HD3	2.31	0.46
1:B:33:LYS:HG2	1:B:119:GLU:HG3	1.97	0.46
1:B:33:LYS:HG2	1:B:119:GLU:CB	2.40	0.46
1:B:322:THR:O	1:B:323:GLY:O	2.34	0.46
1:A:128:VAL:H	1:A:355:GLN:HE22	1.63	0.46
1:B:4:SER:HB3	1:B:6:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ALA:C	1:B:276:ARG:O	2.52	0.46
1:B:422:PRO:O	1:B:424:LEU:N	2.46	0.46
1:A:122:LYS:HE3	1:A:303:TYR:O	2.15	0.46
1:A:385:ASN:HB2	1:A:387:ASN:HD21	1.79	0.46
1:A:385:ASN:ND2	1:A:387:ASN:HD22	2.13	0.46
1:A:133:ARG:HH11	1:A:133:ARG:HD3	1.45	0.46
1:A:94:ILE:HD12	1:A:94:ILE:C	2.36	0.46
1:B:173:PRO:O	1:B:176:PHE:HB3	2.16	0.46
1:A:393:GLY:O	1:A:395:GLY:N	2.48	0.46
1:B:377:PRO:HD3	1:B:413:ALA:HB1	1.98	0.46
1:B:85:TYR:O	1:B:86:PRO:C	2.55	0.45
1:B:189:PHE:HD1	1:B:227:LEU:HB3	1.81	0.45
1:B:452:ARG:CB	1:B:458:GLU:O	2.64	0.45
1:A:128:VAL:H	1:A:355:GLN:NE2	2.13	0.45
1:A:195:PRO:HB3	1:B:107:LEU:HD13	1.97	0.45
1:A:233:THR:HG1	1:A:262:VAL:HA	1.79	0.45
1:A:357:TRP:CE3	1:A:360:MET:HE2	2.51	0.45
1:A:412:GLN:HB3	1:A:433:LEU:CD1	2.46	0.45
1:B:101:ILE:HD12	1:B:101:ILE:HA	1.67	0.45
1:B:373:ALA:HB1	1:B:413:ALA:HB2	1.97	0.45
1:B:376:MET:HE3	1:B:376:MET:HB3	1.83	0.45
1:A:405:ALA:O	1:A:409:SER:HB3	2.17	0.45
1:B:194:GLU:H	1:B:194:GLU:HG3	1.37	0.45
1:A:239:GLU:O	1:A:240:ILE:C	2.52	0.45
1:B:342:MET:SD	1:B:357:TRP:HZ2	2.39	0.45
1:A:30:MET:HG2	1:A:121:ALA:HB2	1.98	0.45
1:B:26:CYS:HB3	1:B:28:TYR:CE1	2.51	0.45
1:B:287:HIS:CD2	1:B:288:ARG:N	2.85	0.45
1:A:204:LEU:O	1:A:208:ILE:HB	2.16	0.45
1:A:426:TYR:HD2	1:A:433:LEU:HD12	1.82	0.45
1:B:159:LEU:O	1:B:159:LEU:HD12	2.17	0.45
1:B:199:GLN:HB3	1:B:201:PHE:CD1	2.51	0.45
1:B:423:VAL:HG11	1:B:448:TYR:CZ	2.51	0.45
1:A:218:ALA:O	1:A:222:THR:HG23	2.17	0.45
1:A:376:MET:HE1	1:A:390:LEU:HD22	1.98	0.45
1:B:75:ASP:HB3	1:B:80:LEU:HB2	1.99	0.45
1:B:327:PHE:HD1	1:B:328:GLY:H	1.63	0.45
1:B:287:HIS:CD2	1:B:288:ARG:H	2.35	0.45
1:B:426:TYR:O	1:B:430:HIS:ND1	2.49	0.45
1:A:420:GLY:O	1:A:422:PRO:HD2	2.17	0.44
1:B:171:LEU:HD12	1:B:176:PHE:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:O	1:A:143:ILE:C	2.54	0.44
1:A:285:HIS:NE2	1:A:321:HIS:NE2	2.34	0.44
1:A:376:MET:HB3	1:A:377:PRO:CD	2.44	0.44
1:B:212:ALA:O	1:B:215:MET:HB3	2.17	0.44
1:B:243:ARG:O	1:B:246:TYR:N	2.51	0.44
1:A:143:ILE:HA	1:A:143:ILE:HD12	1.55	0.44
1:A:176:PHE:CE2	1:A:211:VAL:CG2	3.01	0.44
1:B:430:HIS:ND1	1:B:430:HIS:N	2.65	0.44
1:B:225:ALA:HB1	1:B:257:HIS:CE1	2.52	0.44
1:A:292:GLY:O	1:A:296:SER:HB2	2.17	0.44
1:A:385:ASN:HD22	1:A:387:ASN:H	1.66	0.44
1:A:100:MET:HG3	1:A:103:SER:H	1.82	0.44
1:A:164:ILE:HD11	1:A:391:THR:HG23	1.99	0.44
1:A:325:MET:HB3	1:A:379:PHE:CE1	2.51	0.44
1:A:367:ILE:HG22	1:A:390:LEU:HD12	1.99	0.44
1:B:184:TRP:CZ2	1:B:190:ILE:HG13	2.53	0.44
1:B:268:GLY:O	1:B:269:ALA:C	2.55	0.44
1:B:385:ASN:ND2	1:B:385:ASN:C	2.71	0.44
1:A:191:LYS:HB2	1:A:229:SER:HB3	1.99	0.44
1:B:287:HIS:HD2	1:B:288:ARG:H	1.66	0.44
1:B:72:TYR:CD2	1:B:84:ALA:HB2	2.53	0.44
1:B:95:THR:HG22	1:B:96:ASP:H	1.83	0.44
1:B:115:MET:O	1:B:115:MET:SD	2.76	0.44
1:A:236:ASP:O	1:A:239:GLU:N	2.50	0.44
1:A:317:ALA:O	1:A:363:CYS:HB2	2.18	0.44
1:B:75:ASP:CB	1:B:80:LEU:HB2	2.48	0.44
1:B:375:ARG:HD2	1:B:443:ASP:OD2	2.18	0.43
1:B:380:PHE:CE1	1:B:386:ALA:HB1	2.53	0.43
1:B:422:PRO:HG2	1:B:425:ASP:OD2	2.18	0.43
1:B:71:VAL:HG22	1:B:83:ILE:HG12	2.00	0.43
1:B:191:LYS:HE3	1:B:192:ASN:O	2.18	0.43
1:A:13:LYS:HD2	1:A:16:ASP:OD2	2.19	0.43
1:A:178:GLU:HA	1:A:178:GLU:OE1	2.18	0.43
1:A:444:ALA:O	1:A:445:ASP:HB2	2.18	0.43
1:B:398:GLY:HA3	1:B:440:PHE:HZ	1.80	0.43
1:A:284:LEU:H	1:A:318:SER:CB	2.30	0.43
1:A:321:HIS:HA	1:A:366:ILE:O	2.19	0.43
1:B:268:GLY:O	1:B:271:ALA:N	2.39	0.43
1:B:376:MET:CE	1:B:413:ALA:HB3	2.48	0.43
1:B:163:THR:HB	1:B:183:PHE:CZ	2.54	0.43
1:A:310:LYS:HZ3	1:A:355:GLN:CG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLY:N	1:B:390:LEU:O	2.51	0.43
1:A:165:ILE:HG21	1:A:176:PHE:HD1	1.80	0.43
1:A:270:ALA:HA	1:B:235:ASP:O	2.18	0.43
1:B:172:ARG:HB3	1:B:173:PRO:HD2	2.00	0.43
1:B:225:ALA:HB1	1:B:257:HIS:HE1	1.83	0.43
1:A:99:ALA:CB	1:A:132:TYR:CE1	3.02	0.43
1:A:185:LEU:O	1:A:404:VAL:HG13	2.18	0.43
1:A:427:ALA:HB2	1:A:437:PHE:HE2	1.84	0.43
1:A:67:VAL:O	1:A:89:LEU:HD11	2.19	0.43
1:A:142:ASN:HB2	1:A:143:ILE:H	1.70	0.43
1:A:248:LEU:HD23	1:A:258:VAL:HG11	1.99	0.43
1:B:276:ARG:HG3	1:B:276:ARG:NH1	2.34	0.43
1:A:49:SER:OG	1:A:112:ASN:ND2	2.49	0.43
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.89	0.43
1:B:141:VAL:CG2	1:B:283:PHE:HA	2.49	0.43
1:A:239:GLU:CG	1:B:95:THR:HB	2.44	0.42
1:B:45:PHE:HA	1:B:115:MET:HE3	2.00	0.42
1:B:125:ASP:OD2	1:B:351:PRO:HD2	2.19	0.42
1:B:199:GLN:HB3	1:B:200:PRO:HD2	2.01	0.42
1:B:162:GLY:HA2	1:B:189:PHE:O	2.19	0.42
1:A:3:GLN:NE2	1:A:6:ARG:HD2	2.34	0.42
1:A:374:LEU:HD22	1:A:374:LEU:H	1.84	0.42
1:B:122:LYS:HB2	1:B:300:LYS:O	2.19	0.42
1:A:5:SER:O	1:A:6:ARG:CB	2.65	0.42
1:A:6:ARG:NH1	1:A:65:ARG:HB3	2.34	0.42
1:A:243:ARG:NH2	1:B:100:MET:HE1	2.34	0.42
1:A:161:VAL:CG1	1:A:390:LEU:HD23	2.49	0.42
1:A:247:VAL:HG23	1:A:251:PHE:CE1	2.54	0.42
1:B:56:GLU:HB3	1:B:57:VAL:H	1.64	0.42
1:B:296:SER:HA	1:B:297:PRO:HD3	1.78	0.42
1:A:30:MET:HA	1:A:120:TYR:O	2.19	0.42
1:A:265:TYR:O	1:A:267:ALA:N	2.51	0.42
1:A:357:TRP:CD1	1:A:357:TRP:N	2.79	0.42
1:B:123:MET:CE	1:B:307:VAL:HG11	2.49	0.42
1:B:374:LEU:HD11	1:B:437:PHE:CA	2.44	0.42
1:B:394:GLY:O	1:B:440:PHE:HZ	2.02	0.42
1:B:111:ASN:O	1:B:115:MET:HB2	2.19	0.42
1:B:277:ARG:HE	1:B:277:ARG:HB2	1.77	0.42
1:B:123:MET:HE2	1:B:307:VAL:HG11	2.02	0.42
1:B:229:SER:HA	1:B:259:ALA:O	2.20	0.42
1:A:155:VAL:O	1:A:157:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PRO:O	1:A:204:LEU:C	2.57	0.42
1:A:168:LYS:HE3	1:A:195:PRO:CG	2.50	0.42
1:A:194:GLU:N	1:A:195:PRO:CD	2.83	0.42
1:A:268:GLY:HA3	1:B:268:GLY:HA3	2.02	0.42
1:A:377:PRO:HA	1:A:380:PHE:HD2	1.85	0.42
1:B:133:ARG:O	1:B:136:PHE:HB2	2.20	0.42
1:B:230:ALA:HB3	1:B:247:VAL:HG11	2.01	0.42
1:B:306:PHE:CZ	1:B:342:MET:HG2	2.55	0.42
1:A:101:ILE:O	1:A:104:PHE:HB3	2.20	0.41
1:A:310:LYS:HZ3	1:A:355:GLN:HE21	1.67	0.41
1:B:225:ALA:O	1:B:226:LYS:HD3	2.18	0.41
1:A:239:GLU:HG3	1:B:95:THR:CB	2.41	0.41
1:A:371:MET:O	1:A:376:MET:SD	2.78	0.41
1:A:397:PHE:CE1	1:A:410:LEU:HD21	2.55	0.41
1:A:110:GLY:O	1:A:113:GLN:HB2	2.21	0.41
1:A:171:LEU:O	1:A:172:ARG:O	2.38	0.41
1:A:195:PRO:HB3	1:B:107:LEU:HD11	2.00	0.41
1:A:368:SER:HB3	2:A:600:RUB:O5P	2.20	0.41
1:B:273:THR:O	1:B:277:ARG:HB3	2.19	0.41
1:A:165:ILE:HG21	1:A:176:PHE:CE1	2.54	0.41
1:A:402:GLY:O	1:A:404:VAL:N	2.54	0.41
1:A:94:ILE:HG21	1:B:204:LEU:CD1	2.46	0.41
1:A:310:LYS:NZ	1:A:355:GLN:HE21	2.18	0.41
1:A:322:THR:HG23	1:A:339:ILE:HG21	2.03	0.41
1:B:365:PRO:HB2	1:B:388:VAL:HG22	2.02	0.41
1:B:275:ALA:O	1:B:276:ARG:O	2.38	0.41
1:B:305:ALA:O	1:B:306:PHE:C	2.57	0.41
1:A:6:ARG:O	1:A:6:ARG:HG2	2.21	0.41
1:A:162:GLY:HA3	1:A:189:PHE:O	2.21	0.41
1:A:448:TYR:HD1	1:A:448:TYR:HA	1.64	0.41
1:B:184:TRP:CG	1:B:226:LYS:HG3	2.56	0.41
1:B:193:ASP:OD1	1:B:194:GLU:HG3	2.21	0.41
1:B:194:GLU:CB	1:B:195:PRO:HD3	2.47	0.41
1:B:355:GLN:HG3	1:B:356:SER:N	2.36	0.41
1:A:65:ARG:O	1:A:68:ASP:HB2	2.21	0.41
1:A:91:ASP:HB3	1:A:103:SER:HB2	2.02	0.41
1:A:114:GLY:O	1:A:115:MET:C	2.60	0.41
1:A:272:ILE:HD13	1:A:272:ILE:HA	1.82	0.41
1:B:202:ALA:H	1:B:203:PRO:CD	2.32	0.41
1:B:163:THR:HB	1:B:183:PHE:CE2	2.56	0.40
1:B:168:LYS:HG3	1:B:193:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ARG:O	1:B:277:ARG:C	2.58	0.40
1:B:322:THR:CG2	1:B:323:GLY:N	2.80	0.40
1:A:313:ARG:CG	1:A:313:ARG:NH1	2.79	0.40
1:A:452:ARG:H	1:A:452:ARG:HG2	1.70	0.40
1:B:22:GLU:OE1	1:B:86:PRO:HA	2.21	0.40
1:B:63:PHE:H	1:B:65:ARG:NE	2.18	0.40
1:B:141:VAL:HG11	1:B:281:ASP:O	2.21	0.40
1:B:184:TRP:O	1:B:226:LYS:NZ	2.51	0.40
1:A:248:LEU:HD22	1:A:282:ASN:HD21	1.86	0.40
1:A:274:THR:OG1	1:B:237:PRO:HG3	2.22	0.40
1:A:318:SER:O	1:A:363:CYS:HA	2.22	0.40
1:A:415:GLN:CG	1:A:418:ARG:HH21	2.27	0.40
1:B:85:TYR:CZ	1:B:108:THR:HG22	2.57	0.40
1:B:367:ILE:O	1:B:391:THR:HG22	2.21	0.40
1:A:90:PHE:O	1:A:92:ARG:HD3	2.22	0.40
1:A:426:TYR:O	1:A:430:HIS:N	2.49	0.40
1:B:84:ALA:O	1:B:86:PRO:HD3	2.22	0.40
1:B:374:LEU:HD22	1:B:448:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	457/466 (98%)	330 (72%)	82 (18%)	45 (10%)	0 0
1	B	456/466 (98%)	360 (79%)	60 (13%)	36 (8%)	1 1
All	All	913/932 (98%)	690 (76%)	142 (16%)	81 (9%)	1 0

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	38	TYR
1	A	129	PRO
1	A	136	PHE
1	A	144	SER
1	A	156	ASP
1	A	171	LEU
1	A	252	GLY
1	A	264	GLY
1	A	266	VAL
1	A	267	ALA
1	A	288	ARG
1	A	333	GLU
1	A	357	TRP
1	A	360	MET
1	A	372	ASN
1	A	394	GLY
1	A	422	PRO
1	A	445	ASP
1	A	449	PRO
1	A	451	TRP
1	A	456	GLY
1	A	457	VAL
1	A	459	ASP
1	B	4	SER
1	B	54	ASN
1	B	125	ASP
1	B	192	ASN
1	B	202	ALA
1	B	214	ALA
1	B	269	ALA
1	B	276	ARG
1	B	277	ARG
1	B	289	ALA
1	B	323	GLY
1	B	327	PHE
1	B	330	MET
1	B	335	SER
1	B	423	VAL
1	B	445	ASP
1	B	458	GLU
1	A	5	SER
1	A	157	GLY

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	326	GLY
1	A	358	GLY
1	B	3	GLN
1	B	56	GLU
1	B	58	CYS
1	B	63	PHE
1	B	393	GLY
1	B	403	PRO
1	B	429	GLU
1	A	184	TRP
1	A	221	GLU
1	A	268	GLY
1	A	347	GLU
1	A	373	ALA
1	A	418	ARG
1	B	120	TYR
1	B	373	ALA
1	A	9	ASN
1	A	55	VAL
1	A	186	GLY
1	A	403	PRO
1	B	62	ASP
1	B	246	TYR
1	B	288	ARG
1	A	263	ASP
1	A	421	VAL
1	B	99	ALA
1	B	154	GLU
1	B	326	GLY
1	A	172	ARG
1	A	297	PRO
1	B	186	GLY
1	A	67	VAL
1	B	66	GLY
1	B	86	PRO
1	A	388	VAL
1	B	247	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	348/354 (98%)	266 (76%)	82 (24%)	1 1
1	B	348/354 (98%)	268 (77%)	80 (23%)	1 1
All	All	696/708 (98%)	534 (77%)	162 (23%)	1 1

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	GLN
1	A	5	SER
1	A	6	ARG
1	A	10	LEU
1	A	12	LEU
1	A	17	LEU
1	A	41	THR
1	A	48	GLU
1	A	54	ASN
1	A	55	VAL
1	A	65	ARG
1	A	70	LEU
1	A	71	VAL
1	A	82	LYS
1	A	92	ARG
1	A	93	ASN
1	A	94	ILE
1	A	106	THR
1	A	115	MET
1	A	128	VAL
1	A	135	LEU
1	A	141	VAL
1	A	144	SER
1	A	156	ASP
1	A	161	VAL
1	A	163	THR

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Mol	Chain	Res	Type
1	A	169	LEU
1	A	178	GLU
1	A	191	LYS
1	A	192	ASN
1	A	194	GLU
1	A	196	GLN
1	A	201	PHE
1	A	204	LEU
1	A	206	ASP
1	A	216	ARG
1	A	219	GLN
1	A	220	ASP
1	A	224	GLU
1	A	226	LYS
1	A	237	PRO
1	A	239	GLU
1	A	254	ASN
1	A	256	SER
1	A	278	ARG
1	A	286	TYR
1	A	294	VAL
1	A	301	ARG
1	A	308	HIS
1	A	311	MET
1	A	313	ARG
1	A	318	SER
1	A	325	MET
1	A	327	PHE
1	A	329	LYS
1	A	330	MET
1	A	360	MET
1	A	363	CYS
1	A	374	LEU
1	A	376	MET
1	A	383	LEU
1	A	385	ASN
1	A	387	ASN
1	A	390	LEU
1	A	391	THR
1	A	397	PHE
1	A	409	SER
1	A	410	LEU

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Mol	Chain	Res	Type
1	A	414	TRP
1	A	415	GLN
1	A	421	VAL
1	A	422	PRO
1	A	423	VAL
1	A	424	LEU
1	A	432	GLU
1	A	435	ARG
1	A	446	GLN
1	A	447	ILE
1	A	448	TYR
1	A	449	PRO
1	A	453	LYS
1	B	2	ASP
1	B	3	GLN
1	B	5	SER
1	B	8	VAL
1	B	10	LEU
1	B	14	GLU
1	B	15	GLU
1	B	16	ASP
1	B	28	TYR
1	B	50	SER
1	B	53	THR
1	B	54	ASN
1	B	55	VAL
1	B	58	CYS
1	B	61	ASP
1	B	63	PHE
1	B	64	THR
1	B	65	ARG
1	B	80	LEU
1	B	86	PRO
1	B	95	THR
1	B	107	LEU
1	B	112	ASN
1	B	115	MET
1	B	120	TYR
1	B	126	PHE
1	B	130	GLU
1	B	133	ARG
1	B	146	LEU

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Mol	Chain	Res	Type
1	B	156	ASP
1	B	159	LEU
1	B	163	THR
1	B	165	ILE
1	B	169	LEU
1	B	171	LEU
1	B	174	LYS
1	B	178	GLU
1	B	180	CYS
1	B	188	ASP
1	B	190	ILE
1	B	192	ASN
1	B	194	GLU
1	B	204	LEU
1	B	205	ARG
1	B	208	ILE
1	B	210	LEU
1	B	227	LEU
1	B	229	SER
1	B	249	GLU
1	B	253	GLU
1	B	256	SER
1	B	261	LEU
1	B	263	ASP
1	B	284	LEU
1	B	286	TYR
1	B	303	TYR
1	B	314	LEU
1	B	320	ILE
1	B	327	PHE
1	B	337	ARG
1	B	368	SER
1	B	377	PRO
1	B	381	GLU
1	B	382	ASN
1	B	385	ASN
1	B	391	THR
1	B	403	PRO
1	B	409	SER
1	B	424	LEU
1	B	428	ARG
1	B	430	HIS

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Mol	Chain	Res	Type
1	B	431	LYS
1	B	435	ARG
1	B	437	PHE
1	B	443	ASP
1	B	446	GLN
1	B	452	ARG
1	B	455	LEU
1	B	457	VAL
1	B	459	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	44	HIS
1	A	192	ASN
1	A	219	GLN
1	A	282	ASN
1	A	287	HIS
1	A	308	HIS
1	A	355	GLN
1	A	385	ASN
1	A	387	ASN
1	A	415	GLN
1	B	3	GLN
1	B	111	ASN
1	B	112	ASN
1	B	181	HIS
1	B	287	HIS
1	B	315	GLN
1	B	382	ASN
1	B	385	ASN
1	B	399	HIS
1	B	415	GLN

5.3.3 RNA

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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FMT	A	601	3,1	0,2,2	0.00	-	0,1,1	0.00	-
2	RUB	A	600	3	15,17,17	2.83	8 (53%)	16,25,25	1.49	4 (25%)
2	RUB	B	700	3	15,17,17	1.55	2 (13%)	16,25,25	0.88	0
4	FMT	B	701	3,1	0,2,2	0.00	-	0,1,1	0.00	-

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	RUB	A	600	3	-	11/20/20/20	-
2	RUB	B	700	3	-	15/20/20/20	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	RUB	C5-C4	7.19	1.62	1.51
2	A	600	RUB	C1-C2	3.85	1.57	1.51
2	A	600	RUB	P2-O4P	3.33	1.61	1.50
2	A	600	RUB	P1-O1P	3.17	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	RUB	P1-O1P	3.17	1.60	1.50
2	B	700	RUB	P2-O4P	3.09	1.60	1.50
2	A	600	RUB	P2-O5	2.82	1.69	1.60
2	A	600	RUB	P2-O5P	2.19	1.63	1.54
2	A	600	RUB	O1-C1	2.16	1.44	1.43
2	A	600	RUB	O2-C2	2.07	1.25	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	RUB	O6P-P2-O5	2.48	113.34	106.73
2	A	600	RUB	O3P-P1-O1	2.28	112.79	106.73
2	A	600	RUB	O5-P2-O4P	2.26	112.82	106.47
2	A	600	RUB	O5-C5-C4	2.09	114.93	109.36

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	RUB	O2-C2-C3-O3
2	A	600	RUB	C2-C3-C4-C5
2	A	600	RUB	C2-C3-C4-O4
2	A	600	RUB	O3-C3-C4-C5
2	A	600	RUB	O3-C3-C4-O4
2	A	600	RUB	C5-O5-P2-O4P
2	A	600	RUB	C5-O5-P2-O5P
2	A	600	RUB	C5-O5-P2-O6P
2	B	700	RUB	O1-C1-C2-C3
2	B	700	RUB	C2-C3-C4-C5
2	B	700	RUB	C2-C3-C4-O4
2	B	700	RUB	O3-C3-C4-C5
2	B	700	RUB	O3-C3-C4-O4
2	B	700	RUB	C3-C4-C5-O5
2	B	700	RUB	O4-C4-C5-O5
2	B	700	RUB	C1-O1-P1-O1P
2	B	700	RUB	C1-O1-P1-O2P
2	B	700	RUB	C1-O1-P1-O3P
2	B	700	RUB	C5-O5-P2-O4P
2	B	700	RUB	C5-O5-P2-O5P
2	B	700	RUB	C5-O5-P2-O6P
2	A	600	RUB	O1-C1-C2-O2
2	B	700	RUB	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	600	RUB	C1-C2-C3-O3
2	B	700	RUB	C1-C2-C3-O3
2	A	600	RUB	O1-C1-C2-C3

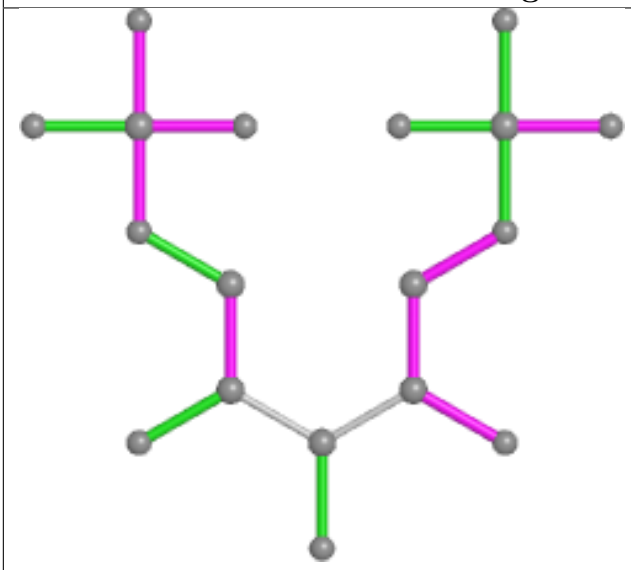
There are no ring outliers.

4 monomers are involved in 10 short contacts:

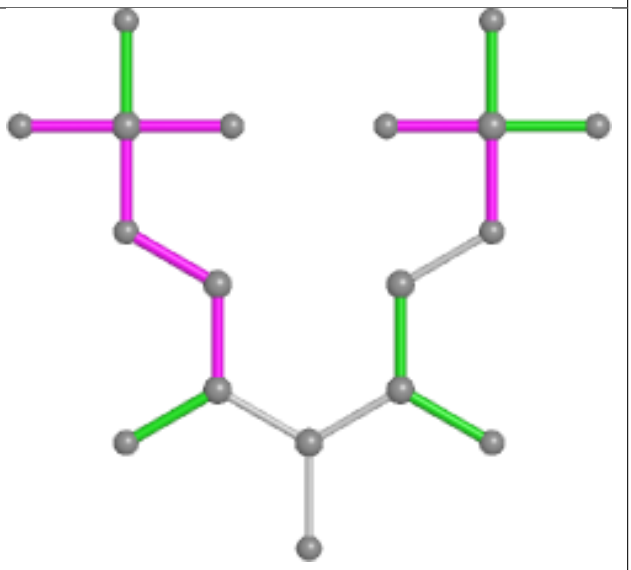
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	FMT	2	0
2	A	600	RUB	3	0
2	B	700	RUB	5	0
4	B	701	FMT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

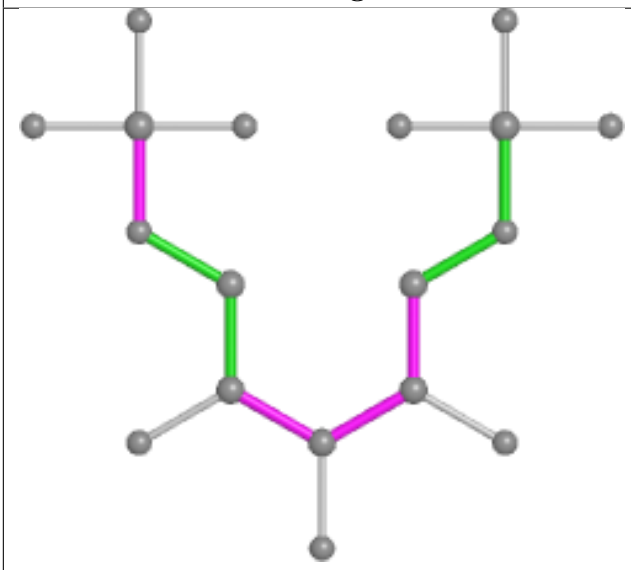
Ligand RUB A 600



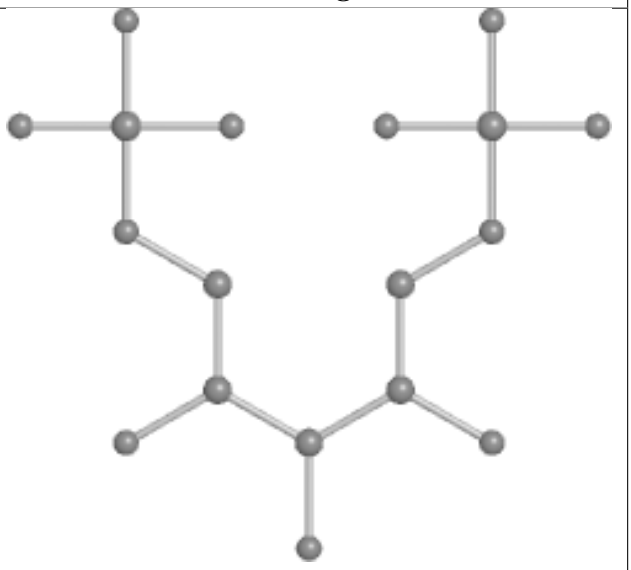
Bond lengths



Bond angles

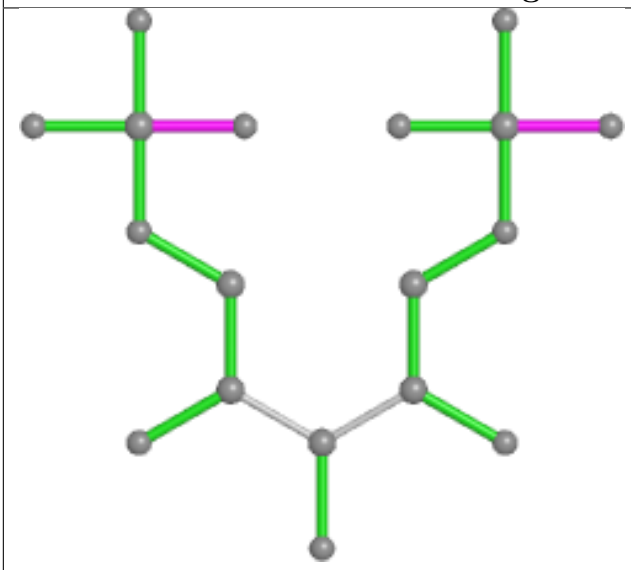


Torsions

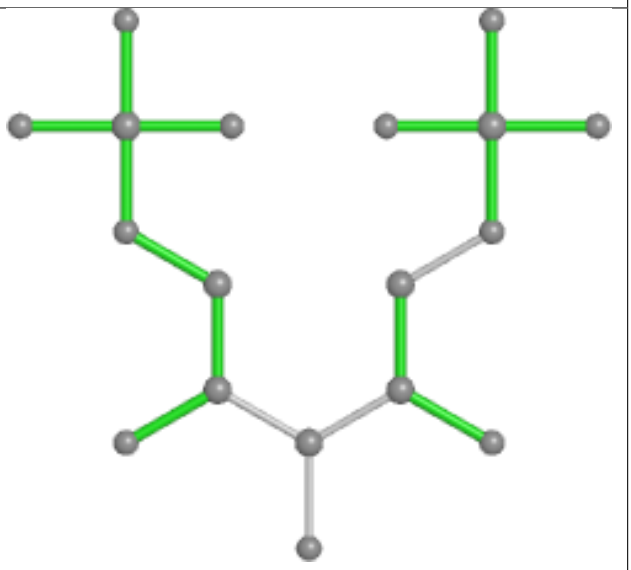


Rings

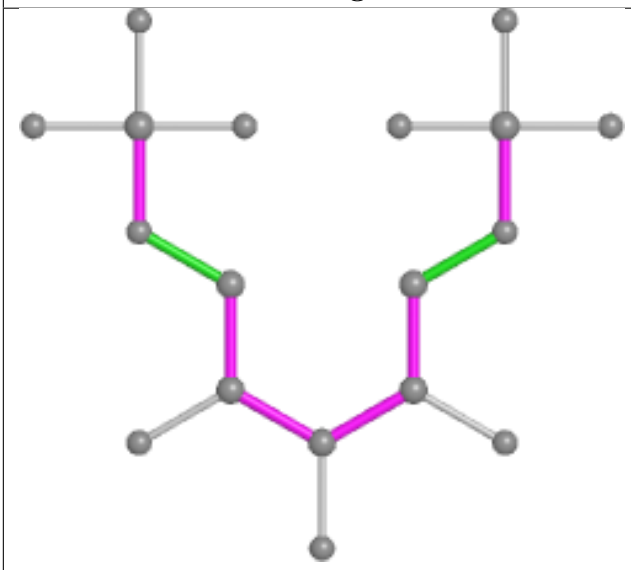
Ligand RUB B 700



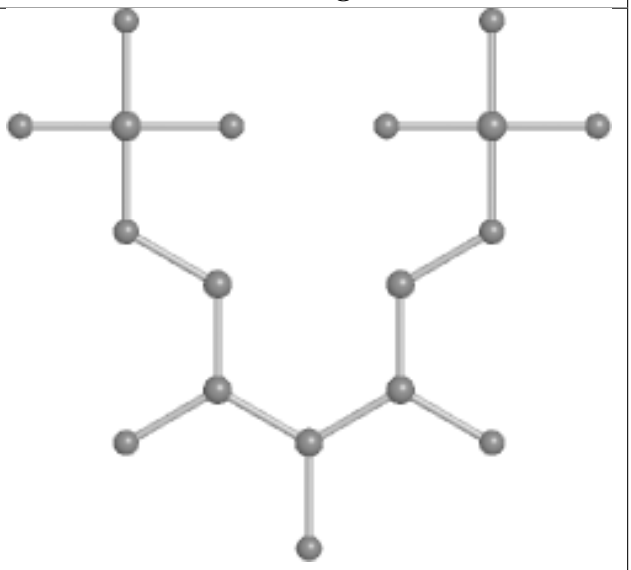
Bond lengths



Bond angles



Torsions



Rings

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.