



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:58 AM UTC

PDB ID : 2ONG / pdb_00002ong
Title : Crystal Structure of of limonene synthase with 2-fluorogeranyl diphosphate (FGPP) enzymatically converted to 2-fluorolinalyl diphosphate (FLPP)
Authors : Hyatt, D.C.; Youn, B.; Croteau, R.; Kang, C.
Deposited on : 2007-01-23
Resolution : 2.70 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

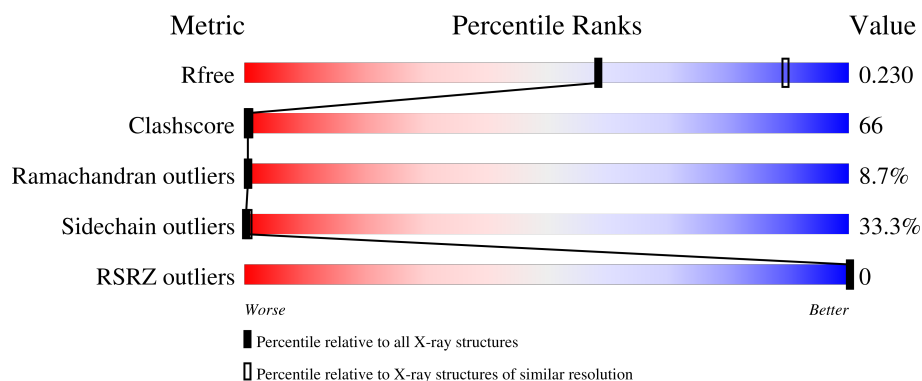
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	 12% 37% 38% 14%
1	B	543	 14% 36% 36% 14%

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
3	F3P	A	600	-	-	X	-
3	F3P	B	1600	-	-	X	-
4	BTB	A	605	-	-	X	-
4	BTB	B	1604	-	-	X	-
4	BTB	B	1605	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9181 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 4S-limonene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4495	2871	761	843	20			
1	B	543	Total	C	N	O	S	0	0	0
			4491	2870	758	843	20			

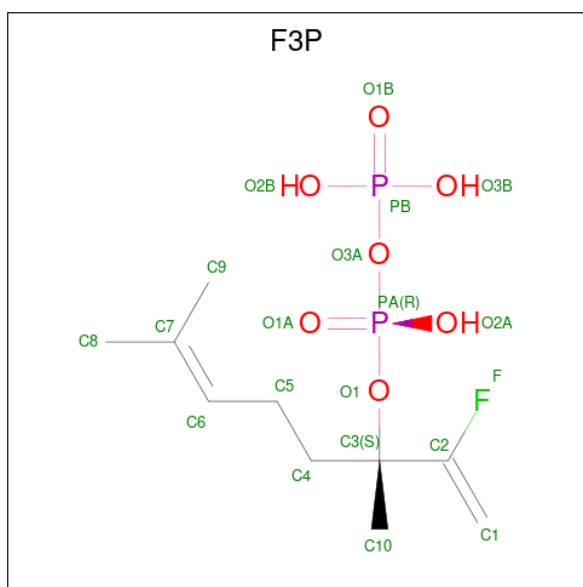
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MET	GLU	engineered mutation	UNP Q40322
B	57	MET	GLU	engineered mutation	UNP Q40322

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

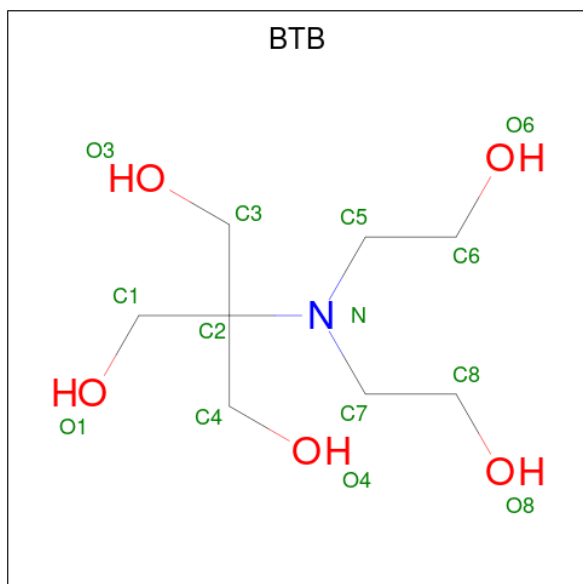
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		

- Molecule 3 is (3S)-2-fluoro-3,7-dimethylocta-1,6-dien-3-yl trihydrogen diphosphate (CCD ID: F3P) (formula: C₁₀H₁₉FO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 20	C 10	F 1	O 7	P 2	0	0
3	B	1	Total 20	C 10	F 1	O 7	P 2	0	0

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

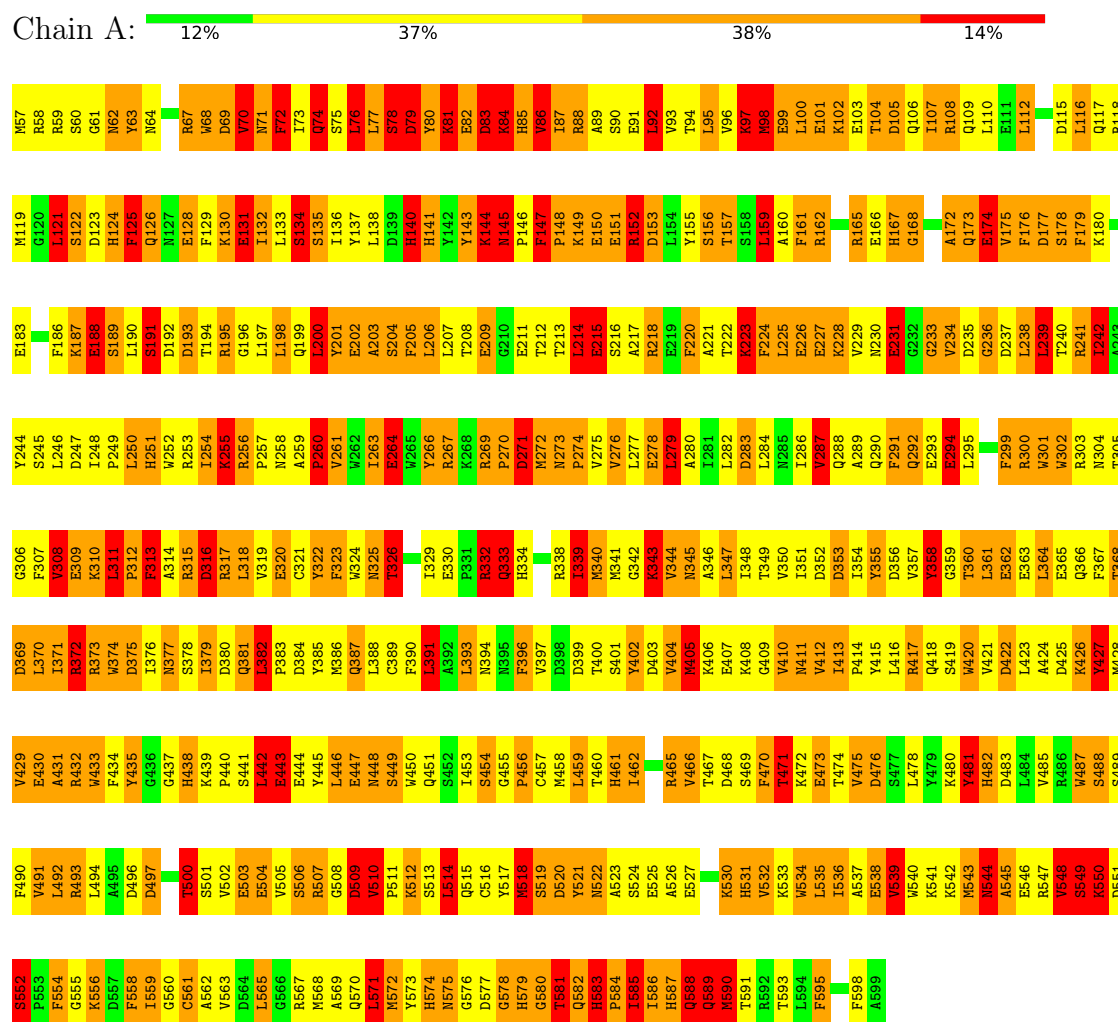
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	54	Total	O	0	0
			54	54		

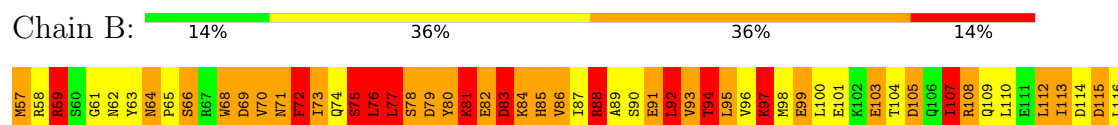
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 4S-limonene synthase



• Molecule 1: 4S-limonene synthase



K550	Q117
D551	R118
S552	M119
F553	G120
F554	E185
G555	L121
K556	L186
D557	L187
F558	K187
T559	D188
G560	D123
C561	H124
A562	F125
V563	N126
D564	Q127
L565	E128
G566	E193
R567	T194
M568	F195
A569	L196
Q570	S189
L571	H190
M572	S191
Y573	D192
H574	E193
M575	T194
G576	F195
D577	K195
G578	G196
H579	L197
G580	L198
T581	Q199
Q582	L200
H583	Y201
P584	E202
I585	A203
I586	S204
H587	F205
Q588	L206
Q589	Y266
M590	L207
T591	T208
R592	E209
T593	G210
L594	E211
F595	T212
E596	T213
P597	L214
F598	E215
A599	R152
	D153
	L154
	Y155
	S158
	L159
	A160
	F161
	R162
	L163
	L164
	R165
	E166
	V229
	H167
	G168
	F169
	E174
	V175
	F176
	D177
	S178
	F179
	K180
	N181
	E182
	E183
	G184
	Y244
	S245
	G246
	D247
	I248
	P249
	L250
	H251
	W252
	R253
	L254
	K255
	R256
	P257
	L258
	A259
	P260
	V261
	W262
	I263
	E264
	W265
	Y266
	R267
	K268
	R269
	P270
	D271
	Q272
	K273
	P274
	V275
	V276
	L277
	E278
	L279
	A280
	I281
	L282
	D283
	L284
	K285
	I286
	V287
	Q288
	A289
	Q290
	F291
	Q292
	E293
	E294
	L295
	K296
	E297
	S298
	P299
	R300
	W301
	W302
	R303
	N304
	G305
	L306
	F307
	V308
	E309
	K310
	L311
	P312
	W313
	A314
	R315
	D316
	R317
	L318
	V319
	E320
	C321
	Y322
	F323
	W324
	N325
	T326
	I329
	R332
	Q333
	H334
	A335
	S336
	A337
	R338
	I339
	M340
	M341
	G342
	K343
	V344
	N345
	A346
	L347
	I348
	T349
	V350
	I351
	D352
	D353
	I354
	V357
	T360
	L361
	E362
	E363
	L364
	A365
	E366
	Q366
	F367
	T368
	D369
	L370
	I371
	R372
	K373
	W374
	D375
	L376
	N377
	S378
	I379
	D380
	Q381
	L382
	P383
	D384
	Y385
	K386
	Q387
	L388
	C389
	F390
	L391
	A392
	L393
	N394
	N395
	F396
	V397
	D398
	D399
	T400
	S401
	Y402
	D403
	Y404
	M405
	K406
	E407
	N408
	G409
	V410
	M411
	V412
	I413
	P414
	Y415
	L416
	R417
	Q418
	S419
	W420
	V421
	D422
	L423
	A424
	R425
	K426
	Y427
	M428
	V429
	E430
	A431
	R432
	W433
	G436
	L437
	H438
	K439
	P440
	S441
	L442
	E443
	E444
	Y445
	L446
	E447
	N448
	S449
	W450
	Q451
	S452
	L453
	S454
	P455
	P456
	C457
	M458
	L459
	T460
	H461
	I462
	F463
	F464
	R465
	V466
	T467
	D468
	S469
	F470
	T471
	K472
	E473
	T474
	Y475
	D476
	S477
	L478
	Y479
	K480
	Y481
	H482
	D483
	L484
	V485
	R486
	W487
	S488
	S489
	F490
	V491
	L492
	R493
	L494
	A495
	D496
	D497
	L498
	G499
	T500
	S501
	V502
	E503
	E504
	V505
	S506
	R507
	G508
	D509
	Y510
	P511
	K512
	S513
	L514
	Q515
	C516
	Y517
	H518
	S519
	D520
	P521
	N522
	A526
	E527
	A528
	R529
	K530
	H531
	W534
	L535
	I536
	A537
	E538
	V539
	W540
	K541
	M542
	M543
	N544
	A545
	E546
	R547
	V548
	S549

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	200.48Å 200.48Å 123.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 10.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 93.1 (10.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.61Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.208 , 0.241 0.220 , 0.230	Depositor DCC
R_{free} test set	3503 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.478 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9181	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, MN, F3P

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	1.18	39/4607 (0.8%)	2.37	351/6234 (5.6%)
1	B	1.15	42/4603 (0.9%)	2.27	324/6230 (5.2%)
All	All	1.17	81/9210 (0.9%)	2.32	675/12464 (5.4%)

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	THR	C-O	12.06	1.38	1.24
1	B	368	THR	C-O	9.90	1.36	1.24
1	B	413	ILE	CA-CB	8.17	1.59	1.53
1	B	255	LYS	N-CA	-6.65	1.38	1.46
1	A	482	HIS	N-CA	-6.45	1.38	1.46
1	B	140	HIS	ND1-CE1	6.42	1.39	1.32
1	A	141	HIS	ND1-CE1	6.09	1.38	1.32
1	B	167	HIS	CE1-NE2	6.07	1.38	1.32
1	A	251	HIS	ND1-CE1	6.06	1.38	1.32
1	B	141	HIS	CE1-NE2	6.04	1.38	1.32
1	A	487	TRP	CG-CD2	-6.01	1.32	1.43
1	A	433	TRP	CG-CD2	-6.00	1.32	1.43
1	A	461	HIS	ND1-CE1	5.99	1.38	1.32
1	B	167	HIS	ND1-CE1	5.99	1.38	1.32
1	B	587	HIS	ND1-CE1	5.96	1.38	1.32
1	A	141	HIS	CE1-NE2	5.93	1.38	1.32
1	A	587	HIS	CE1-NE2	5.93	1.38	1.32
1	B	334	HIS	ND1-CE1	5.92	1.38	1.32
1	A	140	HIS	ND1-CE1	5.92	1.38	1.32
1	A	334	HIS	ND1-CE1	5.91	1.38	1.32
1	B	141	HIS	ND1-CE1	5.91	1.38	1.32
1	A	251	HIS	CE1-NE2	5.90	1.38	1.32
1	B	140	HIS	CE1-NE2	5.88	1.38	1.32
1	A	583	HIS	CE1-NE2	5.87	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	583	HIS	ND1-CE1	5.85	1.38	1.32
1	A	574	HIS	ND1-CE1	5.85	1.38	1.32
1	A	583	HIS	ND1-CE1	5.82	1.38	1.32
1	B	579	HIS	ND1-CE1	5.81	1.38	1.32
1	A	574	HIS	CE1-NE2	5.81	1.38	1.32
1	A	124	HIS	CE1-NE2	5.80	1.38	1.32
1	B	85	HIS	CE1-NE2	5.76	1.38	1.32
1	A	167	HIS	ND1-CE1	5.75	1.38	1.32
1	A	461	HIS	CE1-NE2	5.75	1.38	1.32
1	B	583	HIS	CE1-NE2	5.75	1.38	1.32
1	A	334	HIS	CE1-NE2	5.75	1.38	1.32
1	B	438	HIS	CE1-NE2	5.74	1.38	1.32
1	A	85	HIS	CE1-NE2	5.73	1.38	1.32
1	B	587	HIS	CE1-NE2	5.72	1.38	1.32
1	A	105	ASP	N-CA	-5.70	1.39	1.46
1	B	256	ARG	N-CA	-5.70	1.41	1.46
1	B	438	HIS	ND1-CE1	5.70	1.38	1.32
1	A	124	HIS	ND1-CE1	5.69	1.38	1.32
1	A	579	HIS	ND1-CE1	5.66	1.38	1.32
1	A	587	HIS	ND1-CE1	5.66	1.38	1.32
1	A	482	HIS	CE1-NE2	5.64	1.38	1.32
1	A	438	HIS	ND1-CE1	5.64	1.38	1.32
1	B	579	HIS	CE1-NE2	5.63	1.38	1.32
1	B	124	HIS	ND1-CE1	5.63	1.38	1.32
1	B	251	HIS	ND1-CE1	5.61	1.38	1.32
1	B	461	HIS	ND1-CE1	5.56	1.38	1.32
1	A	438	HIS	CE1-NE2	5.53	1.38	1.32
1	B	482	HIS	CE1-NE2	5.50	1.38	1.32
1	A	140	HIS	CE1-NE2	5.48	1.38	1.32
1	A	167	HIS	CE1-NE2	5.48	1.38	1.32
1	A	545	ALA	C-O	5.47	1.30	1.24
1	B	251	HIS	CE1-NE2	5.47	1.38	1.32
1	B	531	HIS	ND1-CE1	5.47	1.38	1.32
1	A	485	VAL	N-CA	-5.45	1.40	1.46
1	B	209	GLU	N-CA	5.44	1.53	1.46
1	A	579	HIS	CE1-NE2	5.44	1.38	1.32
1	B	400	THR	N-CA	-5.43	1.39	1.46
1	B	467	THR	N-CA	-5.40	1.40	1.46
1	B	574	HIS	ND1-CE1	5.35	1.38	1.32
1	B	531	HIS	CE1-NE2	5.35	1.38	1.32
1	A	326	THR	N-CA	-5.35	1.39	1.46
1	A	85	HIS	ND1-CE1	5.34	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	HIS	ND1-CE1	5.33	1.37	1.32
1	B	461	HIS	CE1-NE2	5.33	1.37	1.32
1	B	334	HIS	CE1-NE2	5.33	1.37	1.32
1	B	574	HIS	CE1-NE2	5.33	1.37	1.32
1	B	482	HIS	ND1-CE1	5.32	1.37	1.32
1	B	124	HIS	CE1-NE2	5.32	1.37	1.32
1	B	485	VAL	N-CA	-5.28	1.39	1.46
1	A	556	LYS	N-CA	-5.21	1.39	1.46
1	B	352	ASP	N-CA	-5.17	1.40	1.46
1	A	482	HIS	ND1-CE1	5.15	1.37	1.32
1	B	388	LEU	N-CA	-5.14	1.40	1.46
1	A	374	TRP	CG-CD2	-5.12	1.34	1.43
1	B	349	THR	N-CA	-5.11	1.40	1.46
1	A	375	ASP	N-CA	-5.02	1.39	1.46
1	B	252	TRP	CG-CD2	-5.02	1.34	1.43

All (675) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	LYS	N-CA-C	-18.45	91.25	111.36
1	A	313	PHE	N-CA-C	-16.93	92.29	113.97
1	A	551	ASP	N-CA-C	-16.47	88.00	111.56
1	A	410	VAL	N-CA-C	15.58	129.93	108.11
1	A	313	PHE	CA-C-N	15.53	142.72	120.82
1	A	313	PHE	C-N-CA	15.53	142.72	120.82
1	A	481	TYR	N-CA-C	-14.63	79.63	110.80
1	A	205	PHE	CA-CB-CG	-14.51	99.29	113.80
1	A	544	ASN	CA-CB-CG	-14.23	98.37	112.60
1	A	80	TYR	N-CA-C	-14.03	96.71	112.57
1	B	238	LEU	N-CA-C	-13.88	94.62	111.69
1	B	422	ASP	CA-CB-CG	13.83	126.43	112.60
1	A	586	ILE	N-CA-C	-13.74	93.40	112.50
1	B	71	ASN	CA-CB-CG	-13.63	98.97	112.60
1	B	480	LYS	N-CA-C	-13.61	96.35	113.23
1	A	167	HIS	CA-CB-CG	-13.56	100.24	113.80
1	B	387	GLN	N-CA-C	-13.31	96.49	113.12
1	B	195	ARG	N-CA-C	-13.26	96.46	111.71
1	A	99	GLU	N-CA-C	-13.20	96.53	111.71
1	A	531	HIS	CA-CB-CG	-13.20	100.60	113.80
1	A	87	ILE	N-CA-C	-12.74	98.55	110.53
1	B	380	ASP	CA-CB-CG	-12.54	100.06	112.60
1	A	271	ASP	CA-CB-CG	12.41	125.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ASP	N-CA-C	12.18	124.24	110.97
1	A	220	PHE	CA-CB-CG	12.15	125.95	113.80
1	B	209	GLU	CB-CG-CD	12.15	133.26	112.60
1	B	79	ASP	CA-CB-CG	12.11	124.71	112.60
1	B	207	LEU	N-CA-C	11.91	126.22	109.31
1	A	581	THR	N-CA-C	-11.87	85.52	110.80
1	A	583	HIS	N-CA-C	11.52	135.26	109.81
1	B	209	GLU	N-CA-C	-11.44	86.43	110.80
1	A	307	PHE	N-CA-C	-11.39	97.98	112.90
1	A	209	GLU	CB-CG-CD	11.38	131.94	112.60
1	A	246	LEU	N-CA-C	-11.35	99.44	113.18
1	A	131	GLU	CB-CG-CD	11.32	131.84	112.60
1	A	238	LEU	N-CA-C	-11.19	98.61	111.03
1	A	105	ASP	CA-CB-CG	-11.17	101.43	112.60
1	B	85	HIS	CA-CB-CG	-11.15	102.65	113.80
1	A	85	HIS	CA-CB-CG	-11.01	102.79	113.80
1	B	585	ILE	N-CA-C	-10.93	101.51	113.43
1	B	91	GLU	N-CA-C	-10.93	100.44	113.88
1	B	342	GLY	N-CA-C	-10.86	99.35	112.49
1	A	482	HIS	CA-CB-CG	-10.85	102.95	113.80
1	A	390	PHE	CA-CB-CG	-10.76	103.04	113.80
1	B	123	ASP	N-CA-C	10.67	124.82	111.69
1	B	334	HIS	CA-CB-CG	-10.57	103.23	113.80
1	A	482	HIS	ND1-CG-CD2	10.54	116.64	106.10
1	A	126	GLN	N-CA-C	10.50	122.80	111.36
1	B	549	SER	CA-C-N	10.47	141.54	121.54
1	B	549	SER	C-N-CA	10.47	141.54	121.54
1	A	519	SER	N-CA-C	-10.44	98.79	112.68
1	B	318	LEU	N-CA-C	10.40	125.07	112.38
1	B	412	VAL	CA-C-N	-10.24	113.79	120.24
1	B	412	VAL	C-N-CA	-10.24	113.79	120.24
1	B	490	PHE	CA-CB-CG	-10.09	103.71	113.80
1	A	550	LYS	N-CA-C	-9.97	99.25	113.21
1	A	342	GLY	N-CA-C	-9.96	100.59	112.64
1	A	63	TYR	N-CA-C	-9.94	94.17	110.17
1	A	85	HIS	ND1-CG-CD2	9.82	115.92	106.10
1	B	377	ASN	N-CA-C	-9.76	99.95	112.93
1	A	353	ASP	CA-CB-CG	-9.74	102.86	112.60
1	A	71	ASN	CA-CB-CG	-9.64	102.96	112.60
1	A	481	TYR	CA-CB-CG	-9.53	96.75	113.90
1	A	128	GLU	N-CA-C	-9.53	98.32	112.04
1	B	468	ASP	CA-C-N	-9.48	106.85	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	ASP	C-N-CA	-9.48	106.85	122.21
1	B	482	HIS	ND1-CG-CD2	9.46	115.56	106.10
1	B	544	ASN	CA-CB-CG	-9.40	103.20	112.60
1	B	365	GLU	N-CA-C	-9.36	101.08	111.28
1	A	427	TYR	N-CA-C	-9.34	100.98	111.82
1	A	407	GLU	N-CA-C	9.30	124.89	113.17
1	B	188	GLU	CB-CG-CD	9.29	128.40	112.60
1	A	538	GLU	CA-C-N	-9.23	107.08	121.02
1	A	538	GLU	C-N-CA	-9.23	107.08	121.02
1	B	263	ILE	CA-CB-CG2	-9.22	94.83	110.50
1	A	148	PRO	CA-C-N	9.21	136.22	122.68
1	A	148	PRO	C-N-CA	9.21	136.22	122.68
1	A	405	MET	N-CA-C	-9.20	101.22	111.07
1	B	85	HIS	ND1-CG-CD2	9.13	115.23	106.10
1	B	353	ASP	CA-CB-CG	-9.10	103.50	112.60
1	B	186	PHE	CA-CB-CG	-9.03	104.77	113.80
1	B	131	GLU	CB-CG-CD	9.02	127.93	112.60
1	A	375	ASP	CA-CB-CG	-8.98	103.62	112.60
1	B	169	PHE	N-CA-C	-8.97	97.20	110.48
1	A	223	LYS	CA-C-N	-8.96	107.56	120.29
1	A	223	LYS	C-N-CA	-8.96	107.56	120.29
1	B	241	ARG	N-CA-C	-8.92	100.71	111.69
1	A	377	ASN	CA-CB-CG	-8.92	103.68	112.60
1	A	565	LEU	N-CA-C	-8.89	101.16	111.03
1	B	211	GLU	N-CA-C	8.88	129.72	110.80
1	A	537	ALA	CA-C-N	8.88	132.18	120.28
1	A	537	ALA	C-N-CA	8.88	132.18	120.28
1	A	552	SER	N-CA-C	-8.81	98.45	109.64
1	A	147	PHE	CA-CB-CG	8.75	122.55	113.80
1	B	134	SER	N-CA-C	-8.71	101.86	111.36
1	B	598	PHE	CA-C-N	8.69	137.35	121.70
1	B	598	PHE	C-N-CA	8.69	137.35	121.70
1	A	448	ASN	CA-CB-CG	-8.67	103.93	112.60
1	A	322	TYR	N-CA-C	-8.65	102.85	113.50
1	A	195	ARG	N-CA-C	-8.65	92.38	110.80
1	A	225	LEU	N-CA-C	-8.64	100.75	111.11
1	A	144	LYS	N-CA-C	8.63	123.02	110.42
1	B	311	LEU	N-CA-C	-8.62	93.27	108.97
1	A	231	GLU	N-CA-C	-8.59	97.74	110.46
1	B	93	VAL	N-CA-C	-8.54	102.01	110.30
1	B	88	ARG	N-CA-C	-8.54	100.60	111.02
1	A	224	PHE	CA-CB-CG	-8.46	105.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	LYS	N-CA-C	8.42	120.37	111.03
1	A	490	PHE	CA-CB-CG	-8.39	105.41	113.80
1	B	167	HIS	CA-CB-CG	-8.35	105.45	113.80
1	A	551	ASP	CA-C-N	8.30	131.93	120.39
1	A	551	ASP	C-N-CA	8.30	131.93	120.39
1	A	176	PHE	CA-CB-CG	-8.27	105.53	113.80
1	B	579	HIS	ND1-CG-CD2	8.27	114.37	106.10
1	A	384	ASP	N-CA-C	8.26	120.36	111.36
1	B	461	HIS	CA-CB-CG	-8.26	105.54	113.80
1	A	448	ASN	N-CA-C	-8.25	101.33	111.40
1	A	575	ASN	N-CA-C	-8.23	102.12	114.64
1	A	355	TYR	N-CA-C	8.22	120.02	111.14
1	A	134	SER	N-CA-C	-8.21	102.02	110.97
1	B	410	VAL	N-CA-C	8.20	122.22	108.86
1	B	407	GLU	N-CA-C	8.18	119.88	110.97
1	A	92	LEU	N-CA-C	-8.18	103.44	113.41
1	A	250	LEU	CA-C-N	-8.16	108.52	120.28
1	A	250	LEU	C-N-CA	-8.16	108.52	120.28
1	A	116	LEU	N-CA-C	-8.15	102.40	111.28
1	B	78	SER	N-CA-C	8.13	123.26	110.17
1	A	561	CYS	N-CA-C	-8.12	102.51	111.36
1	A	316	ASP	CA-CB-CG	8.09	120.69	112.60
1	A	439	LYS	N-CA-C	-8.04	96.53	109.40
1	B	179	PHE	CA-CB-CG	8.00	121.80	113.80
1	B	379	ILE	N-CA-C	-7.99	100.85	112.04
1	B	223	LYS	CA-C-N	-7.94	107.46	120.72
1	B	223	LYS	C-N-CA	-7.94	107.46	120.72
1	A	531	HIS	ND1-CG-CD2	7.93	114.03	106.10
1	B	105	ASP	CA-CB-CG	-7.93	104.67	112.60
1	B	413	ILE	O-C-N	-7.91	114.45	120.07
1	B	318	LEU	CA-C-N	-7.91	107.90	120.55
1	B	318	LEU	C-N-CA	-7.91	107.90	120.55
1	B	339	ILE	CB-CA-C	-7.90	101.68	111.87
1	A	533	LYS	N-CA-C	-7.89	102.61	111.14
1	B	218	ARG	N-CA-C	-7.89	102.67	111.28
1	B	416	LEU	N-CA-C	-7.86	102.79	111.36
1	A	480	LYS	CA-C-N	7.86	136.55	121.54
1	A	480	LYS	C-N-CA	7.86	136.55	121.54
1	B	552	SER	O-C-N	-7.85	112.29	121.32
1	B	275	VAL	N-CA-C	-7.85	100.92	111.44
1	B	403	ASP	CA-CB-CG	-7.78	104.82	112.60
1	A	326	THR	N-CA-C	-7.78	103.25	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	583	HIS	CA-CB-CG	7.75	121.56	113.80
1	A	391	LEU	CA-C-N	-7.72	109.16	120.28
1	A	391	LEU	C-N-CA	-7.72	109.16	120.28
1	B	291	PHE	N-CA-C	-7.72	102.46	111.03
1	A	104	THR	CA-C-N	-7.71	110.50	121.99
1	A	104	THR	C-N-CA	-7.71	110.50	121.99
1	A	230	ASN	CA-CB-CG	7.70	120.30	112.60
1	B	167	HIS	ND1-CG-CD2	7.69	113.79	106.10
1	B	554	PHE	CA-CB-CG	-7.69	106.11	113.80
1	B	124	HIS	CA-CB-CG	7.68	121.48	113.80
1	A	237	ASP	N-CA-C	-7.64	103.42	112.89
1	A	443	GLU	N-CA-C	7.64	119.69	111.36
1	B	350	VAL	N-CA-C	7.64	117.71	110.30
1	B	438	HIS	CA-CB-CG	-7.63	106.17	113.80
1	A	217	ALA	N-CA-C	-7.62	102.91	111.14
1	B	579	HIS	CA-CB-CG	-7.62	106.18	113.80
1	B	97	LYS	N-CA-C	-7.61	94.59	110.80
1	A	485	VAL	CA-C-N	-7.61	108.74	120.31
1	A	485	VAL	C-N-CA	-7.61	108.74	120.31
1	A	356	ASP	CA-CB-CG	7.61	120.21	112.60
1	B	570	GLN	CB-CG-CD	-7.59	99.69	112.60
1	A	72	PHE	N-CA-C	-7.57	102.61	112.68
1	A	200	LEU	N-CA-C	-7.55	102.40	111.69
1	A	523	ALA	N-CA-C	7.53	121.21	110.14
1	A	396	PHE	CA-C-N	-7.50	108.62	120.47
1	A	396	PHE	C-N-CA	-7.50	108.62	120.47
1	A	82	GLU	N-CA-C	7.49	121.42	108.76
1	B	384	ASP	CA-CB-CG	7.49	120.09	112.60
1	A	161	PHE	N-CA-C	-7.48	102.81	110.97
1	B	94	THR	CA-C-N	-7.48	108.98	121.92
1	B	94	THR	C-N-CA	-7.48	108.98	121.92
1	A	247	ASP	CA-CB-CG	7.46	120.06	112.60
1	B	542	LYS	N-CA-C	-7.45	103.14	111.71
1	B	380	ASP	CA-C-N	-7.45	110.79	122.49
1	B	380	ASP	C-N-CA	-7.45	110.79	122.49
1	A	582	GLN	CB-CG-CD	7.44	125.24	112.60
1	A	291	PHE	N-CA-C	-7.41	101.98	111.02
1	A	168	GLY	CA-C-N	-7.40	110.06	122.64
1	A	168	GLY	C-N-CA	-7.40	110.06	122.64
1	B	310	LYS	CA-C-N	-7.38	113.82	123.34
1	B	310	LYS	C-N-CA	-7.38	113.82	123.34
1	A	369	ASP	N-CA-C	7.37	120.36	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	LEU	N-CA-C	-7.36	101.67	110.13
1	B	81	LYS	N-CA-C	-7.35	104.29	113.18
1	A	147	PHE	N-CA-C	7.33	120.20	110.08
1	B	544	ASN	N-CA-C	-7.31	103.01	110.97
1	B	482	HIS	CA-CB-CG	-7.28	106.52	113.80
1	A	177	ASP	N-CA-C	7.28	119.84	111.11
1	A	482	HIS	N-CA-C	-7.26	100.47	110.35
1	B	147	PHE	CA-CB-CG	7.26	121.06	113.80
1	A	300	ARG	N-CA-C	-7.25	102.56	111.33
1	A	167	HIS	ND1-CG-CD2	7.25	113.34	106.10
1	B	226	GLU	N-CA-C	-7.23	103.33	111.07
1	B	584	PRO	CA-C-N	7.23	131.26	122.16
1	B	584	PRO	C-N-CA	7.23	131.26	122.16
1	B	263	ILE	CA-CB-CG1	7.22	122.68	110.40
1	B	244	TYR	CA-C-N	-7.21	107.52	121.58
1	B	244	TYR	C-N-CA	-7.21	107.52	121.58
1	A	551	ASP	CA-CB-CG	-7.21	105.39	112.60
1	A	159	LEU	CA-C-N	-7.20	109.92	120.28
1	A	159	LEU	C-N-CA	-7.20	109.92	120.28
1	A	177	ASP	CA-CB-CG	-7.19	105.41	112.60
1	A	369	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	521	TYR	CA-CB-CG	-7.18	100.98	113.90
1	A	132	ILE	N-CA-C	7.16	117.29	110.42
1	A	580	GLY	N-CA-C	-7.14	96.25	113.18
1	A	404	VAL	N-CA-C	-7.13	104.02	111.58
1	A	518	MET	CB-CG-SD	-7.13	91.31	112.70
1	B	396	PHE	CA-C-N	-7.13	110.69	120.46
1	B	396	PHE	C-N-CA	-7.13	110.69	120.46
1	A	576	GLY	CA-C-N	7.12	135.14	121.54
1	A	576	GLY	C-N-CA	7.12	135.14	121.54
1	A	595	PHE	N-CA-C	7.12	122.40	112.93
1	A	456	PRO	CA-C-N	-7.10	111.21	120.44
1	A	456	PRO	C-N-CA	-7.10	111.21	120.44
1	A	487	TRP	CE2-CD2-CE3	7.08	125.88	118.80
1	A	343	LYS	CA-C-N	-7.08	109.23	120.55
1	A	343	LYS	C-N-CA	-7.08	109.23	120.55
1	A	524	SER	N-CA-C	-7.06	101.21	110.53
1	A	340	MET	CA-C-N	-7.05	108.81	121.14
1	A	340	MET	C-N-CA	-7.05	108.81	121.14
1	A	590	MET	CG-SD-CE	-7.02	85.46	100.90
1	B	574	HIS	ND1-CG-CD2	6.99	113.09	106.10
1	B	205	PHE	CA-C-N	-6.99	111.39	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	PHE	C-N-CA	-6.99	111.39	122.79
1	B	177	ASP	CA-CB-CG	6.99	119.58	112.60
1	B	302	TRP	CB-CG-CD1	-6.96	116.45	126.90
1	A	188	GLU	CB-CG-CD	6.96	124.44	112.60
1	B	534	TRP	CG-CD2-CE3	6.95	140.85	133.90
1	A	251	HIS	ND1-CG-CD2	6.95	113.05	106.10
1	B	258	ASN	CA-CB-CG	-6.94	105.66	112.60
1	B	339	ILE	CA-CB-CG2	-6.94	98.70	110.50
1	B	421	VAL	N-CA-C	6.92	117.71	110.72
1	A	149	LYS	N-CA-C	6.90	120.76	111.24
1	B	378	SER	N-CA-C	-6.88	105.30	113.21
1	A	466	VAL	CA-C-N	-6.88	111.91	122.09
1	A	466	VAL	C-N-CA	-6.88	111.91	122.09
1	A	193	ASP	CA-C-N	-6.87	111.20	122.54
1	A	193	ASP	C-N-CA	-6.87	111.20	122.54
1	B	382	LEU	N-CA-C	-6.86	102.08	110.31
1	A	583	HIS	CA-C-N	6.86	128.41	119.84
1	A	583	HIS	C-N-CA	6.86	128.41	119.84
1	A	345	ASN	N-CA-C	-6.83	103.83	111.28
1	A	203	ALA	N-CA-C	-6.82	105.11	113.50
1	A	172	ALA	N-CA-C	6.81	119.89	110.35
1	B	99	GLU	CB-CG-CD	6.81	124.18	112.60
1	A	587	HIS	ND1-CG-CD2	6.79	112.89	106.10
1	A	320	GLU	N-CA-C	-6.79	102.97	111.11
1	B	299	PHE	N-CA-C	-6.79	103.50	111.03
1	A	422	ASP	N-CA-C	-6.79	102.74	111.02
1	A	97	LYS	CA-C-N	-6.78	109.45	122.06
1	A	97	LYS	C-N-CA	-6.78	109.45	122.06
1	A	571	LEU	N-CA-C	-6.77	101.20	111.56
1	B	322	TYR	N-CA-C	-6.76	104.67	113.12
1	B	72	PHE	CA-CB-CG	6.74	120.54	113.80
1	B	483	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	108	ARG	N-CA-C	-6.73	104.08	112.90
1	B	469	SER	CA-C-N	-6.73	110.63	122.20
1	B	469	SER	C-N-CA	-6.73	110.63	122.20
1	A	475	VAL	CA-C-N	-6.72	110.60	120.28
1	A	475	VAL	C-N-CA	-6.72	110.60	120.28
1	A	333	GLN	N-CA-C	6.71	120.93	112.87
1	A	518	MET	CA-C-N	-6.71	109.98	122.60
1	A	518	MET	C-N-CA	-6.71	109.98	122.60
1	B	309	GLU	CB-CG-CD	6.71	124.01	112.60
1	A	598	PHE	CA-C-N	6.70	133.76	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	PHE	C-N-CA	6.70	133.76	121.70
1	B	393	LEU	CD1-CG-CD2	-6.70	96.06	110.80
1	A	74	GLN	CB-CG-CD	-6.69	101.23	112.60
1	A	476	ASP	CA-CB-CG	-6.68	105.92	112.60
1	B	538	GLU	CA-C-N	-6.67	109.35	120.30
1	B	538	GLU	C-N-CA	-6.67	109.35	120.30
1	B	506	SER	N-CA-C	-6.67	103.93	111.07
1	A	410	VAL	CB-CA-C	-6.65	100.79	110.63
1	B	546	GLU	CB-CG-CD	-6.65	101.30	112.60
1	A	544	ASN	CA-C-N	-6.64	111.55	120.79
1	A	544	ASN	C-N-CA	-6.64	111.55	120.79
1	B	297	GLU	N-CA-C	6.63	118.16	111.07
1	B	302	TRP	CG-CD2-CE3	6.62	140.53	133.90
1	B	391	LEU	CA-C-N	-6.62	110.89	120.29
1	B	391	LEU	C-N-CA	-6.62	110.89	120.29
1	B	201	TYR	N-CA-C	-6.62	103.17	111.11
1	B	565	LEU	N-CA-C	-6.62	104.15	111.36
1	A	199	GLN	N-CA-C	6.62	120.61	112.54
1	A	62	ASN	CA-C-N	-6.61	111.41	122.64
1	A	62	ASN	C-N-CA	-6.61	111.41	122.64
1	B	299	PHE	CA-CB-CG	-6.59	107.21	113.80
1	B	96	VAL	N-CA-C	-6.58	102.86	111.09
1	B	251	HIS	ND1-CG-CD2	6.58	112.68	106.10
1	A	442	LEU	CA-C-N	-6.58	110.95	120.29
1	A	442	LEU	C-N-CA	-6.58	110.95	120.29
1	A	352	ASP	CA-C-N	-6.57	111.47	120.28
1	A	352	ASP	C-N-CA	-6.57	111.47	120.28
1	A	447	GLU	CB-CG-CD	6.57	123.76	112.60
1	B	140	HIS	CA-CB-CG	6.56	120.36	113.80
1	B	583	HIS	ND1-CG-CD2	6.56	112.66	106.10
1	B	534	TRP	CB-CG-CD1	-6.56	117.07	126.90
1	A	302	TRP	CB-CG-CD1	-6.54	117.10	126.90
1	B	205	PHE	CA-CB-CG	-6.53	107.27	113.80
1	A	532	VAL	CA-C-N	-6.52	111.57	120.44
1	A	532	VAL	C-N-CA	-6.52	111.57	120.44
1	A	366	GLN	CB-CG-CD	6.52	123.69	112.60
1	A	153	ASP	CA-C-N	-6.50	111.05	120.29
1	A	153	ASP	C-N-CA	-6.50	111.05	120.29
1	A	130	LYS	N-CA-C	6.50	118.44	111.36
1	B	202	GLU	N-CA-C	6.49	120.66	112.87
1	B	123	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	446	LEU	CA-C-N	-6.49	109.79	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	LEU	C-N-CA	-6.49	109.79	121.14
1	B	381	GLN	CA-C-N	-6.49	111.42	123.55
1	B	381	GLN	C-N-CA	-6.49	111.42	123.55
1	B	468	ASP	CA-CB-CG	-6.48	106.12	112.60
1	B	298	SER	CA-C-N	6.47	129.43	120.63
1	B	298	SER	C-N-CA	6.47	129.43	120.63
1	B	332	ARG	N-CA-C	6.47	120.03	111.75
1	B	381	GLN	CB-CG-CD	-6.46	101.62	112.60
1	B	538	GLU	N-CA-C	6.45	118.39	111.36
1	A	293	GLU	CB-CG-CD	-6.44	101.65	112.60
1	B	145	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	255	LYS	N-CA-C	6.42	124.48	110.80
1	B	400	THR	N-CA-C	-6.42	103.41	111.11
1	B	438	HIS	ND1-CG-CD2	6.41	112.51	106.10
1	B	487	TRP	CA-C-N	-6.39	111.71	120.28
1	B	487	TRP	C-N-CA	-6.39	111.71	120.28
1	B	549	SER	N-CA-C	6.39	124.42	110.80
1	A	345	ASN	CA-CB-CG	-6.39	106.21	112.60
1	A	504	GLU	N-CA-C	-6.39	103.22	111.02
1	A	325	ASN	CA-CB-CG	-6.38	106.22	112.60
1	A	121	LEU	N-CA-C	-6.38	105.46	113.18
1	A	76	LEU	CA-C-N	-6.37	113.35	122.77
1	A	76	LEU	C-N-CA	-6.37	113.35	122.77
1	B	141	HIS	ND1-CG-CD2	6.37	112.47	106.10
1	B	517	TYR	N-CA-C	-6.36	104.27	111.14
1	B	320	GLU	N-CA-C	-6.36	104.27	111.07
1	B	459	LEU	N-CA-C	6.34	118.20	111.28
1	A	377	ASN	N-CA-C	-6.34	103.67	111.40
1	B	427	TYR	N-CA-C	-6.33	104.42	111.71
1	B	274	PRO	CA-C-N	-6.33	109.40	120.29
1	B	274	PRO	C-N-CA	-6.33	109.40	120.29
1	A	287	VAL	CA-CB-CG1	-6.33	99.64	110.40
1	A	244	TYR	CA-C-N	-6.31	110.95	122.38
1	A	244	TYR	C-N-CA	-6.31	110.95	122.38
1	A	402	TYR	N-CA-C	-6.31	104.33	111.14
1	B	433	TRP	CA-C-N	-6.31	112.05	120.63
1	B	433	TRP	C-N-CA	-6.31	112.05	120.63
1	B	389	CYS	CA-C-N	-6.31	111.33	120.29
1	B	389	CYS	C-N-CA	-6.31	111.33	120.29
1	B	417	ARG	N-CA-C	-6.29	103.34	111.02
1	A	539	VAL	CA-C-N	-6.27	111.88	120.28
1	A	539	VAL	C-N-CA	-6.27	111.88	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	TRP	CB-CG-CD1	-6.27	117.49	126.90
1	B	548	VAL	N-CA-C	-6.26	104.49	113.07
1	B	57	MET	CA-C-N	6.26	132.28	121.64
1	B	57	MET	C-N-CA	6.26	132.28	121.64
1	A	503	GLU	CB-CG-CD	6.25	123.23	112.60
1	B	115	ASP	CA-CB-CG	6.25	118.85	112.60
1	B	86	VAL	CA-C-N	-6.25	112.56	120.56
1	B	86	VAL	C-N-CA	-6.25	112.56	120.56
1	B	366	GLN	CB-CG-CD	6.24	123.21	112.60
1	B	76	LEU	N-CA-C	6.23	124.08	110.80
1	B	368	THR	CA-C-N	-6.23	112.42	120.65
1	B	368	THR	C-N-CA	-6.23	112.42	120.65
1	A	242	ILE	CB-CA-C	-6.23	103.73	112.14
1	A	311	LEU	CA-C-N	6.23	127.63	119.84
1	A	311	LEU	C-N-CA	6.23	127.63	119.84
1	A	294	GLU	N-CA-C	-6.21	104.51	111.28
1	B	80	TYR	CA-C-N	-6.21	109.47	121.58
1	B	80	TYR	C-N-CA	-6.21	109.47	121.58
1	B	438	HIS	N-CA-C	6.18	123.97	110.80
1	A	279	LEU	N-CA-C	-6.17	104.47	111.07
1	B	208	THR	CA-C-N	6.16	133.31	121.54
1	B	208	THR	C-N-CA	6.16	133.31	121.54
1	B	583	HIS	CA-C-N	6.16	127.54	119.84
1	B	583	HIS	C-N-CA	6.16	127.54	119.84
1	A	128	GLU	CB-CG-CD	6.16	123.06	112.60
1	A	431	ALA	N-CA-C	-6.15	97.69	110.80
1	A	581	THR	CA-C-N	-6.15	112.30	122.08
1	A	581	THR	C-N-CA	-6.15	112.30	122.08
1	B	150	GLU	N-CA-C	-6.15	97.71	110.80
1	A	481	TYR	CA-C-N	6.13	130.00	120.75
1	A	481	TYR	C-N-CA	6.13	130.00	120.75
1	B	341	MET	CG-SD-CE	-6.13	87.42	100.90
1	A	347	LEU	CA-C-N	-6.13	113.25	120.72
1	A	347	LEU	C-N-CA	-6.13	113.25	120.72
1	A	583	HIS	ND1-CG-CD2	6.13	112.23	106.10
1	B	176	PHE	CA-CB-CG	-6.12	107.68	113.80
1	A	131	GLU	N-CA-C	-6.12	104.53	111.07
1	B	250	LEU	N-CA-C	-6.11	103.77	111.11
1	B	276	VAL	N-CA-C	-6.11	104.67	110.42
1	B	64	ASN	N-CA-C	-6.11	102.98	110.31
1	B	131	GLU	CA-C-N	-6.10	111.53	121.54
1	B	131	GLU	C-N-CA	-6.10	111.53	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	GLU	N-CA-C	6.09	123.78	110.80
1	A	334	HIS	ND1-CG-CD2	6.08	112.18	106.10
1	B	442	LEU	CA-C-N	-6.08	110.86	122.53
1	B	442	LEU	C-N-CA	-6.08	110.86	122.53
1	B	341	MET	N-CA-C	6.06	120.28	113.01
1	B	531	HIS	ND1-CG-CD2	6.06	112.16	106.10
1	A	362	GLU	N-CA-C	-6.05	104.61	111.14
1	B	377	ASN	CA-CB-CG	-6.05	106.55	112.60
1	B	518	MET	CA-C-N	-6.05	112.58	120.44
1	B	518	MET	C-N-CA	-6.05	112.58	120.44
1	A	145	ASN	CA-CB-CG	-6.03	106.57	112.60
1	B	475	VAL	N-CA-C	-6.02	104.87	110.53
1	A	302	TRP	CA-C-N	6.02	128.35	120.28
1	A	302	TRP	C-N-CA	6.02	128.35	120.28
1	A	461	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	299	PHE	CA-CB-CG	-6.02	107.78	113.80
1	B	566	GLY	N-CA-C	-6.02	105.36	113.24
1	A	83	ASP	N-CA-C	6.01	123.60	110.80
1	A	556	LYS	CA-C-N	6.00	128.32	120.28
1	A	556	LYS	C-N-CA	6.00	128.32	120.28
1	B	198	LEU	N-CA-C	-6.00	104.66	111.14
1	A	124	HIS	CA-CB-CG	-5.99	107.81	113.80
1	A	349	THR	CA-C-N	-5.99	112.89	120.56
1	A	349	THR	C-N-CA	-5.99	112.89	120.56
1	A	543	MET	CG-SD-CE	-5.99	87.72	100.90
1	B	564	ASP	CA-CB-CG	-5.99	106.61	112.60
1	A	81	LYS	CA-C-N	-5.99	113.52	122.74
1	A	81	LYS	C-N-CA	-5.99	113.52	122.74
1	B	141	HIS	N-CA-C	5.98	121.88	113.56
1	B	522	ASN	N-CA-C	-5.98	98.07	110.80
1	B	129	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	548	VAL	CG1-CB-CG2	-5.96	97.69	110.80
1	A	302	TRP	CG-CD2-CE3	5.95	139.85	133.90
1	B	340	MET	CG-SD-CE	-5.94	87.83	100.90
1	B	571	LEU	CD1-CG-CD2	-5.92	97.78	110.80
1	B	320	GLU	CB-CG-CD	5.90	122.62	112.60
1	B	419	SER	N-CA-C	-5.89	104.45	111.69
1	B	266	TYR	N-CA-C	-5.86	104.89	111.28
1	B	319	VAL	N-CA-C	-5.85	104.63	111.00
1	B	517	TYR	CA-C-N	-5.84	112.85	120.44
1	B	517	TYR	C-N-CA	-5.84	112.85	120.44
1	B	326	THR	N-CA-C	-5.83	106.00	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ILE	CA-CB-CG2	-5.83	100.59	110.50
1	A	250	LEU	N-CA-C	-5.83	105.01	111.71
1	B	120	GLY	N-CA-C	5.82	122.49	114.92
1	A	95	LEU	N-CA-C	-5.82	104.84	111.07
1	A	320	GLU	CB-CG-CD	5.81	122.48	112.60
1	B	398	ASP	CA-C-N	-5.81	112.54	120.44
1	B	398	ASP	C-N-CA	-5.81	112.54	120.44
1	B	83	ASP	N-CA-C	5.79	123.14	110.80
1	A	264	GLU	CA-C-N	-5.79	110.68	120.58
1	A	264	GLU	C-N-CA	-5.79	110.68	120.58
1	A	391	LEU	CD1-CG-CD2	-5.79	98.07	110.80
1	A	512	LYS	CA-C-N	-5.78	112.93	120.44
1	A	512	LYS	C-N-CA	-5.78	112.93	120.44
1	A	589	GLN	N-CA-C	-5.78	105.07	111.71
1	B	209	GLU	N-CA-CB	5.77	120.25	110.49
1	A	254	ILE	N-CA-C	5.77	116.45	108.84
1	A	549	SER	CA-C-N	5.77	129.04	119.35
1	A	549	SER	C-N-CA	5.77	129.04	119.35
1	A	579	HIS	N-CA-C	-5.75	98.55	110.80
1	B	503	GLU	CB-CG-CD	5.75	122.38	112.60
1	B	462	ILE	N-CA-C	5.75	115.93	110.53
1	A	442	LEU	CD1-CG-CD2	-5.73	98.19	110.80
1	B	59	ARG	CA-C-N	-5.72	112.85	122.29
1	B	59	ARG	C-N-CA	-5.72	112.85	122.29
1	A	539	VAL	N-CA-C	-5.71	104.65	113.16
1	B	387	GLN	CA-C-N	-5.71	112.62	120.28
1	B	387	GLN	C-N-CA	-5.71	112.62	120.28
1	A	454	SER	N-CA-CB	-5.71	107.66	114.17
1	A	530	LYS	CA-C-N	-5.71	112.86	120.79
1	A	530	LYS	C-N-CA	-5.71	112.86	120.79
1	A	125	PHE	CA-C-N	-5.70	112.19	120.29
1	A	125	PHE	C-N-CA	-5.70	112.19	120.29
1	A	409	GLY	CA-C-N	5.70	130.61	123.14
1	A	409	GLY	C-N-CA	5.70	130.61	123.14
1	B	256	ARG	N-CA-C	5.70	120.66	113.25
1	A	263	ILE	CA-C-N	-5.68	110.50	121.58
1	A	263	ILE	C-N-CA	-5.68	110.50	121.58
1	B	408	LYS	N-CA-C	5.68	120.07	113.20
1	B	208	THR	N-CA-C	5.66	122.86	110.80
1	A	576	GLY	N-CA-C	5.66	119.86	111.76
1	A	183	GLU	N-CA-C	-5.66	106.36	113.20
1	A	585	ILE	CA-CB-CG1	-5.66	100.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	LYS	CA-C-N	5.65	132.34	121.54
1	B	480	LYS	C-N-CA	5.65	132.34	121.54
1	B	451	GLN	N-CA-C	-5.64	105.18	112.68
1	B	510	VAL	O-C-N	-5.63	114.68	121.10
1	B	487	TRP	CE2-CD2-CE3	5.62	124.42	118.80
1	B	371	ILE	N-CA-C	-5.62	105.04	110.72
1	B	425	ASP	N-CA-C	5.62	118.95	111.75
1	A	97	LYS	N-CA-C	-5.62	105.06	111.07
1	A	260	PRO	CA-C-N	-5.62	112.61	120.53
1	A	260	PRO	C-N-CA	-5.62	112.61	120.53
1	A	301	TRP	CB-CG-CD1	-5.59	118.52	126.90
1	A	438	HIS	CA-CB-CG	-5.58	108.22	113.80
1	B	192	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	157	THR	CA-C-N	-5.57	112.38	120.29
1	A	157	THR	C-N-CA	-5.57	112.38	120.29
1	B	107	ILE	CA-CB-CG1	-5.56	100.95	110.40
1	A	202	GLU	CA-C-N	-5.55	112.32	121.92
1	A	202	GLU	C-N-CA	-5.55	112.32	121.92
1	B	131	GLU	N-CA-C	-5.55	105.14	111.14
1	B	475	VAL	CG1-CB-CG2	-5.54	98.62	110.80
1	A	574	HIS	ND1-CG-CD2	5.53	111.63	106.10
1	B	481	TYR	CA-CB-CG	-5.51	103.99	113.90
1	A	68	TRP	CE2-CD2-CE3	5.50	124.31	118.80
1	A	264	GLU	CB-CG-CD	-5.50	103.25	112.60
1	B	351	ILE	CA-C-N	-5.50	112.96	120.44
1	B	351	ILE	C-N-CA	-5.50	112.96	120.44
1	B	425	ASP	CA-C-N	-5.49	111.34	120.68
1	B	425	ASP	C-N-CA	-5.49	111.34	120.68
1	B	79	ASP	N-CA-C	5.49	118.78	111.75
1	A	86	VAL	CA-C-N	-5.49	113.53	120.56
1	A	86	VAL	C-N-CA	-5.49	113.53	120.56
1	A	354	ILE	N-CA-C	-5.49	105.15	110.42
1	A	554	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	292	GLN	CA-C-N	-5.48	113.31	120.44
1	A	292	GLN	C-N-CA	-5.48	113.31	120.44
1	A	352	ASP	CA-CB-CG	-5.48	107.12	112.60
1	A	441	SER	CA-C-N	-5.48	112.94	120.28
1	A	441	SER	C-N-CA	-5.48	112.94	120.28
1	A	491	VAL	CB-CA-C	-5.47	104.97	111.97
1	B	334	HIS	ND1-CG-CD2	5.46	111.56	106.10
1	A	387	GLN	N-CA-C	-5.46	103.21	111.56
1	A	358	TYR	N-CA-C	5.45	122.41	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	461	HIS	ND1-CG-CD2	5.45	111.55	106.10
1	A	475	VAL	CB-CA-C	-5.45	104.88	112.02
1	B	147	PHE	CA-C-N	5.45	126.65	119.84
1	B	147	PHE	C-N-CA	5.45	126.65	119.84
1	A	389	CYS	N-CA-C	-5.45	104.21	111.24
1	A	370	LEU	N-CA-C	-5.45	105.50	111.82
1	A	179	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	332	ARG	CA-C-N	-5.44	111.90	120.60
1	B	332	ARG	C-N-CA	-5.44	111.90	120.60
1	B	596	GLU	CA-C-N	5.43	125.73	119.92
1	B	596	GLU	C-N-CA	5.43	125.73	119.92
1	B	350	VAL	CB-CA-C	-5.43	105.03	111.81
1	A	438	HIS	ND1-CG-CD2	5.42	111.52	106.10
1	A	420	TRP	CA-CB-CG	-5.42	103.31	113.60
1	A	79	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	439	LYS	N-CA-C	-5.41	96.93	108.93
1	B	265	TRP	N-CA-C	-5.40	105.05	111.69
1	B	205	PHE	N-CA-C	-5.40	106.54	113.02
1	B	313	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	216	SER	N-CA-C	-5.39	106.75	113.38
1	A	509	ASP	N-CA-C	-5.39	99.32	110.80
1	A	491	VAL	CA-C-N	-5.39	113.00	120.38
1	A	491	VAL	C-N-CA	-5.39	113.00	120.38
1	B	576	GLY	CA-C-N	5.38	131.82	121.54
1	B	576	GLY	C-N-CA	5.38	131.82	121.54
1	B	502	VAL	N-CA-C	5.38	120.53	109.34
1	B	482	HIS	CA-C-N	-5.38	112.66	120.29
1	B	482	HIS	C-N-CA	-5.38	112.66	120.29
1	B	68	TRP	CA-CB-CG	-5.37	103.39	113.60
1	B	246	LEU	N-CA-C	-5.37	105.99	112.54
1	A	267	ARG	N-CA-C	-5.35	105.14	110.97
1	B	316	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	382	LEU	CD1-CG-CD2	-5.34	99.05	110.80
1	B	479	TYR	N-CA-C	5.33	122.16	110.80
1	A	556	LYS	N-CA-C	5.33	122.15	110.80
1	B	398	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	264	GLU	CB-CG-CD	-5.33	103.55	112.60
1	A	356	ASP	N-CA-C	5.32	118.58	112.57
1	A	433	TRP	CD1-CG-CD2	5.32	114.82	106.30
1	A	323	PHE	N-CA-C	5.31	119.02	112.54
1	B	420	TRP	CG-CD1-NE1	-5.31	103.29	110.20
1	A	140	HIS	ND1-CG-CD2	5.31	111.41	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	590	MET	CA-C-N	5.30	128.12	120.38
1	B	590	MET	C-N-CA	5.30	128.12	120.38
1	B	154	LEU	N-CA-C	5.29	116.73	111.07
1	A	311	LEU	N-CA-C	-5.29	98.12	109.81
1	A	179	PHE	CA-C-N	-5.28	114.52	122.81
1	A	179	PHE	C-N-CA	-5.28	114.52	122.81
1	B	132	ILE	N-CA-C	5.28	119.46	112.76
1	B	536	ILE	CB-CA-C	-5.27	105.13	112.04
1	B	272	MET	N-CA-C	5.27	122.02	110.80
1	A	583	HIS	CA-CB-CG	5.27	119.07	113.80
1	B	362	GLU	N-CA-C	-5.27	105.45	111.14
1	A	583	HIS	N-CA-CB	-5.25	101.02	110.37
1	B	163	LEU	CA-C-N	-5.25	113.24	120.28
1	B	163	LEU	C-N-CA	-5.25	113.24	120.28
1	B	128	GLU	N-CA-C	-5.25	103.53	111.56
1	B	572	MET	CG-SD-CE	-5.25	89.36	100.90
1	A	283	ASP	N-CA-C	-5.24	104.63	111.02
1	B	324	TRP	CG-CD1-NE1	-5.24	103.39	110.20
1	A	151	GLU	CB-CG-CD	5.23	121.49	112.60
1	A	266	TYR	N-CA-C	-5.23	105.76	111.82
1	B	413	ILE	CB-CA-C	-5.23	108.81	114.35
1	B	536	ILE	N-CA-C	-5.22	104.67	110.62
1	B	92	LEU	CA-C-N	-5.21	114.18	120.70
1	B	92	LEU	C-N-CA	-5.21	114.18	120.70
1	A	446	LEU	CA-C-N	-5.21	111.82	120.68
1	A	446	LEU	C-N-CA	-5.21	111.82	120.68
1	B	577	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	483	ASP	N-CA-C	-5.20	105.69	111.36
1	A	339	ILE	N-CA-C	-5.20	105.53	110.42
1	A	433	TRP	CG-CD1-NE1	-5.20	103.44	110.20
1	B	426	LYS	N-CA-C	-5.20	105.68	112.23
1	A	124	HIS	ND1-CG-CD2	5.19	111.29	106.10
1	B	339	ILE	CA-CB-CG1	5.19	119.23	110.40
1	A	162	ARG	CA-C-N	-5.18	112.43	120.31
1	A	162	ARG	C-N-CA	-5.18	112.43	120.31
1	A	471	THR	N-CA-C	-5.18	102.52	110.14
1	A	411	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	468	ASP	N-CA-C	5.18	119.31	112.89
1	B	580	GLY	CA-C-N	5.17	131.42	121.54
1	B	580	GLY	C-N-CA	5.17	131.42	121.54
1	B	142	TYR	N-CA-C	5.17	121.81	110.80
1	B	324	TRP	CD1-CG-CD2	5.17	114.57	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	CB-CA-C	-5.16	105.32	112.24
1	A	150	GLU	N-CA-C	-5.16	106.25	113.37
1	A	94	THR	CA-C-N	-5.16	113.73	120.44
1	A	94	THR	C-N-CA	-5.16	113.73	120.44
1	B	146	PRO	CA-C-N	5.16	134.38	121.80
1	B	146	PRO	C-N-CA	5.16	134.38	121.80
1	B	317	ARG	CA-C-N	-5.15	112.35	120.60
1	B	317	ARG	C-N-CA	-5.15	112.35	120.60
1	A	251	HIS	N-CA-C	5.15	117.63	111.71
1	A	214	LEU	N-CA-C	-5.14	105.59	111.14
1	A	316	ASP	CA-C-N	-5.14	113.67	121.53
1	A	316	ASP	C-N-CA	-5.14	113.67	121.53
1	A	215	GLU	CA-C-N	-5.13	113.38	122.26
1	A	215	GLU	C-N-CA	-5.13	113.38	122.26
1	B	124	HIS	CA-C-N	5.13	130.99	122.73
1	B	124	HIS	C-N-CA	5.13	130.99	122.73
1	A	579	HIS	ND1-CG-CD2	5.12	111.22	106.10
1	B	313	PHE	N-CA-C	5.12	121.71	110.80
1	A	116	LEU	CA-C-N	-5.12	113.02	120.29
1	A	116	LEU	C-N-CA	-5.12	113.02	120.29
1	A	98	MET	CA-C-N	-5.12	112.91	120.28
1	A	98	MET	C-N-CA	-5.12	112.91	120.28
1	B	582	GLN	CB-CG-CD	5.12	121.30	112.60
1	A	536	ILE	CB-CA-C	-5.11	105.24	112.14
1	A	487	TRP	CG-CD2-CE3	-5.11	128.79	133.90
1	B	248	ILE	CA-CB-CG2	-5.11	101.81	110.50
1	A	99	GLU	CB-CG-CD	5.11	121.28	112.60
1	B	357	VAL	CA-C-N	-5.11	111.79	121.54
1	B	357	VAL	C-N-CA	-5.11	111.79	121.54
1	A	143	TYR	CA-CB-CG	5.10	123.09	113.90
1	B	529	ARG	N-CA-C	-5.10	105.90	111.82
1	B	113	ILE	CA-C-N	-5.10	113.44	120.28
1	B	113	ILE	C-N-CA	-5.10	113.44	120.28
1	A	372	ARG	CA-C-N	-5.10	114.52	122.73
1	A	372	ARG	C-N-CA	-5.10	114.52	122.73
1	B	460	THR	N-CA-C	-5.09	105.81	111.36
1	B	82	GLU	N-CA-C	5.08	121.63	110.80
1	A	487	TRP	NE1-CE2-CD2	5.08	114.01	107.40
1	A	558	PHE	N-CA-C	5.08	116.51	110.97
1	A	588	GLN	CA-C-N	5.07	127.58	120.28
1	A	588	GLN	C-N-CA	5.07	127.58	120.28
1	B	263	ILE	CA-C-N	-5.07	111.14	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	ILE	C-N-CA	-5.07	111.14	121.18
1	B	166	GLU	N-CA-C	-5.07	105.65	111.07
1	A	514	LEU	CA-C-N	-5.07	113.55	120.44
1	A	514	LEU	C-N-CA	-5.07	113.55	120.44
1	B	552	SER	N-CA-C	-5.07	98.61	109.81
1	A	209	GLU	N-CA-C	-5.06	102.89	110.23
1	B	431	ALA	CA-C-N	-5.06	111.93	120.58
1	B	431	ALA	C-N-CA	-5.06	111.93	120.58
1	B	75	SER	N-CA-C	5.05	120.37	110.56
1	B	339	ILE	N-CA-C	-5.05	105.67	110.42
1	A	510	VAL	O-C-N	-5.05	115.35	121.10
1	A	344	VAL	CA-C-N	-5.04	113.52	120.28
1	A	344	VAL	C-N-CA	-5.04	113.52	120.28
1	A	438	HIS	N-CA-C	-5.04	102.23	110.20
1	B	582	GLN	N-CA-C	-5.04	103.85	111.56
1	A	126	GLN	CA-C-N	-5.03	113.27	122.38
1	A	126	GLN	C-N-CA	-5.03	113.27	122.38
1	B	495	ALA	N-CA-C	-5.03	105.88	111.36
1	B	262	TRP	CA-C-N	-5.02	114.23	120.56
1	B	262	TRP	C-N-CA	-5.02	114.23	120.56
1	B	348	ILE	CB-CA-C	-5.01	105.56	111.97
1	B	140	HIS	ND1-CG-CD2	5.01	111.11	106.10

There are no chirality outliers.

There are no planarity outliers.

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	4495	0	4346	592	0
1	B	4491	0	4342	536	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	20	0	18	9	0
3	B	20	0	18	13	0
4	A	28	0	38	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	38	40	0
5	A	39	0	0	1	0
5	B	54	0	0	2	0
All	All	9181	0	8800	1186	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 66.

All (1186) 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)
4:B:1604:BTB:N	4:B:1604:BTB:C2	1.68	1.56
4:B:1605:BTB:N	4:B:1605:BTB:C2	1.69	1.51
4:A:605:BTB:N	4:A:605:BTB:C2	1.71	1.49
1:B:579:HIS:CD2	3:B:1600:F3P:H92	1.67	1.28
4:B:1605:BTB:C7	4:B:1605:BTB:H32	1.72	1.19
4:B:1605:BTB:H32	4:B:1605:BTB:H71	1.24	1.18
4:B:1604:BTB:N	4:B:1604:BTB:C1	2.10	1.14
4:B:1604:BTB:C7	4:B:1604:BTB:H42	1.78	1.12
1:B:218:ARG:HG3	1:B:218:ARG:HH11	1.14	1.11
1:B:302:TRP:HB2	1:B:318:LEU:HD13	1.28	1.11
4:B:1605:BTB:N	4:B:1605:BTB:C3	2.12	1.10
4:A:605:BTB:N	4:A:605:BTB:C3	2.19	1.05
4:B:1604:BTB:H32	4:B:1604:BTB:C5	1.86	1.05
1:A:324:TRP:HE1	1:A:579:HIS:HB2	1.19	1.03
1:B:579:HIS:HD2	3:B:1600:F3P:H92	1.24	1.02
1:B:254:ILE:HD12	1:B:254:ILE:H	1.25	1.01
4:B:1604:BTB:H42	4:B:1604:BTB:H72	1.02	1.01
1:A:315:ARG:HB2	1:A:317:ARG:HE	1.25	1.01
4:B:1604:BTB:N	4:B:1604:BTB:C3	2.25	0.99
1:B:411:ASN:ND2	1:B:413:ILE:HG23	1.78	0.98
4:B:1605:BTB:N	4:B:1605:BTB:C1	2.25	0.98
4:B:1604:BTB:H72	4:B:1604:BTB:C4	1.93	0.98
4:B:1604:BTB:H32	4:B:1604:BTB:H52	1.45	0.97
1:A:315:ARG:HH21	3:A:600:F3P:H102	1.27	0.97
4:A:605:BTB:H42	4:A:605:BTB:C5	1.95	0.97
1:B:211:GLU:HG2	1:B:214:LEU:HD12	1.46	0.97
1:A:282:LEU:HG	1:A:286:ILE:HD11	1.44	0.96
1:B:145:ASN:HD22	1:B:146:PRO:HD3	1.28	0.96
4:B:1604:BTB:N	4:B:1604:BTB:H12	1.81	0.95
1:A:311:LEU:HD12	1:A:385:TYR:HB2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLN:H	1:A:333:GLN:HE21	1.01	0.94
4:A:605:BTB:C1	4:A:605:BTB:H71	1.97	0.94
1:B:502:VAL:HG13	1:B:503:GLU:H	1.31	0.94
3:B:1600:F3P:C2	3:B:1600:F3P:H61	1.96	0.93
1:B:59:ARG:HG3	1:B:59:ARG:HH11	1.34	0.93
1:A:376:ILE:HD11	1:A:391:LEU:HD12	1.49	0.92
4:A:605:BTB:N	4:A:605:BTB:C4	2.33	0.91
1:B:272:MET:HE1	1:B:277:LEU:HB2	1.49	0.91
4:B:1605:BTB:C7	4:B:1605:BTB:C3	2.48	0.90
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.37	0.90
4:A:605:BTB:N	4:A:605:BTB:C1	2.34	0.89
1:A:333:GLN:HE21	1:A:333:GLN:N	1.70	0.89
1:A:403:ASP:HA	1:A:406:LYS:HE3	1.54	0.89
1:A:585:ILE:HG13	1:A:588:GLN:HB2	1.55	0.89
1:B:583:HIS:HB2	1:B:586:ILE:HB	1.55	0.88
4:A:605:BTB:H71	4:A:605:BTB:H12	1.56	0.87
4:B:1605:BTB:N	4:B:1605:BTB:C4	2.37	0.87
1:A:465:ARG:HH11	1:A:465:ARG:HG3	1.36	0.87
1:B:95:LEU:HD11	1:B:275:VAL:HG21	1.56	0.87
1:B:575:ASN:HD22	1:B:586:ILE:HD11	1.40	0.87
4:A:605:BTB:C1	4:A:605:BTB:C7	2.54	0.86
4:B:1604:BTB:N	4:B:1604:BTB:C4	2.39	0.85
4:B:1604:BTB:C7	4:B:1604:BTB:C4	2.52	0.85
4:A:605:BTB:H42	4:A:605:BTB:H52	1.58	0.85
1:A:471:THR:HG23	1:A:474:THR:H	1.42	0.85
4:B:1605:BTB:H71	4:B:1605:BTB:C3	2.03	0.84
1:A:320:GLU:HG3	1:A:590:MET:HE1	1.59	0.84
1:A:324:TRP:NE1	1:A:579:HIS:HB2	1.92	0.84
4:A:605:BTB:H12	4:A:605:BTB:C7	2.07	0.84
1:A:402:TYR:HD1	1:B:391:LEU:HD23	1.42	0.84
1:A:578:GLY:C	1:A:580:GLY:H	1.86	0.84
3:B:1600:F3P:H61	3:B:1600:F3P:H12	1.59	0.84
1:B:165:ARG:HB3	1:B:206:LEU:HD23	1.58	0.84
1:B:514:LEU:O	1:B:518:MET:HG2	1.78	0.83
1:B:371:ILE:HD13	1:B:372:ARG:N	1.93	0.83
1:A:456:PRO:O	1:A:460:THR:HG23	1.79	0.83
1:B:579:HIS:CD2	3:B:1600:F3P:C9	2.58	0.82
1:A:504:GLU:O	1:A:509:ASP:HB2	1.79	0.82
1:B:554:PHE:HB2	1:B:559:ILE:HG22	1.62	0.81
1:A:493:ARG:HD3	1:A:493:ARG:C	2.05	0.81
3:B:1600:F3P:H61	3:B:1600:F3P:C1	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:605:BTB:H62	4:A:605:BTB:O3	1.81	0.81
4:A:605:BTB:N	4:A:605:BTB:H32	1.96	0.80
1:A:510:VAL:HG23	1:A:511:PRO:HD2	1.63	0.80
1:B:302:TRP:CB	1:B:318:LEU:HD13	2.11	0.80
1:A:68:TRP:HB3	1:A:73:ILE:HD11	1.63	0.80
1:A:173:GLN:HE22	1:A:211:GLU:C	1.90	0.79
1:B:493:ARG:HG3	1:B:494:LEU:N	1.96	0.79
1:A:174:GLU:O	1:A:177:ASP:HB2	1.83	0.79
1:A:493:ARG:HG2	1:A:493:ARG:HH11	1.47	0.79
1:A:256:ARG:HG2	1:A:256:ARG:NH1	1.95	0.79
3:B:1600:F3P:H61	3:B:1600:F3P:H103	1.62	0.79
1:B:241:ARG:HH21	1:B:244:TYR:HD2	1.27	0.79
1:A:340:MET:O	1:A:344:VAL:HG23	1.83	0.79
1:A:177:ASP:O	1:A:180:LYS:HG3	1.82	0.79
1:A:315:ARG:NH2	3:A:600:F3P:H102	1.97	0.79
1:B:119:MET:HG3	1:B:262:TRP:HD1	1.48	0.79
4:B:1605:BTB:N	4:B:1605:BTB:H32	1.86	0.79
1:B:401:SER:HB3	1:B:413:ILE:HG22	1.64	0.78
1:B:458:MET:O	1:B:462:ILE:HG13	1.81	0.78
1:A:70:VAL:O	1:A:74:GLN:HG2	1.82	0.78
1:A:228:LYS:HZ1	1:A:234:VAL:H	1.30	0.78
1:A:370:LEU:HD13	1:A:382:LEU:HD21	1.66	0.78
1:B:527:GLU:HA	1:B:530:LYS:HZ2	1.48	0.78
1:B:145:ASN:ND2	1:B:146:PRO:HD3	1.98	0.78
1:A:78:SER:HB2	1:A:81:LYS:HG3	1.65	0.78
1:A:283:ASP:HA	1:A:286:ILE:HD12	1.65	0.78
1:A:501:SER:HA	1:A:512:LYS:HG3	1.63	0.78
1:A:453:ILE:HG12	1:A:492:LEU:HG	1.66	0.77
1:A:136:ILE:O	1:A:140:HIS:HB2	1.83	0.77
1:A:315:ARG:HH11	1:A:353:ASP:CG	1.91	0.77
1:B:577:ASP:HB2	1:B:582:GLN:HB3	1.66	0.77
1:B:73:ILE:HG21	1:B:299:PHE:CD2	2.20	0.77
1:A:483:ASP:HB3	1:A:487:TRP:CZ3	2.20	0.76
1:B:92:LEU:HD22	1:B:278:GLU:HG2	1.66	0.76
1:A:256:ARG:HH11	1:A:256:ARG:CG	1.98	0.76
1:A:465:ARG:HG3	1:A:465:ARG:NH1	1.96	0.76
1:A:98:MET:O	1:A:102:LYS:HB2	1.86	0.76
4:B:1605:BTB:C7	4:B:1605:BTB:H12	2.16	0.76
1:A:413:ILE:HG12	1:A:414:PRO:HD3	1.68	0.76
1:B:145:ASN:ND2	1:B:145:ASN:H	1.83	0.75
1:B:411:ASN:HD21	1:B:413:ILE:HG23	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1600:F3P:H61	3:B:1600:F3P:C10	2.16	0.75
1:A:201:TYR:HB2	1:A:221:ALA:HB1	1.67	0.75
1:A:188:GLU:CD	1:A:188:GLU:H	1.94	0.75
1:A:449:SER:HB2	1:A:493:ARG:HH11	1.51	0.74
1:B:165:ARG:HB3	1:B:206:LEU:CD2	2.17	0.74
1:B:315:ARG:HD3	1:B:353:ASP:OD2	1.86	0.74
1:A:193:ASP:O	1:A:197:LEU:HB2	1.88	0.74
1:B:218:ARG:HG3	1:B:218:ARG:NH1	1.94	0.74
4:B:1605:BTB:N	4:B:1605:BTB:H12	2.01	0.74
4:B:1604:BTB:C5	4:B:1604:BTB:C3	2.65	0.74
1:B:401:SER:CB	1:B:413:ILE:HG22	2.18	0.74
1:B:554:PHE:HB3	1:B:558:PHE:HD2	1.51	0.73
1:A:238:LEU:HG	1:A:242:ILE:HD11	1.68	0.73
1:B:483:ASP:HB3	1:B:487:TRP:NE1	2.03	0.73
1:A:345:ASN:HB3	3:A:600:F3P:C9	2.18	0.73
1:B:323:PHE:CD2	1:B:590:MET:HG2	2.23	0.73
1:B:514:LEU:HD11	1:B:529:ARG:HA	1.69	0.73
1:A:273:ASN:HD21	1:A:275:VAL:HG23	1.53	0.73
1:B:103:GLU:HB3	1:B:109:GLN:HG3	1.70	0.73
1:A:514:LEU:H	1:A:514:LEU:HD12	1.52	0.73
1:B:73:ILE:HG21	1:B:299:PHE:CG	2.24	0.73
1:A:102:LYS:HE2	1:A:102:LYS:HA	1.70	0.73
1:B:89:ALA:HA	1:B:92:LEU:HD12	1.71	0.73
1:B:510:VAL:HG12	1:B:511:PRO:HD2	1.69	0.73
1:B:116:LEU:HD23	1:B:121:LEU:HD12	1.71	0.73
1:B:148:PRO:HB3	1:B:178:SER:OG	1.89	0.73
1:A:442:LEU:HD22	1:A:516:CYS:HB2	1.69	0.72
1:B:484:LEU:HD23	1:B:554:PHE:CD2	2.24	0.72
1:A:333:GLN:H	1:A:333:GLN:NE2	1.83	0.72
1:A:459:LEU:HD13	1:A:565:LEU:HD22	1.71	0.72
1:B:209:GLU:O	1:B:210:GLY:C	2.31	0.72
1:B:59:ARG:HG3	1:B:59:ARG:NH1	1.94	0.72
1:A:174:GLU:H	1:A:174:GLU:CD	1.97	0.71
1:A:201:TYR:HB2	1:A:221:ALA:CB	2.20	0.71
1:A:222:THR:O	1:A:226:GLU:HB2	1.90	0.71
1:A:259:ALA:O	1:A:263:ILE:HG12	1.91	0.71
1:B:302:TRP:HB2	1:B:318:LEU:CD1	2.15	0.71
1:B:254:ILE:HD12	1:B:254:ILE:N	2.03	0.71
1:A:496:ASP:O	1:A:500:THR:HG23	1.90	0.71
4:B:1605:BTB:C2	4:B:1605:BTB:C7	2.69	0.70
4:B:1604:BTB:N	4:B:1604:BTB:H32	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LYS:HG3	1:A:146:PRO:HD2	1.73	0.70
1:B:242:ILE:HG22	1:B:243:ALA:N	2.06	0.70
1:A:131:GLU:HG3	1:A:132:ILE:N	2.05	0.70
1:A:544:ASN:O	1:A:548:VAL:HG23	1.91	0.70
1:A:150:GLU:C	1:A:152:ARG:H	2.00	0.70
1:A:577:ASP:HB3	1:A:582:GLN:H	1.56	0.70
1:A:458:MET:HE2	1:A:565:LEU:CD1	2.22	0.70
1:B:571:LEU:C	1:B:571:LEU:HD23	2.17	0.70
1:B:317:ARG:HH21	1:B:581:THR:HA	1.56	0.69
1:A:162:ARG:HH11	1:A:162:ARG:HG2	1.56	0.69
1:B:367:PHE:CD1	1:B:386:MET:HE3	2.28	0.69
1:B:218:ARG:HH11	1:B:218:ARG:CG	1.99	0.69
1:A:67:ARG:HD3	1:A:587:HIS:CD2	2.27	0.69
1:B:530:LYS:HZ2	1:B:530:LYS:HB3	1.58	0.69
1:A:229:VAL:HG13	1:A:239:LEU:HD13	1.73	0.69
1:A:548:VAL:O	1:A:549:SER:HB3	1.93	0.69
1:B:97:LYS:HD3	1:B:128:GLU:OE1	1.93	0.69
1:B:177:ASP:OD2	1:B:180:LYS:HE3	1.92	0.69
1:B:221:ALA:O	1:B:225:LEU:HB2	1.93	0.69
1:B:341:MET:HE1	1:B:458:MET:HA	1.74	0.69
1:A:345:ASN:HB3	3:A:600:F3P:H93	1.74	0.69
1:B:183:GLU:HB2	1:B:185:GLU:HG3	1.75	0.69
1:A:577:ASP:OD1	1:A:584:PRO:HD3	1.92	0.69
1:B:433:TRP:CE3	1:B:440:PRO:HG3	2.27	0.69
4:B:1604:BTB:C2	4:B:1604:BTB:C7	2.71	0.69
1:A:115:ASP:O	1:A:119:MET:HG3	1.94	0.68
1:B:581:THR:HG23	1:B:582:GLN:N	2.08	0.68
1:B:80:TYR:HA	1:B:85:HIS:CD2	2.27	0.68
1:B:231:GLU:O	1:B:234:VAL:HG23	1.94	0.68
1:A:161:PHE:HD2	1:A:203:ALA:HB1	1.58	0.68
1:A:315:ARG:HD3	1:A:353:ASP:OD2	1.93	0.68
1:B:211:GLU:CG	1:B:214:LEU:HD12	2.23	0.68
1:B:269:ARG:O	1:B:272:MET:HB3	1.94	0.68
1:B:382:LEU:HB3	1:B:386:MET:HE2	1.75	0.68
1:B:579:HIS:HD2	3:B:1600:F3P:C9	2.02	0.68
1:A:317:ARG:HH11	1:A:317:ARG:HB3	1.58	0.68
1:A:302:TRP:HB2	1:A:318:LEU:HG	1.76	0.67
1:B:93:VAL:HG13	1:B:94:THR:H	1.59	0.67
3:B:1600:F3P:H103	3:B:1600:F3P:C6	2.22	0.67
1:A:149:LYS:C	1:A:151:GLU:H	1.99	0.67
1:B:527:GLU:HA	1:B:530:LYS:NZ	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:TRP:HA	1:A:568:MET:HE2	1.76	0.67
4:B:1605:BTB:H12	4:B:1605:BTB:H72	1.76	0.67
1:A:494:LEU:HD13	1:A:535:LEU:HB3	1.76	0.67
1:B:137:TYR:CD1	1:B:142:TYR:HB2	2.29	0.67
1:B:222:THR:O	1:B:226:GLU:HG2	1.93	0.67
1:A:145:ASN:ND2	1:A:174:GLU:HG3	2.10	0.67
1:A:294:GLU:HB3	1:A:339:ILE:CD1	2.24	0.67
1:B:116:LEU:CD2	1:B:121:LEU:HD12	2.25	0.67
1:B:554:PHE:CB	1:B:559:ILE:HG22	2.23	0.67
1:A:238:LEU:O	1:A:242:ILE:HG12	1.94	0.67
1:B:227:GLU:O	1:B:231:GLU:HG2	1.95	0.67
1:A:144:LYS:HG3	1:A:146:PRO:CD	2.25	0.66
1:B:72:PHE:CD1	1:B:72:PHE:C	2.73	0.66
1:B:86:VAL:HA	1:B:286:ILE:HD13	1.77	0.66
1:B:502:VAL:HG13	1:B:503:GLU:N	2.08	0.66
1:A:497:ASP:O	1:A:501:SER:HB2	1.95	0.66
1:A:95:LEU:HB2	1:A:275:VAL:HG11	1.78	0.66
1:B:290:GLN:O	1:B:294:GLU:HG3	1.95	0.66
1:B:337:ALA:O	1:B:341:MET:HB2	1.96	0.66
1:B:93:VAL:HG13	1:B:94:THR:N	2.10	0.66
1:A:153:ASP:HB3	1:A:156:SER:HB3	1.78	0.66
1:A:401:SER:HB2	1:A:413:ILE:HG22	1.78	0.66
1:A:136:ILE:HG23	1:A:140:HIS:HD2	1.61	0.65
1:A:413:ILE:O	1:A:417:ARG:HB2	1.96	0.65
1:B:586:ILE:HD13	1:B:589:GLN:HE21	1.61	0.65
1:A:289:ALA:O	1:A:292:GLN:HB2	1.96	0.65
1:A:67:ARG:HD2	1:A:583:HIS:CE1	2.32	0.65
1:A:202:GLU:OE2	1:A:250:LEU:HG	1.96	0.65
1:A:282:LEU:HG	1:A:286:ILE:CD1	2.25	0.65
1:A:401:SER:CB	1:A:413:ILE:HG22	2.27	0.65
1:B:428:MET:HE3	1:B:431:ALA:HB3	1.79	0.65
1:B:121:LEU:HD21	1:B:280:ALA:HA	1.77	0.65
1:B:581:THR:HG23	1:B:582:GLN:H	1.61	0.65
1:A:198:LEU:HA	1:A:225:LEU:HD21	1.79	0.65
1:B:310:LYS:C	1:B:312:PRO:HD3	2.21	0.65
1:B:534:TRP:O	1:B:537:ALA:HB3	1.97	0.65
1:A:402:TYR:CD1	1:B:391:LEU:HD23	2.29	0.64
1:B:72:PHE:C	1:B:72:PHE:HD1	2.05	0.64
1:B:73:ILE:O	1:B:76:LEU:HD22	1.97	0.64
1:B:103:GLU:CD	1:B:104:THR:H	2.05	0.64
1:B:164:LEU:HB3	1:B:169:PHE:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASP:O	1:B:317:ARG:HD3	1.96	0.64
4:B:1605:BTB:H12	4:B:1605:BTB:H52	1.79	0.64
1:A:179:PHE:HB3	1:A:190:LEU:HD11	1.79	0.64
1:B:442:LEU:HG	1:B:442:LEU:O	1.98	0.64
1:A:152:ARG:HG3	1:A:152:ARG:HH11	1.62	0.64
1:B:243:ALA:HA	1:B:246:LEU:HB2	1.78	0.64
1:B:284:LEU:HD22	1:B:598:PHE:HB2	1.79	0.64
1:A:204:SER:O	1:A:207:LEU:HD22	1.97	0.64
1:A:433:TRP:CE3	1:A:440:PRO:HG3	2.32	0.64
1:A:510:VAL:HG23	1:A:511:PRO:CD	2.27	0.64
1:B:592:ARG:HG3	1:B:592:ARG:HH11	1.63	0.64
1:A:121:LEU:HD11	1:A:280:ALA:HA	1.79	0.64
1:A:458:MET:HE2	1:A:565:LEU:HD11	1.80	0.64
1:B:159:LEU:HD23	1:B:199:GLN:CD	2.22	0.64
1:A:315:ARG:HH22	3:A:600:F3P:H13	1.63	0.64
1:B:107:ILE:HD12	1:B:110:LEU:HD12	1.80	0.64
1:B:484:LEU:HD23	1:B:554:PHE:HD2	1.63	0.64
1:A:105:ASP:HB3	1:A:108:ARG:HB2	1.78	0.64
4:A:605:BTB:C2	4:A:605:BTB:C7	2.73	0.63
4:B:1605:BTB:C1	4:B:1605:BTB:C5	2.76	0.63
3:B:1600:F3P:C2	3:B:1600:F3P:C6	2.70	0.63
1:A:67:ARG:HD3	1:A:587:HIS:HD2	1.62	0.63
1:B:512:LYS:H	1:B:515:GLN:NE2	1.97	0.63
1:A:462:ILE:O	1:A:466:VAL:HG22	1.99	0.63
4:A:605:BTB:H71	4:A:605:BTB:O1	1.98	0.63
1:B:75:SER:O	1:B:77:LEU:N	2.31	0.63
1:B:82:GLU:O	1:B:84:LYS:HD2	1.98	0.63
1:B:236:GLY:O	1:B:239:LEU:HB2	1.98	0.63
1:A:162:ARG:HG2	1:A:162:ARG:NH1	2.11	0.63
1:B:95:LEU:CD1	1:B:275:VAL:HG21	2.26	0.63
1:B:475:VAL:O	1:B:478:LEU:HB3	1.98	0.63
4:B:1605:BTB:H12	4:B:1605:BTB:C5	2.28	0.63
1:B:257:PRO:HA	1:B:593:THR:HG21	1.81	0.63
1:B:547:ARG:HA	1:B:559:ILE:HD13	1.81	0.63
1:B:209:GLU:O	1:B:211:GLU:N	2.32	0.62
1:B:251:HIS:O	1:B:567:ARG:NH1	2.31	0.62
1:B:256:ARG:HB3	1:B:257:PRO:HD3	1.80	0.62
1:A:78:SER:HB2	1:A:81:LYS:CG	2.28	0.62
1:B:336:SER:HA	1:B:339:ILE:HG12	1.81	0.62
1:B:583:HIS:CB	1:B:586:ILE:HB	2.27	0.62
1:A:108:ARG:HB2	1:A:108:ARG:CZ	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:HA	1:A:180:LYS:HD2	1.80	0.62
1:B:471:THR:O	1:B:472:LYS:C	2.42	0.62
1:B:504:GLU:O	1:B:509:ASP:HB2	1.99	0.62
1:B:311:LEU:HD21	1:B:354:ILE:HD11	1.81	0.62
1:B:137:TYR:CE2	1:B:143:TYR:HB3	2.34	0.62
1:B:208:THR:HG21	1:B:545:ALA:HB2	1.82	0.62
1:B:281:ILE:HG23	1:B:598:PHE:HD2	1.64	0.62
1:A:179:PHE:C	1:A:187:LYS:HD3	2.25	0.62
1:B:70:VAL:HG23	1:B:74:GLN:HG3	1.80	0.62
1:A:361:LEU:HD12	1:A:435:TYR:HB3	1.79	0.62
1:A:547:ARG:C	1:A:549:SER:H	2.06	0.62
1:B:483:ASP:HB3	1:B:487:TRP:HE1	1.65	0.62
1:B:76:LEU:HD23	1:B:77:LEU:H	1.65	0.62
1:B:446:LEU:HD12	1:B:490:PHE:HE1	1.65	0.62
1:B:586:ILE:HA	1:B:589:GLN:HG3	1.81	0.61
1:A:212:THR:O	1:A:213:THR:C	2.39	0.61
1:A:570:GLN:O	1:A:574:HIS:HB2	2.00	0.61
1:B:575:ASN:ND2	1:B:586:ILE:HD11	2.12	0.61
1:A:103:GLU:CD	1:A:105:ASP:H	2.08	0.61
1:B:544:ASN:HA	1:B:547:ARG:HH11	1.65	0.61
1:A:166:GLU:C	1:A:168:GLY:H	2.07	0.61
1:A:188:GLU:O	1:A:191:SER:HB3	2.00	0.61
1:B:311:LEU:HG	1:B:313:PHE:CZ	2.35	0.61
1:A:347:LEU:O	1:A:351:ILE:HG13	2.01	0.61
1:A:405:MET:HE1	1:B:387:GLN:C	2.25	0.61
1:B:201:TYR:HB2	1:B:221:ALA:CB	2.31	0.61
1:B:87:ILE:O	1:B:91:GLU:HG3	1.99	0.61
1:B:315:ARG:HD3	1:B:315:ARG:H	1.64	0.61
4:A:605:BTB:N	4:A:605:BTB:H12	2.13	0.61
1:A:311:LEU:N	1:A:312:PRO:HD3	2.14	0.61
1:B:272:MET:HE1	1:B:277:LEU:CB	2.27	0.60
1:A:105:ASP:HB3	1:A:108:ARG:CB	2.32	0.60
1:A:274:PRO:O	1:A:275:VAL:C	2.43	0.60
1:A:368:THR:O	1:A:371:ILE:HB	2.01	0.60
1:B:411:ASN:HD22	1:B:413:ILE:HG23	1.64	0.60
1:A:228:LYS:NZ	1:A:234:VAL:H	2.00	0.60
1:A:256:ARG:HB3	1:A:257:PRO:HD3	1.81	0.60
1:A:577:ASP:HB2	1:A:584:PRO:CD	2.31	0.60
1:B:63:TYR:CZ	1:B:315:ARG:HD2	2.37	0.60
1:B:530:LYS:HB3	1:B:530:LYS:NZ	2.16	0.60
1:B:547:ARG:HB2	1:B:559:ILE:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:GLY:O	1:B:559:ILE:HG23	2.01	0.60
1:A:175:VAL:HG12	1:A:176:PHE:CD1	2.36	0.60
1:A:323:PHE:O	1:A:326:THR:HB	2.02	0.60
1:A:571:LEU:HD23	1:A:571:LEU:C	2.26	0.60
1:A:92:LEU:HA	1:A:95:LEU:HG	1.82	0.60
1:A:493:ARG:HG2	1:A:493:ARG:NH1	2.16	0.60
1:A:96:VAL:HA	1:A:99:GLU:HG3	1.81	0.60
1:A:531:HIS:O	1:A:534:TRP:HB3	2.01	0.59
1:B:79:ASP:O	1:B:82:GLU:HG3	2.02	0.59
1:B:95:LEU:HD11	1:B:275:VAL:HG11	1.84	0.59
1:B:209:GLU:H	1:B:541:LYS:HD2	1.67	0.59
1:B:571:LEU:HD23	1:B:572:MET:N	2.18	0.59
1:A:345:ASN:HA	1:A:348:ILE:HD12	1.85	0.59
1:A:555:GLY:O	1:A:559:ILE:HG23	2.02	0.59
1:B:216:SER:HA	1:B:219:GLU:CD	2.28	0.59
1:B:145:ASN:HD22	1:B:145:ASN:H	1.50	0.59
1:B:296:LYS:O	1:B:299:PHE:HB3	2.03	0.59
1:A:559:ILE:HG13	1:A:560:GLY:N	2.16	0.59
4:B:1605:BTB:N	4:B:1605:BTB:H42	2.17	0.59
1:A:278:GLU:HG3	1:A:279:LEU:N	2.17	0.59
1:B:128:GLU:O	1:B:132:ILE:HD12	2.03	0.59
1:B:350:VAL:HG12	1:B:351:ILE:N	2.18	0.59
1:B:77:LEU:HG	1:B:296:LYS:NZ	2.18	0.58
1:A:168:GLY:HA2	1:A:548:VAL:CG1	2.33	0.58
1:A:378:SER:HB3	1:A:381:GLN:OE1	2.02	0.58
1:B:174:GLU:CD	1:B:174:GLU:H	2.10	0.58
1:B:456:PRO:HD3	1:B:489:SER:OG	2.03	0.58
1:B:93:VAL:HG22	1:B:97:LYS:HE2	1.84	0.58
1:B:312:PRO:O	1:B:314:ALA:N	2.36	0.58
1:A:121:LEU:HB3	1:A:125:PHE:HE2	1.68	0.58
1:A:266:TYR:O	1:A:269:ARG:HB3	2.02	0.58
1:B:459:LEU:HD12	1:B:462:ILE:HD12	1.85	0.58
1:B:587:HIS:ND1	1:B:587:HIS:C	2.60	0.58
1:A:79:ASP:N	1:A:81:LYS:HG3	2.19	0.58
1:A:345:ASN:CB	3:A:600:F3P:H93	2.33	0.58
4:A:605:BTB:N	4:A:605:BTB:H42	2.13	0.58
1:A:173:GLN:NE2	1:A:213:THR:N	2.51	0.58
1:A:194:THR:HA	1:A:197:LEU:HB2	1.84	0.58
1:B:61:GLY:O	1:B:62:ASN:HB2	2.02	0.58
1:B:83:ASP:C	1:B:85:HIS:N	2.55	0.58
1:A:315:ARG:NH1	1:A:353:ASP:CG	2.61	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:O	1:A:91:GLU:HG3	2.02	0.58
1:A:577:ASP:OD2	1:A:582:GLN:HB2	2.03	0.58
1:B:70:VAL:O	1:B:74:GLN:HG3	2.03	0.58
1:B:315:ARG:NH1	1:B:349:THR:HG23	2.19	0.58
1:B:314:ALA:HA	1:B:353:ASP:OD2	2.03	0.58
1:B:75:SER:O	1:B:77:LEU:HD12	2.03	0.58
1:B:320:GLU:HB3	1:B:579:HIS:O	2.04	0.58
1:B:103:GLU:OE1	1:B:103:GLU:HA	2.04	0.57
1:B:159:LEU:HD23	1:B:199:GLN:OE1	2.04	0.57
1:B:492:LEU:HA	1:B:569:ALA:HB1	1.86	0.57
1:A:168:GLY:HA2	1:A:548:VAL:HG13	1.85	0.57
1:B:282:LEU:HG	1:B:286:ILE:HD11	1.86	0.57
1:B:582:GLN:HG2	1:B:584:PRO:HD3	1.85	0.57
1:B:114:ASP:O	1:B:118:ARG:HG2	2.02	0.57
1:B:128:GLU:OE2	1:B:128:GLU:N	2.38	0.57
1:A:277:LEU:HD13	1:A:277:LEU:C	2.29	0.57
1:A:311:LEU:HG	1:A:313:PHE:CZ	2.40	0.57
1:B:592:ARG:HH11	1:B:592:ARG:CG	2.17	0.57
1:A:86:VAL:HA	1:A:89:ALA:HB3	1.85	0.57
1:A:315:ARG:NH2	3:A:600:F3P:O2A	2.38	0.57
1:A:449:SER:HB2	1:A:493:ARG:NH1	2.18	0.57
1:A:577:ASP:HB2	1:A:584:PRO:HD2	1.86	0.57
1:B:254:ILE:HG12	1:B:568:MET:HA	1.85	0.57
1:B:267:ARG:HA	1:B:272:MET:HE3	1.87	0.57
1:B:544:ASN:O	1:B:547:ARG:HG2	2.03	0.57
1:A:86:VAL:HG23	1:A:286:ILE:HG21	1.85	0.57
1:A:315:ARG:NH2	3:A:600:F3P:H13	2.20	0.57
1:A:554:PHE:HB3	1:A:558:PHE:HD2	1.69	0.57
1:B:93:VAL:HG22	1:B:97:LYS:HG3	1.86	0.57
4:B:1605:BTB:C7	4:B:1605:BTB:C1	2.79	0.57
1:A:90:SER:O	1:A:93:VAL:HG12	2.04	0.57
1:A:190:LEU:O	1:A:192:ASP:N	2.37	0.57
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.11	0.57
1:B:188:GLU:H	1:B:188:GLU:CD	2.12	0.57
1:A:453:ILE:O	1:A:453:ILE:HG13	2.03	0.57
1:A:493:ARG:HD3	1:A:493:ARG:O	2.04	0.57
1:A:527:GLU:OE1	1:A:527:GLU:HA	2.04	0.57
1:A:70:VAL:HG12	1:A:74:GLN:NE2	2.19	0.56
1:A:106:GLN:HG2	1:A:136:ILE:HG12	1.86	0.56
1:A:325:ASN:HB3	1:A:338:ARG:HG3	1.87	0.56
1:B:87:ILE:O	1:B:88:ARG:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:HD13	1:B:125:PHE:CD1	2.40	0.56
1:B:371:ILE:HG12	1:B:421:VAL:HG22	1.86	0.56
1:A:204:SER:HB2	1:A:218:ARG:NH1	2.20	0.56
1:A:209:GLU:OE1	5:A:700:HOH:O	2.18	0.56
1:A:270:PRO:O	1:A:271:ASP:C	2.48	0.56
1:A:283:ASP:CG	1:A:332:ARG:HH22	2.13	0.56
1:A:311:LEU:HD21	1:A:350:VAL:CG1	2.35	0.56
1:A:324:TRP:CZ2	1:A:572:MET:HG2	2.38	0.56
1:A:379:ILE:HD13	1:A:387:GLN:HG2	1.86	0.56
1:A:413:ILE:HG12	1:A:414:PRO:CD	2.35	0.56
1:A:491:VAL:O	1:A:492:LEU:C	2.47	0.56
1:B:283:ASP:CG	1:B:332:ARG:HH22	2.13	0.56
1:B:301:TRP:HZ2	1:B:347:LEU:HD21	1.70	0.56
1:B:515:GLN:HA	1:B:518:MET:HG3	1.86	0.56
1:A:69:ASP:OD2	1:A:69:ASP:C	2.47	0.56
1:A:128:GLU:O	1:A:129:PHE:C	2.44	0.56
1:A:378:SER:O	1:A:379:ILE:C	2.47	0.56
1:A:207:LEU:H	1:A:207:LEU:CD2	2.19	0.56
1:A:279:LEU:HD12	1:A:279:LEU:O	2.06	0.56
1:A:100:LEU:HD12	1:A:112:LEU:HD12	1.86	0.56
1:A:276:VAL:O	1:A:277:LEU:C	2.48	0.56
1:A:493:ARG:C	1:A:493:ARG:CD	2.78	0.56
1:B:87:ILE:HA	1:B:90:SER:OG	2.06	0.56
1:B:493:ARG:O	1:B:496:ASP:N	2.38	0.56
1:A:317:ARG:HB3	1:A:317:ARG:NH1	2.20	0.56
1:B:323:PHE:O	1:B:326:THR:HB	2.06	0.56
1:A:266:TYR:CE2	1:A:272:MET:HG2	2.40	0.56
1:A:274:PRO:C	1:A:276:VAL:N	2.62	0.56
1:A:455:GLY:O	1:A:459:LEU:HB2	2.05	0.56
1:B:344:VAL:HG12	1:B:348:ILE:CD1	2.36	0.56
1:A:224:PHE:O	1:A:225:LEU:C	2.47	0.56
1:A:559:ILE:HD12	1:A:559:ILE:O	2.05	0.56
1:B:317:ARG:HD2	1:B:320:GLU:OE2	2.06	0.56
1:A:376:ILE:O	1:A:379:ILE:HB	2.05	0.55
1:A:473:GLU:O	1:A:474:THR:C	2.47	0.55
1:A:192:ASP:O	1:A:194:THR:HG23	2.07	0.55
1:A:290:GLN:NE2	1:A:294:GLU:HG2	2.21	0.55
1:A:500:THR:HG1	1:A:501:SER:H	1.53	0.55
1:B:299:PHE:HA	1:B:318:LEU:HD22	1.87	0.55
1:B:341:MET:HE1	1:B:458:MET:CA	2.37	0.55
1:A:70:VAL:C	1:A:74:GLN:HG2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:O	1:A:99:GLU:HG2	2.06	0.55
1:A:116:LEU:HD13	1:A:125:PHE:CD2	2.41	0.55
1:A:573:TYR:HE1	1:A:578:GLY:HA2	1.70	0.55
1:B:92:LEU:HD13	1:B:279:LEU:HA	1.89	0.55
1:B:428:MET:HG3	1:B:432:ARG:HE	1.72	0.55
1:A:367:PHE:HB2	1:A:386:MET:SD	2.47	0.55
1:A:547:ARG:HB2	1:A:559:ILE:HD13	1.88	0.55
1:B:83:ASP:O	1:B:85:HIS:N	2.40	0.55
1:B:116:LEU:HD22	1:B:125:PHE:CE1	2.41	0.55
1:B:211:GLU:HG2	1:B:214:LEU:CD1	2.26	0.55
1:B:267:ARG:HH22	1:B:599:ALA:HA	1.71	0.55
1:A:194:THR:HA	1:A:197:LEU:CB	2.37	0.55
1:A:318:LEU:HD13	1:A:318:LEU:O	2.07	0.55
1:A:493:ARG:O	1:A:494:LEU:C	2.49	0.55
1:B:259:ALA:O	1:B:260:PRO:C	2.45	0.55
1:B:360:THR:HG23	1:B:363:GLU:OE1	2.07	0.55
1:B:513:SER:O	1:B:514:LEU:C	2.49	0.55
1:B:559:ILE:O	1:B:559:ILE:HD12	2.06	0.55
1:A:151:GLU:O	1:A:152:ARG:O	2.23	0.55
1:B:309:GLU:HG3	1:B:310:LYS:HG2	1.87	0.55
1:B:547:ARG:HB2	1:B:559:ILE:HD11	1.87	0.55
1:A:123:ASP:CG	1:A:332:ARG:HD2	2.31	0.54
1:A:205:PHE:CZ	1:A:249:PRO:HG3	2.42	0.54
1:A:294:GLU:HB3	1:A:339:ILE:HD11	1.88	0.54
1:A:431:ALA:O	1:A:432:ARG:C	2.50	0.54
1:A:465:ARG:HH11	1:A:465:ARG:CG	2.11	0.54
1:A:100:LEU:CD1	1:A:112:LEU:HD12	2.37	0.54
1:A:405:MET:CE	1:B:388:LEU:HA	2.37	0.54
1:B:204:SER:O	1:B:207:LEU:HD13	2.07	0.54
1:A:98:MET:C	1:A:100:LEU:N	2.59	0.54
1:A:521:TYR:CD2	1:A:521:TYR:N	2.75	0.54
1:B:93:VAL:CG1	1:B:94:THR:H	2.20	0.54
1:B:370:LEU:O	1:B:374:TRP:N	2.41	0.54
1:A:161:PHE:CZ	1:A:165:ARG:NE	2.74	0.54
1:A:585:ILE:C	1:A:587:HIS:N	2.60	0.54
1:B:77:LEU:HG	1:B:296:LYS:CE	2.37	0.54
1:A:115:ASP:OD1	1:A:269:ARG:NH2	2.40	0.54
1:B:95:LEU:HA	1:B:98:MET:HB2	1.89	0.54
1:A:201:TYR:C	1:A:201:TYR:CD2	2.85	0.54
1:A:223:LYS:HD3	1:A:224:PHE:CZ	2.43	0.54
1:B:299:PHE:HE1	1:B:303:ARG:HD2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1604:BTB:C5	4:B:1604:BTB:H12	2.36	0.54
1:A:422:ASP:O	1:A:423:LEU:C	2.50	0.54
1:A:458:MET:HE2	1:A:565:LEU:HD13	1.89	0.54
1:B:86:VAL:HG23	1:B:286:ILE:HD13	1.89	0.54
1:A:79:ASP:C	1:A:81:LYS:H	2.15	0.54
1:B:377:ASN:C	1:B:379:ILE:H	2.16	0.54
1:A:302:TRP:HB2	1:A:318:LEU:CG	2.38	0.54
1:A:361:LEU:HD12	1:A:435:TYR:CB	2.37	0.54
1:B:97:LYS:C	1:B:101:GLU:CD	2.76	0.54
1:B:190:LEU:C	1:B:192:ASP:N	2.65	0.54
1:B:428:MET:O	1:B:429:VAL:C	2.50	0.54
1:B:575:ASN:HB2	1:B:584:PRO:HG2	1.90	0.54
1:B:588:GLN:O	1:B:592:ARG:HB2	2.08	0.54
4:B:1604:BTB:H12	4:B:1604:BTB:C6	2.38	0.54
1:A:212:THR:O	1:A:215:GLU:N	2.41	0.54
1:B:176:PHE:HA	1:B:179:PHE:CE2	2.42	0.54
1:B:497:ASP:CG	1:B:512:LYS:HB3	2.32	0.54
1:B:540:TRP:O	1:B:543:MET:HB3	2.08	0.54
1:B:544:ASN:HD22	1:B:547:ARG:NH1	2.06	0.54
1:B:546:GLU:O	1:B:549:SER:HB3	2.08	0.54
1:A:77:LEU:O	1:A:78:SER:O	2.25	0.53
1:A:319:VAL:HG12	1:A:590:MET:CE	2.37	0.53
1:A:363:GLU:HG2	1:A:383:PRO:HG3	1.89	0.53
1:B:83:ASP:O	1:B:84:LYS:C	2.51	0.53
1:B:456:PRO:O	1:B:460:THR:HG23	2.07	0.53
1:A:172:ALA:HB1	1:A:174:GLU:HG2	1.89	0.53
1:A:70:VAL:O	1:A:72:PHE:N	2.42	0.53
1:A:559:ILE:O	1:A:562:ALA:HB3	2.09	0.53
1:B:453:ILE:HG23	1:B:453:ILE:O	2.07	0.53
1:A:264:GLU:HB2	1:A:267:ARG:CZ	2.36	0.53
1:A:423:LEU:HD12	1:A:423:LEU:O	2.08	0.53
1:A:426:LYS:N	1:A:426:LYS:HD3	2.22	0.53
1:B:426:LYS:O	1:B:429:VAL:HG23	2.08	0.53
1:B:516:CYS:O	1:B:520:ASP:HB2	2.08	0.53
1:A:123:ASP:CG	1:A:332:ARG:HH11	2.16	0.53
1:A:391:LEU:HD22	1:B:405:MET:HE3	1.89	0.53
1:B:95:LEU:HD11	1:B:275:VAL:CG2	2.35	0.53
1:B:202:GLU:CD	1:B:250:LEU:HD22	2.33	0.53
1:B:416:LEU:HD22	1:B:461:HIS:CE1	2.43	0.53
1:B:576:GLY:C	1:B:578:GLY:H	2.14	0.53
1:A:364:LEU:HB3	1:A:428:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:HA	1:A:449:SER:OG	2.09	0.53
1:B:367:PHE:O	1:B:368:THR:C	2.51	0.53
1:A:256:ARG:HB2	1:A:330:GLU:OE2	2.08	0.53
1:B:77:LEU:HG	1:B:296:LYS:HE2	1.90	0.53
1:A:260:PRO:O	1:A:261:VAL:C	2.51	0.53
1:A:329:ILE:HB	1:A:338:ARG:HD3	1.91	0.53
1:B:329:ILE:HG21	1:B:334:HIS:HB2	1.90	0.53
1:B:543:MET:O	1:B:543:MET:HG3	2.08	0.53
1:A:302:TRP:HB2	1:A:318:LEU:CD2	2.39	0.53
1:A:323:PHE:CD2	1:A:572:MET:HE1	2.43	0.53
1:A:559:ILE:HD12	1:A:559:ILE:C	2.34	0.53
1:B:494:LEU:O	1:B:498:LEU:HB2	2.09	0.53
1:A:306:GLY:HA2	1:A:308:VAL:HG23	1.91	0.53
1:A:500:THR:OG1	1:A:501:SER:N	2.21	0.53
1:B:365:GLU:OE2	1:B:428:MET:HE2	2.09	0.53
1:A:82:GLU:N	1:A:82:GLU:OE1	2.42	0.52
1:A:177:ASP:OD2	1:A:180:LYS:HD2	2.08	0.52
1:A:283:ASP:O	1:A:286:ILE:N	2.42	0.52
1:A:323:PHE:HD2	1:A:572:MET:HE1	1.74	0.52
1:A:102:LYS:HA	1:A:102:LYS:CE	2.35	0.52
1:A:155:TYR:HB2	1:A:196:GLY:CA	2.39	0.52
1:B:299:PHE:CE1	1:B:303:ARG:HD2	2.44	0.52
1:A:70:VAL:HG12	1:A:74:GLN:CD	2.34	0.52
1:A:152:ARG:NH1	1:A:178:SER:OG	2.43	0.52
1:A:241:ARG:NH2	1:A:245:SER:OG	2.42	0.52
1:A:417:ARG:O	1:A:421:VAL:HG23	2.09	0.52
1:A:155:TYR:HA	1:A:196:GLY:HA2	1.90	0.52
1:A:273:ASN:HD21	1:A:275:VAL:CG2	2.22	0.52
1:A:587:HIS:O	1:A:591:THR:HG23	2.10	0.52
1:B:103:GLU:OE2	1:B:105:ASP:N	2.43	0.52
1:A:302:TRP:CB	1:A:318:LEU:HG	2.38	0.52
1:A:505:VAL:HG23	1:A:506:SER:N	2.23	0.52
1:A:578:GLY:C	1:A:580:GLY:N	2.58	0.52
1:B:115:ASP:CG	1:B:269:ARG:HH12	2.17	0.52
1:A:435:TYR:C	1:A:437:GLY:H	2.17	0.52
1:A:456:PRO:HD3	1:A:489:SER:OG	2.09	0.52
1:B:97:LYS:O	1:B:100:LEU:N	2.42	0.52
1:B:201:TYR:HB2	1:B:221:ALA:HB3	1.92	0.52
1:B:207:LEU:H	1:B:207:LEU:HD22	1.74	0.52
1:B:282:LEU:HG	1:B:286:ILE:CD1	2.39	0.52
1:B:376:ILE:HA	1:B:379:ILE:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LYS:O	1:B:531:HIS:C	2.50	0.52
1:A:75:SER:O	1:A:76:LEU:C	2.53	0.52
1:A:95:LEU:HD12	1:A:275:VAL:HG13	1.91	0.52
1:A:547:ARG:CB	1:A:559:ILE:HD13	2.39	0.52
1:B:502:VAL:CG1	1:B:503:GLU:H	2.14	0.52
1:A:145:ASN:N	1:A:146:PRO:HD2	2.25	0.52
4:A:605:BTB:C5	4:A:605:BTB:C4	2.72	0.52
1:B:223:LYS:HB3	1:B:223:LYS:HZ2	1.75	0.52
1:B:506:SER:C	1:B:508:GLY:H	2.18	0.52
1:B:551:ASP:O	1:B:552:SER:C	2.52	0.52
1:B:194:THR:C	1:B:196:GLY:N	2.62	0.52
1:B:578:GLY:O	1:B:580:GLY:N	2.42	0.52
1:A:252:TRP:HB3	1:A:570:GLN:NE2	2.26	0.52
1:A:518:MET:HE3	1:A:525:GLU:HA	1.92	0.52
1:B:78:SER:O	1:B:81:LYS:HG2	2.10	0.52
1:B:267:ARG:NH2	1:B:599:ALA:HA	2.25	0.52
1:B:377:ASN:OD1	1:B:377:ASN:N	2.42	0.52
1:A:144:LYS:HG3	1:A:146:PRO:CG	2.41	0.51
1:A:547:ARG:HD2	1:A:563:VAL:HG21	1.92	0.51
1:B:103:GLU:CD	1:B:104:THR:N	2.68	0.51
1:A:75:SER:O	1:A:77:LEU:N	2.44	0.51
1:A:149:LYS:C	1:A:151:GLU:N	2.68	0.51
1:A:369:ASP:HA	1:A:372:ARG:HB2	1.92	0.51
1:A:442:LEU:HD12	1:A:446:LEU:HG	1.92	0.51
1:A:547:ARG:HB2	1:A:559:ILE:CD1	2.40	0.51
1:B:484:LEU:HD12	1:B:484:LEU:O	2.10	0.51
1:A:269:ARG:HG3	1:A:270:PRO:HD2	1.92	0.51
1:A:273:ASN:ND2	1:A:275:VAL:HG23	2.23	0.51
1:A:433:TRP:HA	1:A:438:HIS:HB3	1.93	0.51
1:B:426:LYS:HA	1:B:429:VAL:CG2	2.40	0.51
1:B:546:GLU:HA	1:B:549:SER:HB2	1.93	0.51
1:A:135:SER:O	1:A:136:ILE:C	2.53	0.51
1:A:173:GLN:NE2	1:A:211:GLU:C	2.65	0.51
1:A:304:ASN:O	1:B:406:LYS:HE3	2.10	0.51
1:A:311:LEU:HD21	1:A:350:VAL:HG13	1.93	0.51
1:B:334:HIS:HB3	1:B:337:ALA:HB3	1.91	0.51
1:A:317:ARG:O	1:A:318:LEU:C	2.52	0.51
1:A:401:SER:HB3	1:A:412:VAL:HG23	1.91	0.51
1:B:119:MET:HG3	1:B:262:TRP:CD1	2.36	0.51
1:A:291:PHE:O	1:A:292:GLN:C	2.54	0.51
1:A:370:LEU:HD13	1:A:382:LEU:CD2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD21	1:A:420:TRP:CE2	2.46	0.51
1:A:80:TYR:HA	1:A:85:HIS:CD2	2.45	0.51
1:A:81:LYS:H	1:A:81:LYS:CD	2.22	0.51
1:A:175:VAL:HG12	1:A:176:PHE:CE1	2.46	0.51
1:B:116:LEU:HD13	1:B:125:PHE:CG	2.46	0.51
1:A:144:LYS:HE2	1:A:146:PRO:HD2	1.93	0.51
1:B:181:ASN:C	1:B:181:ASN:OD1	2.51	0.51
1:B:232:GLY:HA2	1:B:239:LEU:CD2	2.40	0.51
1:B:264:GLU:HB3	1:B:267:ARG:NH1	2.25	0.51
1:A:283:ASP:O	1:A:284:LEU:C	2.53	0.51
1:A:530:LYS:O	1:A:531:HIS:C	2.47	0.51
1:B:585:ILE:O	1:B:585:ILE:HG13	2.05	0.51
1:A:110:LEU:HD21	1:A:136:ILE:CD1	2.41	0.50
1:A:128:GLU:OE2	1:A:128:GLU:N	2.44	0.50
1:A:204:SER:C	1:A:206:LEU:N	2.69	0.50
1:A:472:LYS:HD3	1:A:476:ASP:OD2	2.10	0.50
1:B:75:SER:OG	1:B:76:LEU:N	2.44	0.50
1:B:201:TYR:HB2	1:B:221:ALA:HB1	1.92	0.50
1:B:207:LEU:H	1:B:207:LEU:CD2	2.24	0.50
1:B:306:GLY:O	1:B:310:LYS:HG3	2.11	0.50
4:B:1604:BTB:C2	4:B:1604:BTB:C5	2.85	0.50
1:A:97:LYS:O	1:A:100:LEU:HB3	2.10	0.50
1:A:180:LYS:NZ	1:A:213:THR:HG23	2.26	0.50
1:A:535:LEU:O	1:A:539:VAL:HG13	2.11	0.50
1:B:433:TRP:CZ3	1:B:440:PRO:HG3	2.46	0.50
1:A:229:VAL:HA	1:A:239:LEU:CD2	2.40	0.50
1:B:191:SER:HA	1:B:224:PHE:CD2	2.47	0.50
1:B:371:ILE:CD1	1:B:372:ARG:N	2.72	0.50
1:A:83:ASP:O	1:A:84:LYS:C	2.55	0.50
1:A:370:LEU:HG	1:A:375:ASP:HB3	1.93	0.50
1:A:388:LEU:HG	1:B:402:TYR:OH	2.11	0.50
1:B:413:ILE:O	1:B:417:ARG:HB2	2.12	0.50
1:B:410:VAL:HG22	1:B:411:ASN:N	2.26	0.50
1:A:121:LEU:HB3	1:A:125:PHE:CE2	2.47	0.50
1:B:281:ILE:HG23	1:B:598:PHE:CD2	2.46	0.50
1:B:93:VAL:CG1	1:B:94:THR:N	2.75	0.50
1:B:95:LEU:CG	1:B:275:VAL:HG21	2.41	0.50
1:A:301:TRP:CZ3	1:A:346:ALA:HB3	2.47	0.50
1:B:301:TRP:CG	1:B:343:LYS:HD3	2.47	0.50
1:A:373:ARG:O	1:A:374:TRP:C	2.54	0.50
1:B:132:ILE:HG22	1:B:132:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:SER:HB3	1:B:200:LEU:HA	1.92	0.50
1:B:242:ILE:HG23	1:B:246:LEU:HD12	1.92	0.50
1:B:325:ASN:CG	1:B:341:MET:HB3	2.37	0.50
1:B:457:CYS:O	1:B:461:HIS:CD2	2.64	0.50
1:A:544:ASN:O	1:A:545:ALA:C	2.55	0.49
1:B:89:ALA:CA	1:B:92:LEU:HD12	2.42	0.49
1:B:139:ASP:C	1:B:141:HIS:H	2.20	0.49
1:B:223:LYS:HG2	1:B:224:PHE:CD1	2.47	0.49
1:B:238:LEU:HD23	1:B:239:LEU:N	2.27	0.49
1:A:97:LYS:HE3	1:A:128:GLU:OE1	2.12	0.49
1:A:341:MET:HE1	1:A:458:MET:CB	2.43	0.49
1:A:405:MET:HE2	1:B:388:LEU:HA	1.95	0.49
1:A:514:LEU:O	1:A:518:MET:HG3	2.13	0.49
1:B:318:LEU:HA	1:B:321:CYS:HB2	1.94	0.49
1:B:581:THR:CG2	1:B:582:GLN:H	2.25	0.49
1:B:581:THR:CG2	1:B:582:GLN:N	2.75	0.49
1:A:377:ASN:C	1:A:379:ILE:H	2.19	0.49
1:B:277:LEU:HD13	1:B:277:LEU:C	2.38	0.49
1:B:586:ILE:HD13	1:B:589:GLN:NE2	2.27	0.49
1:A:145:ASN:HD22	1:A:145:ASN:C	2.21	0.49
1:A:238:LEU:O	1:A:239:LEU:C	2.54	0.49
1:A:543:MET:O	1:A:547:ARG:HG2	2.12	0.49
1:A:144:LYS:HG3	1:A:146:PRO:HG2	1.94	0.49
1:A:179:PHE:O	1:A:187:LYS:HB2	2.12	0.49
1:B:344:VAL:HG12	1:B:348:ILE:HD13	1.94	0.49
1:B:482:HIS:CD2	1:B:554:PHE:HE2	2.31	0.49
1:A:110:LEU:HD21	1:A:136:ILE:HD12	1.93	0.49
1:A:514:LEU:HD12	1:A:514:LEU:N	2.24	0.49
1:B:315:ARG:H	1:B:315:ARG:CD	2.25	0.49
1:B:323:PHE:CE1	1:B:326:THR:HG21	2.48	0.49
1:B:458:MET:HE1	1:B:565:LEU:HD13	1.95	0.49
1:B:471:THR:H	1:B:474:THR:HG23	1.77	0.49
1:B:592:ARG:CG	1:B:592:ARG:NH1	2.75	0.49
1:A:165:ARG:HB3	1:A:206:LEU:CD2	2.42	0.49
1:A:172:ALA:HB1	1:A:174:GLU:OE1	2.13	0.49
1:B:429:VAL:HG12	5:B:778:HOH:O	2.13	0.49
1:A:207:LEU:N	1:A:207:LEU:HD23	2.27	0.48
1:B:112:LEU:HD13	1:B:116:LEU:HG	1.95	0.48
1:B:241:ARG:HH22	1:B:250:LEU:HD13	1.78	0.48
1:B:558:PHE:O	1:B:559:ILE:C	2.55	0.48
1:A:98:MET:O	1:A:99:GLU:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:HG12	1:A:156:SER:HB2	1.94	0.48
1:B:61:GLY:HA3	1:B:63:TYR:CE2	2.47	0.48
1:B:232:GLY:HA2	1:B:239:LEU:HD21	1.94	0.48
1:B:294:GLU:HG2	1:B:339:ILE:HD11	1.95	0.48
1:B:535:LEU:HD21	4:B:1604:BTB:H12	1.94	0.48
1:A:60:SER:C	1:A:62:ASN:H	2.21	0.48
1:A:101:GLU:OE2	1:A:132:ILE:HD11	2.13	0.48
1:A:345:ASN:CB	3:A:600:F3P:C9	2.90	0.48
1:B:583:HIS:CA	1:B:586:ILE:HB	2.43	0.48
1:A:89:ALA:HA	1:A:92:LEU:HD12	1.95	0.48
1:A:136:ILE:HG23	1:A:140:HIS:CD2	2.45	0.48
1:A:190:LEU:HB2	1:A:220:PHE:HZ	1.79	0.48
1:A:204:SER:C	1:A:206:LEU:H	2.21	0.48
1:A:241:ARG:HH21	1:A:245:SER:CB	2.26	0.48
1:A:379:ILE:CG2	1:A:380:ASP:N	2.77	0.48
1:A:408:LYS:HE2	1:A:467:THR:O	2.14	0.48
1:A:426:LYS:HA	1:A:429:VAL:HG23	1.94	0.48
1:B:585:ILE:C	1:B:587:HIS:N	2.67	0.48
1:A:89:ALA:HA	1:A:282:LEU:HD23	1.95	0.48
1:A:119:MET:HB3	1:A:263:ILE:HD13	1.95	0.48
1:A:374:TRP:CE3	1:A:417:ARG:HG3	2.48	0.48
1:B:145:ASN:HD22	1:B:146:PRO:CD	2.13	0.48
1:B:311:LEU:HG	1:B:313:PHE:CE2	2.49	0.48
1:B:428:MET:O	1:B:431:ALA:N	2.46	0.48
1:A:254:ILE:O	1:A:254:ILE:HG23	2.12	0.48
1:A:282:LEU:O	1:A:286:ILE:HG13	2.12	0.48
1:A:98:MET:O	1:A:98:MET:HG2	2.13	0.48
1:B:202:GLU:OE2	1:B:250:LEU:HD22	2.14	0.48
1:B:261:VAL:O	1:B:262:TRP:C	2.55	0.48
1:B:329:ILE:CG2	1:B:334:HIS:HB2	2.43	0.48
1:B:369:ASP:O	1:B:372:ARG:HB3	2.13	0.48
1:A:140:HIS:O	1:A:141:HIS:C	2.56	0.48
1:A:70:VAL:CG1	1:A:303:ARG:HD3	2.43	0.48
1:A:117:GLN:HG2	1:A:129:PHE:CE1	2.49	0.48
1:A:287:VAL:O	1:A:290:GLN:HB3	2.13	0.48
1:A:442:LEU:CD1	1:A:446:LEU:HG	2.44	0.48
1:B:103:GLU:HB3	1:B:109:GLN:CG	2.43	0.48
1:B:302:TRP:CZ3	1:B:307:PHE:HD2	2.31	0.48
1:B:492:LEU:HA	1:B:569:ALA:CB	2.44	0.48
1:B:576:GLY:O	1:B:578:GLY:N	2.30	0.48
1:A:404:VAL:CG1	1:A:410:VAL:HG23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:MET:HG3	1:A:432:ARG:HE	1.79	0.48
1:A:460:THR:HG21	1:A:481:TYR:HE1	1.78	0.48
1:B:112:LEU:HD22	1:B:112:LEU:HA	1.77	0.48
1:B:155:TYR:HB2	1:B:196:GLY:HA2	1.94	0.48
1:B:368:THR:O	1:B:371:ILE:HD13	2.13	0.48
1:A:391:LEU:HD23	1:B:402:TYR:HD1	1.79	0.47
1:A:220:PHE:CE1	1:A:224:PHE:HE2	2.33	0.47
1:A:256:ARG:HB2	1:A:330:GLU:CD	2.39	0.47
1:A:309:GLU:HG3	1:A:310:LYS:N	2.27	0.47
1:B:188:GLU:CD	1:B:188:GLU:N	2.72	0.47
1:B:493:ARG:O	1:B:494:LEU:C	2.55	0.47
1:B:526:ALA:O	1:B:530:LYS:N	2.41	0.47
3:B:1600:F3P:H103	3:B:1600:F3P:C7	2.44	0.47
1:A:144:LYS:NZ	1:A:146:PRO:HG2	2.29	0.47
1:A:344:VAL:O	1:A:348:ILE:HG13	2.14	0.47
1:A:550:LYS:HG2	1:A:552:SER:HA	1.95	0.47
1:B:190:LEU:O	1:B:192:ASP:N	2.48	0.47
1:B:256:ARG:HD3	1:B:291:PHE:HZ	1.80	0.47
4:B:1605:BTB:C2	4:B:1605:BTB:C5	2.86	0.47
1:A:283:ASP:CA	1:A:286:ILE:HD12	2.41	0.47
4:A:604:BTB:H62	4:A:604:BTB:C4	2.45	0.47
4:A:604:BTB:H62	4:A:604:BTB:H41	1.96	0.47
1:B:73:ILE:HG21	1:B:299:PHE:CE2	2.49	0.47
1:B:261:VAL:HG22	1:B:262:TRP:N	2.29	0.47
1:B:369:ASP:OD2	1:B:372:ARG:NH2	2.47	0.47
1:B:454:SER:O	1:B:455:GLY:C	2.57	0.47
1:A:503:GLU:O	1:A:504:GLU:C	2.55	0.47
1:B:86:VAL:HA	1:B:286:ILE:CD1	2.43	0.47
1:B:299:PHE:O	1:B:302:TRP:N	2.48	0.47
1:A:454:SER:O	1:A:457:CYS:N	2.47	0.47
1:A:133:LEU:O	1:A:134:SER:C	2.57	0.47
1:A:188:GLU:CD	1:A:188:GLU:N	2.70	0.47
1:A:198:LEU:CA	1:A:225:LEU:HD21	2.43	0.47
1:A:446:LEU:C	1:A:449:SER:HG	2.22	0.47
1:B:190:LEU:C	1:B:192:ASP:H	2.22	0.47
1:B:343:LYS:O	1:B:347:LEU:HG	2.14	0.47
1:B:442:LEU:HB3	1:B:520:ASP:OD1	2.15	0.47
1:B:462:ILE:O	1:B:466:VAL:HG22	2.14	0.47
1:B:558:PHE:C	1:B:560:GLY:N	2.69	0.47
1:A:145:ASN:HB3	1:A:146:PRO:HD3	1.95	0.47
1:A:420:TRP:HA	1:A:420:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:SER:O	1:A:505:VAL:HG22	2.14	0.47
1:A:503:GLU:HA	1:A:506:SER:HB2	1.97	0.47
1:B:182:GLU:H	1:B:182:GLU:HG3	1.31	0.47
1:B:510:VAL:HG12	1:B:511:PRO:CD	2.42	0.47
1:A:68:TRP:HZ3	1:A:320:GLU:OE2	1.97	0.47
1:A:110:LEU:HB3	1:A:159:LEU:HD13	1.97	0.47
1:A:492:LEU:HA	1:A:569:ALA:CB	2.44	0.47
1:B:371:ILE:HD13	1:B:372:ARG:H	1.76	0.47
1:A:89:ALA:O	1:A:92:LEU:HD12	2.15	0.47
1:A:445:TYR:C	1:A:447:GLU:N	2.72	0.47
1:B:146:PRO:C	1:B:148:PRO:HD2	2.40	0.47
1:B:161:PHE:HD2	1:B:203:ALA:HB1	1.79	0.47
1:B:194:THR:O	1:B:195:ARG:C	2.54	0.47
1:B:259:ALA:N	1:B:260:PRO:HD2	2.30	0.47
1:B:588:GLN:HA	1:B:591:THR:HG22	1.96	0.47
1:A:190:LEU:C	1:A:192:ASP:N	2.73	0.46
1:A:294:GLU:HB2	1:A:322:TYR:CE1	2.50	0.46
1:B:84:LYS:HD2	1:B:85:HIS:H	1.80	0.46
1:B:254:ILE:HG13	1:B:567:ARG:HB3	1.97	0.46
1:B:512:LYS:HG2	1:B:515:GLN:HE22	1.80	0.46
1:A:319:VAL:HG12	1:A:590:MET:HE3	1.97	0.46
1:B:241:ARG:NH2	1:B:245:SER:OG	2.48	0.46
1:B:457:CYS:O	1:B:461:HIS:HD2	1.97	0.46
1:B:515:GLN:HA	1:B:518:MET:CG	2.46	0.46
1:A:362:GLU:OE2	1:A:362:GLU:HA	2.15	0.46
1:A:502:VAL:O	1:A:505:VAL:HG22	2.16	0.46
1:B:253:ARG:O	1:B:254:ILE:C	2.58	0.46
4:B:1605:BTB:C1	4:B:1605:BTB:H52	2.44	0.46
1:A:324:TRP:CE2	1:A:572:MET:HG2	2.51	0.46
1:A:374:TRP:CZ3	1:A:417:ARG:HG3	2.50	0.46
1:B:82:GLU:O	1:B:85:HIS:HB2	2.16	0.46
1:B:212:THR:O	1:B:213:THR:C	2.59	0.46
1:A:313:PHE:HB3	1:A:358:TYR:CD1	2.51	0.46
1:A:201:TYR:HD2	1:A:202:GLU:HG2	1.81	0.46
1:A:290:GLN:O	1:A:291:PHE:C	2.56	0.46
1:A:585:ILE:O	1:A:585:ILE:HG23	2.14	0.46
1:B:83:ASP:C	1:B:85:HIS:H	2.24	0.46
1:A:276:VAL:O	1:A:279:LEU:N	2.49	0.46
1:A:432:ARG:O	1:A:433:TRP:C	2.58	0.46
1:A:488:SER:HB2	1:A:562:ALA:O	2.16	0.46
1:A:543:MET:O	1:A:543:MET:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:O	1:B:123:ASP:N	2.49	0.46
1:B:294:GLU:HA	1:B:339:ILE:HD12	1.97	0.46
1:B:518:MET:O	1:B:519:SER:C	2.53	0.46
1:B:556:LYS:HE3	5:B:790:HOH:O	2.15	0.46
1:A:85:HIS:O	1:A:88:ARG:HB3	2.14	0.46
1:A:207:LEU:CD2	1:A:207:LEU:N	2.77	0.46
1:A:259:ALA:O	1:A:260:PRO:C	2.55	0.46
1:A:301:TRP:CD2	1:A:343:LYS:HB3	2.51	0.46
1:A:369:ASP:OD2	1:A:373:ARG:NH1	2.49	0.46
1:A:501:SER:OG	1:A:512:LYS:HG3	2.16	0.46
1:B:85:HIS:O	1:B:282:LEU:HD21	2.16	0.46
1:B:176:PHE:CD2	1:B:200:LEU:HD12	2.51	0.46
1:B:200:LEU:O	1:B:201:TYR:C	2.57	0.46
1:A:259:ALA:C	1:A:263:ILE:HG12	2.40	0.46
1:A:418:GLN:O	1:A:419:SER:C	2.58	0.46
1:B:255:LYS:H	1:B:255:LYS:HG2	1.19	0.46
1:A:471:THR:O	1:A:475:VAL:HG23	2.15	0.46
1:B:442:LEU:HD13	1:B:517:TYR:CA	2.46	0.46
1:A:63:TYR:CG	1:A:315:ARG:HB3	2.51	0.45
1:A:83:ASP:O	1:A:85:HIS:N	2.49	0.45
1:A:93:VAL:CG2	1:A:124:HIS:HB3	2.46	0.45
1:A:103:GLU:OE1	1:A:104:THR:N	2.34	0.45
1:A:145:ASN:ND2	1:A:145:ASN:C	2.73	0.45
1:A:149:LYS:HA	1:A:152:ARG:NH2	2.31	0.45
1:A:150:GLU:C	1:A:152:ARG:N	2.70	0.45
1:B:181:ASN:N	1:B:185:GLU:O	2.47	0.45
1:B:205:PHE:CZ	1:B:249:PRO:HG3	2.51	0.45
1:B:304:ASN:O	1:B:305:THR:C	2.59	0.45
1:B:439:LYS:HD2	1:B:439:LYS:HA	1.66	0.45
1:B:517:TYR:C	1:B:517:TYR:CD2	2.95	0.45
1:B:518:MET:HG2	1:B:518:MET:H	1.56	0.45
1:A:70:VAL:C	1:A:72:PHE:N	2.74	0.45
1:A:145:ASN:HA	1:A:172:ALA:CB	2.46	0.45
1:B:269:ARG:HG2	1:B:271:ASP:OD2	2.16	0.45
1:B:415:TYR:OH	1:B:472:LYS:HD2	2.15	0.45
1:A:166:GLU:C	1:A:168:GLY:N	2.72	0.45
1:A:193:ASP:OD2	1:A:193:ASP:C	2.59	0.45
1:A:258:ASN:O	1:A:259:ALA:C	2.55	0.45
1:A:443:GLU:O	1:A:444:GLU:C	2.56	0.45
1:A:547:ARG:C	1:A:549:SER:N	2.73	0.45
1:B:383:PRO:HD2	1:B:386:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:O	1:A:311:LEU:HD23	2.16	0.45
1:A:315:ARG:HB2	1:A:317:ARG:NE	2.10	0.45
1:A:421:VAL:O	1:A:422:ASP:C	2.58	0.45
1:A:481:TYR:HD1	1:A:481:TYR:HA	1.50	0.45
1:B:547:ARG:CA	1:B:559:ILE:HD13	2.47	0.45
1:A:229:VAL:HA	1:A:239:LEU:HD21	1.98	0.45
1:A:416:LEU:HD22	1:A:461:HIS:CE1	2.52	0.45
1:A:442:LEU:HD23	1:A:517:TYR:HA	1.99	0.45
1:B:488:SER:O	1:B:489:SER:C	2.58	0.45
1:A:379:ILE:CD1	1:A:387:GLN:HG2	2.47	0.45
1:B:94:THR:O	1:B:98:MET:HB2	2.16	0.45
1:B:302:TRP:O	1:B:305:THR:OG1	2.34	0.45
1:A:69:ASP:OD2	1:A:72:PHE:N	2.49	0.45
1:A:457:CYS:O	1:A:461:HIS:HD2	2.00	0.45
1:A:482:HIS:CG	1:A:554:PHE:HE2	2.35	0.45
1:B:188:GLU:C	1:B:190:LEU:N	2.74	0.45
1:B:329:ILE:HD13	1:B:337:ALA:CB	2.47	0.45
1:B:491:VAL:O	1:B:492:LEU:C	2.57	0.45
1:A:211:GLU:OE2	1:A:214:LEU:HD23	2.17	0.45
1:A:501:SER:CA	1:A:512:LYS:HG3	2.40	0.45
1:B:84:LYS:HD2	1:B:85:HIS:N	2.31	0.45
1:B:248:ILE:O	1:B:253:ARG:NH1	2.49	0.45
1:B:346:ALA:O	1:B:347:LEU:C	2.58	0.45
1:B:377:ASN:C	1:B:379:ILE:N	2.75	0.45
1:B:432:ARG:O	1:B:436:GLY:N	2.46	0.45
1:B:470:PHE:CD2	1:B:470:PHE:N	2.83	0.45
1:B:477:SER:O	1:B:480:LYS:HG2	2.16	0.45
1:A:539:VAL:O	1:A:540:TRP:C	2.57	0.45
1:A:582:GLN:C	1:A:583:HIS:ND1	2.75	0.45
1:B:415:TYR:CZ	1:B:475:VAL:HG11	2.52	0.45
1:A:478:LEU:HA	1:A:482:HIS:HB2	1.99	0.45
1:A:496:ASP:HB2	1:A:573:TYR:CE2	2.52	0.45
1:A:520:ASP:C	1:A:522:ASN:H	2.25	0.45
1:A:559:ILE:HD12	1:A:563:VAL:HG23	1.98	0.45
1:B:154:LEU:HD11	1:B:200:LEU:HD13	1.99	0.45
1:B:192:ASP:O	1:B:193:ASP:C	2.59	0.45
1:B:281:ILE:HG23	1:B:598:PHE:HB3	1.99	0.45
1:B:425:ASP:O	1:B:429:VAL:HG22	2.17	0.45
1:A:411:ASN:OD1	1:A:413:ILE:HG23	2.17	0.44
1:B:179:PHE:HB3	1:B:190:LEU:HD11	1.99	0.44
1:B:291:PHE:O	1:B:292:GLN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:CG1	1:A:156:SER:HB2	2.47	0.44
1:A:145:ASN:HA	1:A:172:ALA:HB2	1.99	0.44
1:A:332:ARG:HG2	1:A:333:GLN:N	2.32	0.44
1:A:344:VAL:HG22	1:A:396:PHE:CZ	2.51	0.44
1:A:510:VAL:HG23	1:A:511:PRO:N	2.33	0.44
1:A:534:TRP:CE3	1:A:535:LEU:HD13	2.52	0.44
1:B:155:TYR:CD1	1:B:199:GLN:HG2	2.52	0.44
1:A:60:SER:O	1:A:62:ASN:N	2.50	0.44
1:A:72:PHE:C	1:A:72:PHE:CD2	2.95	0.44
1:A:145:ASN:N	1:A:146:PRO:CD	2.79	0.44
1:A:152:ARG:HH11	1:A:152:ARG:CG	2.28	0.44
1:A:301:TRP:HZ3	1:A:346:ALA:CB	2.30	0.44
1:A:323:PHE:CE1	1:A:326:THR:HG21	2.52	0.44
1:A:496:ASP:HA	1:A:573:TYR:CD2	2.52	0.44
1:B:146:PRO:HB2	1:B:147:PHE:H	1.51	0.44
1:B:218:ARG:NH1	1:B:218:ARG:CG	2.67	0.44
1:B:229:VAL:HG23	1:B:242:ILE:HG21	2.00	0.44
1:B:294:GLU:HB3	1:B:339:ILE:HD13	1.99	0.44
1:B:411:ASN:ND2	1:B:413:ILE:H	2.15	0.44
1:A:63:TYR:CE1	1:A:315:ARG:HD2	2.52	0.44
1:A:208:THR:C	1:A:541:LYS:HD2	2.42	0.44
1:A:227:GLU:O	1:A:231:GLU:HG3	2.17	0.44
1:A:367:PHE:O	1:A:368:THR:C	2.61	0.44
1:A:442:LEU:HD12	1:A:446:LEU:CG	2.47	0.44
1:B:88:ARG:O	1:B:89:ALA:C	2.60	0.44
1:B:238:LEU:HD23	1:B:239:LEU:HD12	2.00	0.44
1:A:442:LEU:HD12	1:A:446:LEU:CD1	2.48	0.44
1:A:532:VAL:O	1:A:536:ILE:HG13	2.17	0.44
1:B:137:TYR:CZ	1:B:143:TYR:HB3	2.53	0.44
1:B:222:THR:HG23	1:B:226:GLU:OE2	2.18	0.44
1:B:264:GLU:H	1:B:264:GLU:HG3	1.54	0.44
1:A:138:LEU:C	1:A:140:HIS:H	2.25	0.44
1:B:139:ASP:O	1:B:141:HIS:N	2.51	0.44
1:B:141:HIS:O	1:B:143:TYR:N	2.51	0.44
1:B:158:SER:HB2	1:B:199:GLN:HB3	2.00	0.44
1:B:311:LEU:HD11	1:B:385:TYR:O	2.18	0.44
1:B:329:ILE:HD13	1:B:337:ALA:HB1	2.00	0.44
1:B:570:GLN:O	1:B:574:HIS:HB2	2.16	0.44
1:A:83:ASP:O	1:A:87:ILE:HG12	2.18	0.44
1:A:152:ARG:HB2	1:A:157:THR:OG1	2.18	0.44
1:A:301:TRP:O	1:A:305:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD21	1:A:375:ASP:O	2.17	0.44
1:A:402:TYR:CE1	1:B:392:ALA:HB2	2.53	0.44
1:B:397:VAL:O	1:B:401:SER:HB2	2.18	0.44
1:B:449:SER:OG	1:B:493:ARG:HG2	2.18	0.44
1:A:87:ILE:O	1:A:88:ARG:C	2.58	0.44
1:B:416:LEU:HD22	1:B:461:HIS:ND1	2.32	0.44
1:B:484:LEU:HB2	1:B:546:GLU:HG2	2.00	0.44
1:A:98:MET:O	1:A:102:LYS:N	2.49	0.43
1:A:165:ARG:HB3	1:A:206:LEU:HD23	1.99	0.43
1:B:63:TYR:CE1	1:B:315:ARG:HD2	2.52	0.43
1:B:128:GLU:C	1:B:132:ILE:HD12	2.42	0.43
1:B:288:GLN:O	1:B:291:PHE:HB2	2.18	0.43
1:B:340:MET:O	1:B:344:VAL:HG23	2.17	0.43
1:A:266:TYR:HE2	1:A:277:LEU:HB2	1.83	0.43
1:B:238:LEU:C	1:B:240:THR:N	2.75	0.43
1:B:447:GLU:O	1:B:447:GLU:HG3	2.18	0.43
1:B:458:MET:HE2	1:B:565:LEU:HD22	1.99	0.43
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.80	0.43
1:A:187:LYS:HB3	1:A:190:LEU:HG	2.01	0.43
1:A:200:LEU:O	1:A:201:TYR:C	2.59	0.43
1:A:344:VAL:O	1:A:345:ASN:C	2.60	0.43
1:A:518:MET:HE3	1:A:525:GLU:CA	2.48	0.43
1:B:103:GLU:CD	1:B:108:ARG:NH1	2.76	0.43
1:B:588:GLN:HA	1:B:591:THR:CG2	2.48	0.43
1:A:586:ILE:O	1:A:590:MET:HB2	2.18	0.43
1:B:453:ILE:HG23	1:B:492:LEU:HD23	1.99	0.43
1:A:76:LEU:HD21	1:A:595:PHE:CE1	2.53	0.43
1:A:311:LEU:N	1:A:312:PRO:CD	2.82	0.43
1:B:86:VAL:HA	1:B:89:ALA:HB3	2.00	0.43
1:B:310:LYS:O	1:B:312:PRO:HD3	2.18	0.43
1:B:469:SER:C	1:B:470:PHE:CD2	2.96	0.43
1:A:377:ASN:C	1:A:379:ILE:N	2.77	0.43
1:A:454:SER:O	1:A:455:GLY:C	2.62	0.43
1:A:472:LYS:NZ	1:A:476:ASP:OD2	2.50	0.43
1:A:513:SER:O	1:A:514:LEU:C	2.58	0.43
1:A:577:ASP:O	1:A:578:GLY:O	2.37	0.43
1:A:579:HIS:O	1:A:579:HIS:CG	2.71	0.43
1:B:115:ASP:C	1:B:117:GLN:N	2.74	0.43
1:B:423:LEU:HD22	1:B:423:LEU:O	2.19	0.43
1:A:70:VAL:C	1:A:72:PHE:H	2.27	0.43
1:A:147:PHE:CE2	1:A:149:LYS:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLY:O	1:A:240:THR:HG23	2.19	0.43
1:A:418:GLN:HG2	1:A:422:ASP:OD1	2.18	0.43
1:A:431:ALA:O	1:A:434:PHE:N	2.52	0.43
1:A:487:TRP:NE1	1:A:542:LYS:HD3	2.33	0.43
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.44	0.43
1:B:86:VAL:CA	1:B:286:ILE:HD13	2.46	0.43
1:B:89:ALA:CA	1:B:282:LEU:HD23	2.49	0.43
1:B:97:LYS:O	1:B:98:MET:C	2.60	0.43
1:B:145:ASN:ND2	1:B:145:ASN:N	2.60	0.43
1:B:307:PHE:O	1:B:311:LEU:C	2.61	0.43
1:B:500:THR:HG22	1:B:501:SER:N	2.32	0.43
1:A:173:GLN:HE21	1:A:213:THR:CB	2.31	0.43
1:B:176:PHE:HA	1:B:179:PHE:HE2	1.83	0.43
1:B:242:ILE:CG2	1:B:243:ALA:N	2.72	0.43
1:A:317:ARG:HD2	1:A:579:HIS:CE1	2.54	0.43
1:B:86:VAL:O	1:B:89:ALA:HB3	2.19	0.43
1:B:86:VAL:O	1:B:90:SER:N	2.41	0.43
1:B:162:ARG:NH1	1:B:250:LEU:HD23	2.33	0.43
1:A:144:LYS:CG	1:A:146:PRO:HG2	2.49	0.43
1:A:207:LEU:H	1:A:207:LEU:HD23	1.83	0.43
1:A:266:TYR:O	1:A:272:MET:HG3	2.19	0.43
1:A:283:ASP:OD2	1:A:332:ARG:NH2	2.52	0.43
1:A:393:LEU:HD21	1:A:420:TRP:CD2	2.54	0.43
1:B:266:TYR:CE2	1:B:272:MET:HE2	2.54	0.43
4:B:1605:BTB:H61	4:B:1605:BTB:O4	2.19	0.43
1:A:205:PHE:HD1	1:A:252:TRP:CZ2	2.37	0.42
1:A:544:ASN:ND2	1:A:547:ARG:HH11	2.17	0.42
1:B:126:GLN:C	1:B:128:GLU:H	2.27	0.42
1:B:128:GLU:O	1:B:129:PHE:C	2.60	0.42
1:B:396:PHE:O	1:B:397:VAL:C	2.56	0.42
1:B:462:ILE:O	1:B:463:PHE:C	2.60	0.42
1:A:79:ASP:N	1:A:79:ASP:OD2	2.52	0.42
1:A:273:ASN:OD1	1:A:275:VAL:N	2.51	0.42
1:A:575:ASN:OD1	1:A:575:ASN:N	2.51	0.42
1:B:272:MET:HE2	1:B:272:MET:HB2	1.73	0.42
1:B:344:VAL:HG22	1:B:396:PHE:CZ	2.54	0.42
1:A:225:LEU:HD22	1:A:242:ILE:HG23	2.01	0.42
1:A:404:VAL:HG12	1:A:410:VAL:HG23	1.99	0.42
1:A:424:ALA:O	1:A:425:ASP:C	2.62	0.42
1:A:449:SER:O	1:A:451:GLN:N	2.52	0.42
1:B:69:ASP:OD1	1:B:72:PHE:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ASP:O	1:B:372:ARG:N	2.52	0.42
1:B:484:LEU:HD11	1:B:562:ALA:CB	2.49	0.42
1:B:543:MET:O	1:B:544:ASN:C	2.58	0.42
1:A:152:ARG:NH2	1:A:178:SER:HB3	2.34	0.42
1:A:482:HIS:CG	1:A:554:PHE:CE2	3.07	0.42
1:A:493:ARG:HD3	1:A:497:ASP:HB2	2.00	0.42
1:A:568:MET:O	1:A:572:MET:HB2	2.18	0.42
1:B:241:ARG:NH2	1:B:245:SER:CB	2.82	0.42
1:B:454:SER:O	1:B:457:CYS:N	2.53	0.42
1:B:548:VAL:O	1:B:548:VAL:CG1	2.67	0.42
1:A:415:TYR:O	1:A:416:LEU:C	2.59	0.42
1:A:470:PHE:CD1	1:A:470:PHE:N	2.85	0.42
1:B:339:ILE:O	1:B:340:MET:C	2.61	0.42
1:B:549:SER:OG	1:B:550:LYS:N	2.52	0.42
1:B:586:ILE:HG22	1:B:590:MET:HE2	2.01	0.42
1:A:118:ARG:NH1	1:A:255:LYS:HE3	2.35	0.42
1:A:200:LEU:C	1:A:202:GLU:N	2.73	0.42
1:A:231:GLU:OE2	1:A:233:GLY:HA2	2.19	0.42
1:A:152:ARG:NH1	1:A:175:VAL:O	2.52	0.42
1:A:287:VAL:O	1:A:288:GLN:C	2.63	0.42
1:A:449:SER:HA	1:A:493:ARG:HH12	1.85	0.42
1:A:561:CYS:O	1:A:562:ALA:C	2.61	0.42
1:A:589:GLN:H	1:A:589:GLN:HG2	1.50	0.42
1:B:70:VAL:HG22	1:B:71:ASN:N	2.34	0.42
1:B:255:LYS:HZ3	1:B:255:LYS:HB3	1.84	0.42
1:B:324:TRP:C	1:B:326:THR:H	2.26	0.42
1:B:413:ILE:HG12	1:B:414:PRO:HD3	2.02	0.42
1:B:551:ASP:C	1:B:552:SER:O	2.62	0.42
1:A:79:ASP:C	1:A:81:LYS:N	2.75	0.42
1:A:144:LYS:CE	1:A:146:PRO:HG2	2.50	0.42
1:A:260:PRO:O	1:A:263:ILE:N	2.52	0.42
1:A:360:THR:O	1:A:364:LEU:HB2	2.19	0.42
1:B:350:VAL:O	1:B:353:ASP:N	2.53	0.42
1:B:586:ILE:HA	1:B:589:GLN:HE21	1.85	0.42
1:A:173:GLN:HE21	1:A:213:THR:HB	1.85	0.42
1:A:341:MET:HE1	1:A:458:MET:HB2	2.00	0.42
1:A:425:ASP:O	1:A:428:MET:HB3	2.20	0.42
1:B:301:TRP:CZ2	1:B:347:LEU:HD21	2.51	0.42
1:B:510:VAL:CG1	1:B:511:PRO:HD2	2.45	0.42
1:A:83:ASP:C	1:A:85:HIS:N	2.77	0.42
1:A:165:ARG:NH2	1:A:211:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:C	1:A:192:ASP:H	2.28	0.42
1:A:458:MET:O	1:A:462:ILE:HG13	2.19	0.42
1:B:65:PRO:O	1:B:66:SER:C	2.63	0.42
1:B:103:GLU:OE1	1:B:103:GLU:CA	2.68	0.42
1:B:349:THR:OG1	3:B:1600:F3P:H11	2.20	0.42
4:B:1604:BTB:H52	4:B:1604:BTB:H81	1.67	0.42
1:A:433:TRP:CZ3	1:A:440:PRO:HG3	2.55	0.41
1:A:449:SER:C	1:A:451:GLN:H	2.27	0.41
1:B:70:VAL:C	1:B:72:PHE:N	2.76	0.41
1:B:424:ALA:O	1:B:427:TYR:HB2	2.20	0.41
1:B:429:VAL:HG21	1:B:448:ASN:HD21	1.85	0.41
1:A:279:LEU:HD12	1:A:279:LEU:C	2.46	0.41
1:B:487:TRP:O	1:B:488:SER:C	2.60	0.41
1:A:70:VAL:HA	1:A:299:PHE:CE1	2.56	0.41
1:A:112:LEU:HD13	1:A:116:LEU:HG	2.02	0.41
1:A:423:LEU:HD11	1:A:427:TYR:CE2	2.55	0.41
1:B:226:GLU:O	1:B:227:GLU:C	2.62	0.41
1:B:294:GLU:HG2	1:B:339:ILE:CD1	2.50	0.41
1:B:484:LEU:HD11	1:B:562:ALA:HB3	2.03	0.41
1:B:571:LEU:C	1:B:571:LEU:CD2	2.86	0.41
1:A:92:LEU:O	1:A:93:VAL:C	2.63	0.41
1:A:180:LYS:HZ1	1:A:213:THR:HG23	1.84	0.41
1:A:316:ASP:C	1:A:317:ARG:HG2	2.44	0.41
4:A:605:BTB:H42	4:A:605:BTB:C6	2.50	0.41
1:B:68:TRP:HZ3	1:B:320:GLU:OE2	2.03	0.41
1:B:374:TRP:HE1	1:B:394:ASN:HD22	1.68	0.41
1:B:469:SER:C	1:B:470:PHE:HD2	2.28	0.41
1:B:580:GLY:O	1:B:581:THR:HB	2.20	0.41
1:B:595:PHE:O	1:B:597:PRO:HD3	2.19	0.41
1:A:201:TYR:O	1:A:204:SER:OG	2.39	0.41
1:A:253:ARG:NH1	1:A:253:ARG:HG3	2.35	0.41
1:A:311:LEU:HG	1:A:313:PHE:CE2	2.56	0.41
1:A:329:ILE:HD11	1:A:462:ILE:HD13	2.03	0.41
1:A:351:ILE:O	1:A:355:TYR:HD2	2.01	0.41
1:A:433:TRP:CD1	1:A:438:HIS:CD2	3.08	0.41
1:A:518:MET:HG3	1:A:518:MET:H	1.68	0.41
1:B:585:ILE:O	1:B:586:ILE:C	2.63	0.41
1:A:93:VAL:O	1:A:97:LYS:HB2	2.20	0.41
1:A:238:LEU:O	1:A:240:THR:N	2.54	0.41
1:A:241:ARG:HH21	1:A:245:SER:HB2	1.84	0.41
1:A:424:ALA:O	1:A:427:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASP:C	1:B:141:HIS:N	2.75	0.41
1:B:219:GLU:O	1:B:220:PHE:C	2.63	0.41
1:B:235:ASP:HB3	1:B:236:GLY:H	1.62	0.41
1:B:373:ARG:HB2	1:B:373:ARG:CZ	2.51	0.41
1:B:383:PRO:O	1:B:384:ASP:C	2.62	0.41
1:B:586:ILE:CA	1:B:589:GLN:HG3	2.49	0.41
1:A:89:ALA:CA	1:A:282:LEU:HD23	2.51	0.41
1:A:93:VAL:HG22	1:A:97:LYS:HD2	2.01	0.41
1:A:189:SER:C	1:A:191:SER:N	2.78	0.41
1:A:413:ILE:N	1:A:414:PRO:CD	2.84	0.41
1:A:428:MET:HE3	1:A:431:ALA:HB3	2.03	0.41
1:A:442:LEU:HD23	1:A:517:TYR:CA	2.51	0.41
1:A:442:LEU:HD23	1:A:517:TYR:N	2.36	0.41
1:B:126:GLN:C	1:B:128:GLU:N	2.78	0.41
1:B:220:PHE:CZ	1:B:224:PHE:HE2	2.39	0.41
1:B:228:LYS:HG3	1:B:234:VAL:HG11	2.02	0.41
1:B:449:SER:C	1:B:451:GLN:N	2.77	0.41
1:B:508:GLY:O	1:B:509:ASP:HB2	2.19	0.41
1:A:110:LEU:HD11	1:A:160:ALA:HB2	2.02	0.41
1:A:116:LEU:HD22	1:A:121:LEU:HD23	2.03	0.41
1:A:123:ASP:OD2	1:A:332:ARG:NH1	2.48	0.41
1:A:123:ASP:HB2	1:A:332:ARG:NH1	2.35	0.41
1:A:214:LEU:HD12	1:A:214:LEU:HA	1.71	0.41
1:A:233:GLY:HA3	1:A:239:LEU:HD23	2.03	0.41
1:B:177:ASP:O	1:B:179:PHE:N	2.54	0.41
1:B:200:LEU:HD23	1:B:221:ALA:HB2	2.01	0.41
1:B:205:PHE:CE2	1:B:249:PRO:HG3	2.56	0.41
1:B:465:ARG:HA	1:B:465:ARG:HD2	1.62	0.41
1:A:117:GLN:HE21	1:A:129:PHE:HE1	1.67	0.41
1:A:162:ARG:HD3	1:A:202:GLU:O	2.21	0.41
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.84	0.41
1:A:504:GLU:C	1:A:509:ASP:HB2	2.42	0.41
1:A:507:ARG:NH1	1:A:508:GLY:O	2.54	0.41
1:A:546:GLU:OE1	1:A:550:LYS:HD2	2.21	0.41
1:B:113:ILE:HG23	1:B:129:PHE:CE1	2.56	0.41
1:B:176:PHE:HA	1:B:179:PHE:CD2	2.56	0.41
1:B:188:GLU:OE2	1:B:189:SER:N	2.52	0.41
1:B:228:LYS:HD3	1:B:228:LYS:HA	1.62	0.41
1:B:341:MET:CE	1:B:458:MET:HG2	2.51	0.41
1:B:395:ASN:O	1:B:399:ASP:N	2.51	0.41
1:B:423:LEU:HD22	1:B:423:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ILE:O	1:B:454:SER:CB	2.69	0.41
1:B:493:ARG:O	1:B:496:ASP:HB3	2.20	0.41
1:B:550:LYS:H	1:B:550:LYS:HG3	1.31	0.41
1:A:79:ASP:HA	1:A:81:LYS:HD2	2.03	0.41
1:A:155:TYR:CA	1:A:196:GLY:HA2	2.51	0.41
1:A:201:TYR:HB2	1:A:221:ALA:HB3	2.00	0.41
1:A:251:HIS:O	1:A:567:ARG:NE	2.45	0.41
1:A:274:PRO:O	1:A:276:VAL:N	2.54	0.41
1:A:487:TRP:O	1:A:488:SER:C	2.62	0.41
1:B:309:GLU:CG	1:B:310:LYS:HG2	2.50	0.41
1:B:317:ARG:HG3	1:B:580:GLY:HA3	2.03	0.41
1:A:128:GLU:C	1:A:130:LYS:N	2.78	0.40
4:A:604:BTB:H11	4:A:604:BTB:H71	1.86	0.40
1:B:323:PHE:HE1	1:B:326:THR:HG21	1.86	0.40
1:B:361:LEU:O	1:B:365:GLU:HG2	2.21	0.40
1:A:205:PHE:HE1	1:A:252:TRP:CH2	2.39	0.40
1:A:269:ARG:HG3	1:A:270:PRO:CD	2.51	0.40
1:A:314:ALA:HB1	1:A:350:VAL:HG22	2.04	0.40
1:A:435:TYR:HD2	1:A:435:TYR:HA	1.76	0.40
1:B:81:LYS:HG2	1:B:81:LYS:H	1.56	0.40
1:B:175:VAL:C	1:B:177:ASP:N	2.78	0.40
1:B:455:GLY:O	1:B:458:MET:HB2	2.21	0.40
1:A:70:VAL:O	1:A:74:GLN:N	2.54	0.40
1:A:79:ASP:CA	1:A:81:LYS:HD2	2.52	0.40
1:A:525:GLU:O	1:A:526:ALA:C	2.65	0.40
1:B:145:ASN:N	1:B:146:PRO:CD	2.84	0.40
1:B:147:PHE:N	1:B:148:PRO:HD2	2.36	0.40
1:B:313:PHE:CE1	1:B:354:ILE:HG13	2.57	0.40
1:B:360:THR:OG1	1:B:363:GLU:HB2	2.21	0.40
1:B:411:ASN:HD22	1:B:413:ILE:H	1.69	0.40
1:B:413:ILE:N	1:B:414:PRO:CD	2.84	0.40
1:B:555:GLY:O	1:B:556:LYS:C	2.64	0.40
1:A:81:LYS:CD	1:A:81:LYS:N	2.84	0.40
1:A:108:ARG:O	1:A:109:GLN:C	2.63	0.40
1:A:270:PRO:C	1:A:272:MET:N	2.79	0.40
1:A:311:LEU:HD21	1:A:350:VAL:HG11	2.03	0.40
1:A:425:ASP:O	1:A:428:MET:N	2.55	0.40
1:A:430:GLU:HG2	1:A:510:VAL:HG11	2.03	0.40
1:A:549:SER:OG	1:A:550:LYS:N	2.53	0.40
1:A:579:HIS:ND1	1:A:579:HIS:C	2.79	0.40
1:A:589:GLN:HE21	1:A:589:GLN:HB3	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:VAL:O	1:B:277:LEU:C	2.64	0.40
1:B:396:PHE:CD2	1:B:396:PHE:C	2.97	0.40
1:B:456:PRO:O	1:B:457:CYS:C	2.63	0.40
1:A:134:SER:O	1:A:137:TYR:HB3	2.21	0.40
1:A:173:GLN:HE22	1:A:212:THR:N	2.18	0.40
1:A:229:VAL:HA	1:A:239:LEU:HD22	2.04	0.40
1:A:482:HIS:ND1	1:A:482:HIS:C	2.78	0.40
1:B:260:PRO:O	1:B:261:VAL:C	2.62	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	541/543 (100%)	400 (74%)	93 (17%)	48 (9%)	0	0
1	B	541/543 (100%)	409 (76%)	86 (16%)	46 (8%)	0	1
All	All	1082/1086 (100%)	809 (75%)	179 (16%)	94 (9%)	0	0

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	78	SER
1	A	83	ASP
1	A	125	PHE
1	A	152	ARG
1	A	191	SER
1	A	235	ASP
1	A	272	MET
1	A	357	VAL
1	A	358	TYR

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Mol	Chain	Res	Type
1	A	381	GLN
1	A	500	THR
1	A	520	ASP
1	A	578	GLY
1	A	584	PRO
1	B	76	LEU
1	B	83	ASP
1	B	146	PRO
1	B	147	PHE
1	B	150	GLU
1	B	210	GLY
1	B	211	GLU
1	B	235	ASP
1	B	313	PHE
1	B	437	GLY
1	B	502	VAL
1	B	577	ASP
1	B	579	HIS
1	B	581	THR
1	B	584	PRO
1	A	61	GLY
1	A	71	ASN
1	A	122	SER
1	A	174	GLU
1	A	178	SER
1	A	255	LYS
1	A	270	PRO
1	A	312	PRO
1	A	432	ARG
1	A	481	TYR
1	A	509	ASP
1	A	549	SER
1	B	77	LEU
1	B	122	SER
1	B	142	TYR
1	B	178	SER
1	B	271	ASP
1	B	272	MET
1	B	312	PRO
1	B	357	VAL
1	B	438	HIS
1	B	455	GLY

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Mol	Chain	Res	Type
1	B	500	THR
1	B	549	SER
1	B	578	GLY
1	A	79	ASP
1	A	332	ARG
1	A	359	GLY
1	A	450	TRP
1	B	140	HIS
1	B	148	PRO
1	B	174	GLU
1	B	191	SER
1	B	193	ASP
1	B	481	TYR
1	A	70	VAL
1	A	84	LYS
1	A	135	SER
1	A	236	GLY
1	B	139	ASP
1	B	208	THR
1	B	270	PRO
1	B	374	TRP
1	B	454	SER
1	B	501	SER
1	A	140	HIS
1	A	167	HIS
1	A	239	LEU
1	A	274	PRO
1	A	308	VAL
1	A	449	SER
1	A	581	THR
1	A	583	HIS
1	B	151	GLU
1	B	149	LYS
1	B	376	ILE
1	A	148	PRO
1	A	233	GLY
1	A	234	VAL
1	A	276	VAL
1	B	232	GLY
1	B	508	GLY
1	B	260	PRO
1	A	260	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	490/492 (100%)	331 (68%)	159 (32%)	0	1
1	B	490/492 (100%)	323 (66%)	167 (34%)	0	0
All	All	980/984 (100%)	654 (67%)	326 (33%)	0	1

All (326) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	MET
1	A	58	ARG
1	A	59	ARG
1	A	64	ASN
1	A	67	ARG
1	A	69	ASP
1	A	70	VAL
1	A	72	PHE
1	A	74	GLN
1	A	76	LEU
1	A	77	LEU
1	A	78	SER
1	A	79	ASP
1	A	81	LYS
1	A	83	ASP
1	A	84	LYS
1	A	86	VAL
1	A	88	ARG
1	A	92	LEU
1	A	97	LYS
1	A	98	MET
1	A	100	LEU
1	A	101	GLU
1	A	102	LYS
1	A	107	ILE
1	A	108	ARG
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	121	LEU
1	A	122	SER
1	A	126	GLN
1	A	131	GLU
1	A	134	SER
1	A	143	TYR
1	A	144	LYS
1	A	145	ASN
1	A	147	PHE
1	A	152	ARG
1	A	156	SER
1	A	159	LEU
1	A	165	ARG
1	A	173	GLN
1	A	174	GLU
1	A	175	VAL
1	A	186	PHE
1	A	187	LYS
1	A	188	GLU
1	A	189	SER
1	A	191	SER
1	A	195	ARG
1	A	198	LEU
1	A	200	LEU
1	A	201	TYR
1	A	204	SER
1	A	206	LEU
1	A	214	LEU
1	A	215	GLU
1	A	218	ARG
1	A	223	LYS
1	A	226	GLU
1	A	227	GLU
1	A	228	LYS
1	A	231	GLU
1	A	239	LEU
1	A	241	ARG
1	A	242	ILE
1	A	255	LYS
1	A	256	ARG
1	A	261	VAL
1	A	264	GLU

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Mol	Chain	Res	Type
1	A	269	ARG
1	A	271	ASP
1	A	273	ASN
1	A	278	GLU
1	A	279	LEU
1	A	287	VAL
1	A	294	GLU
1	A	295	LEU
1	A	300	ARG
1	A	308	VAL
1	A	309	GLU
1	A	310	LYS
1	A	311	LEU
1	A	313	PHE
1	A	315	ARG
1	A	316	ASP
1	A	317	ARG
1	A	318	LEU
1	A	321	CYS
1	A	326	THR
1	A	332	ARG
1	A	333	GLN
1	A	339	ILE
1	A	343	LYS
1	A	360	THR
1	A	361	LEU
1	A	364	LEU
1	A	365	GLU
1	A	371	ILE
1	A	372	ARG
1	A	373	ARG
1	A	379	ILE
1	A	382	LEU
1	A	391	LEU
1	A	393	LEU
1	A	394	ASN
1	A	397	VAL
1	A	399	ASP
1	A	400	THR
1	A	405	MET
1	A	412	VAL
1	A	413	ILE

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Mol	Chain	Res	Type
1	A	417	ARG
1	A	426	LYS
1	A	427	TYR
1	A	429	VAL
1	A	430	GLU
1	A	435	TYR
1	A	442	LEU
1	A	443	GLU
1	A	448	ASN
1	A	459	LEU
1	A	462	ILE
1	A	465	ARG
1	A	469	SER
1	A	470	PHE
1	A	471	THR
1	A	473	GLU
1	A	488	SER
1	A	492	LEU
1	A	493	ARG
1	A	497	ASP
1	A	500	THR
1	A	506	SER
1	A	507	ARG
1	A	509	ASP
1	A	510	VAL
1	A	514	LEU
1	A	515	GLN
1	A	518	MET
1	A	519	SER
1	A	522	ASN
1	A	535	LEU
1	A	538	GLU
1	A	539	VAL
1	A	544	ASN
1	A	548	VAL
1	A	550	LYS
1	A	552	SER
1	A	556	LYS
1	A	559	ILE
1	A	571	LEU
1	A	572	MET
1	A	581	THR

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Mol	Chain	Res	Type
1	A	583	HIS
1	A	585	ILE
1	A	588	GLN
1	A	589	GLN
1	A	590	MET
1	A	593	THR
1	B	57	MET
1	B	58	ARG
1	B	59	ARG
1	B	64	ASN
1	B	66	SER
1	B	69	ASP
1	B	70	VAL
1	B	72	PHE
1	B	73	ILE
1	B	75	SER
1	B	76	LEU
1	B	77	LEU
1	B	81	LYS
1	B	83	ASP
1	B	84	LYS
1	B	88	ARG
1	B	92	LEU
1	B	94	THR
1	B	95	LEU
1	B	97	LYS
1	B	99	GLU
1	B	103	GLU
1	B	107	ILE
1	B	112	LEU
1	B	118	ARG
1	B	119	MET
1	B	122	SER
1	B	123	ASP
1	B	124	HIS
1	B	127	ASN
1	B	131	GLU
1	B	145	ASN
1	B	147	PHE
1	B	149	LYS
1	B	150	GLU
1	B	152	ARG

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Mol	Chain	Res	Type
1	B	159	LEU
1	B	163	LEU
1	B	165	ARG
1	B	174	GLU
1	B	178	SER
1	B	182	GLU
1	B	185	GLU
1	B	188	GLU
1	B	189	SER
1	B	192	ASP
1	B	197	LEU
1	B	199	GLN
1	B	200	LEU
1	B	202	GLU
1	B	206	LEU
1	B	207	LEU
1	B	208	THR
1	B	209	GLU
1	B	211	GLU
1	B	215	GLU
1	B	216	SER
1	B	218	ARG
1	B	219	GLU
1	B	222	THR
1	B	223	LYS
1	B	225	LEU
1	B	226	GLU
1	B	227	GLU
1	B	228	LYS
1	B	229	VAL
1	B	231	GLU
1	B	234	VAL
1	B	237	ASP
1	B	238	LEU
1	B	240	THR
1	B	241	ARG
1	B	242	ILE
1	B	245	SER
1	B	250	LEU
1	B	253	ARG
1	B	254	ILE
1	B	255	LYS

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Mol	Chain	Res	Type
1	B	261	VAL
1	B	263	ILE
1	B	264	GLU
1	B	267	ARG
1	B	272	MET
1	B	275	VAL
1	B	276	VAL
1	B	278	GLU
1	B	293	GLU
1	B	305	THR
1	B	308	VAL
1	B	309	GLU
1	B	310	LYS
1	B	311	LEU
1	B	315	ARG
1	B	319	VAL
1	B	321	CYS
1	B	326	THR
1	B	332	ARG
1	B	336	SER
1	B	349	THR
1	B	357	VAL
1	B	361	LEU
1	B	362	GLU
1	B	371	ILE
1	B	376	ILE
1	B	378	SER
1	B	381	GLN
1	B	382	LEU
1	B	393	LEU
1	B	394	ASN
1	B	397	VAL
1	B	406	LYS
1	B	407	GLU
1	B	408	LYS
1	B	412	VAL
1	B	413	ILE
1	B	417	ARG
1	B	419	SER
1	B	423	LEU
1	B	426	LYS
1	B	429	VAL

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Mol	Chain	Res	Type
1	B	439	LYS
1	B	444	GLU
1	B	446	LEU
1	B	449	SER
1	B	451	GLN
1	B	453	ILE
1	B	454	SER
1	B	459	LEU
1	B	465	ARG
1	B	468	ASP
1	B	469	SER
1	B	470	PHE
1	B	471	THR
1	B	474	THR
1	B	475	VAL
1	B	477	SER
1	B	480	LYS
1	B	486	ARG
1	B	498	LEU
1	B	503	GLU
1	B	506	SER
1	B	510	VAL
1	B	513	SER
1	B	514	LEU
1	B	515	GLN
1	B	518	MET
1	B	529	ARG
1	B	530	LYS
1	B	536	ILE
1	B	539	VAL
1	B	547	ARG
1	B	548	VAL
1	B	550	LYS
1	B	551	ASP
1	B	552	SER
1	B	556	LYS
1	B	559	ILE
1	B	563	VAL
1	B	565	LEU
1	B	570	GLN
1	B	571	LEU
1	B	585	ILE

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Mol	Chain	Res	Type
1	B	587	HIS
1	B	588	GLN
1	B	589	GLN
1	B	592	ARG
1	B	593	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	117	GLN
1	A	145	ASN
1	A	173	GLN
1	A	258	ASN
1	A	288	GLN
1	A	290	GLN
1	A	333	GLN
1	A	345	ASN
1	A	418	GLN
1	A	461	HIS
1	A	544	ASN
1	A	587	HIS
1	B	106	GLN
1	B	145	ASN
1	B	345	ASN
1	B	381	GLN
1	B	395	ASN
1	B	411	ASN
1	B	448	ASN
1	B	451	GLN
1	B	461	HIS
1	B	482	HIS
1	B	515	GLN
1	B	544	ASN
1	B	574	HIS
1	B	575	ASN
1	B	579	HIS
1	B	588	GLN
1	B	589	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	BTB	B	1604	-	13,13,13	4.55	6 (46%)	7,16,16	1.13	1 (14%)
3	F3P	B	1600	2	14,19,19	2.49	4 (28%)	20,29,29	2.05	2 (10%)
3	F3P	A	600	2	14,19,19	2.54	5 (35%)	20,29,29	1.67	3 (15%)
4	BTB	A	604	-	13,13,13	2.01	4 (30%)	7,16,16	0.57	0
4	BTB	B	1605	-	13,13,13	4.32	6 (46%)	7,16,16	1.08	1 (14%)
4	BTB	A	605	-	13,13,13	4.54	6 (46%)	7,16,16	1.18	1 (14%)

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
4	BTB	B	1604	-	-	11/21/21/21	-
3	F3P	B	1600	2	-	3/17/25/25	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	F3P	A	600	2	-	4/17/25/25	-
4	BTB	A	604	-	-	2/21/21/21	-
4	BTB	B	1605	-	-	8/21/21/21	-
4	BTB	A	605	-	-	12/21/21/21	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	BTB	C2-N	11.69	1.71	1.48
4	B	1605	BTB	C2-N	10.65	1.69	1.48
4	B	1604	BTB	C2-N	10.43	1.68	1.48
4	B	1604	BTB	C5-N	7.93	1.59	1.48
4	A	605	BTB	C5-N	7.78	1.59	1.48
3	A	600	F3P	C6-C7	7.08	1.53	1.32
3	B	1600	F3P	C6-C7	7.05	1.53	1.32
4	B	1605	BTB	C5-N	6.47	1.57	1.48
4	B	1604	BTB	C7-N	6.15	1.56	1.48
4	B	1604	BTB	C4-C2	5.78	1.60	1.53
4	B	1605	BTB	C7-N	5.51	1.55	1.48
4	A	605	BTB	C4-C2	5.11	1.59	1.53
4	A	604	BTB	C2-N	4.79	1.57	1.48
4	B	1605	BTB	C4-C2	4.67	1.58	1.53
4	B	1605	BTB	C1-C2	4.60	1.58	1.53
4	A	605	BTB	C1-C2	4.30	1.58	1.53
4	A	605	BTB	C7-N	3.98	1.53	1.48
4	B	1604	BTB	C1-C2	3.45	1.57	1.53
4	A	604	BTB	C5-N	3.29	1.52	1.48
4	B	1605	BTB	C3-C2	3.11	1.57	1.53
4	B	1604	BTB	C3-C2	3.09	1.56	1.53
3	B	1600	F3P	PA-O1A	2.98	1.61	1.50
3	A	600	F3P	PA-O1A	2.91	1.60	1.50
3	B	1600	F3P	C9-C7	-2.63	1.43	1.50
3	A	600	F3P	C9-C7	-2.59	1.43	1.50
4	A	604	BTB	C1-C2	2.53	1.56	1.53
3	A	600	F3P	C8-C7	-2.52	1.43	1.50
3	B	1600	F3P	C8-C7	-2.52	1.43	1.50
4	A	604	BTB	C3-C2	2.44	1.56	1.53
4	A	605	BTB	C3-C2	2.36	1.56	1.53
3	A	600	F3P	F-C2	-2.02	1.33	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1600	F3P	O1-C3-C10	-6.21	86.95	108.11
3	B	1600	F3P	C5-C6-C7	-4.78	111.69	127.64
3	A	600	F3P	C5-C6-C7	-4.57	112.42	127.64
3	A	600	F3P	C10-C3-C2	3.09	116.41	110.69
4	A	605	BTB	C6-C5-N	2.61	121.79	111.59
4	B	1605	BTB	C6-C5-N	2.47	121.24	111.59
3	A	600	F3P	PA-O1-C3	-2.08	123.80	128.03
4	B	1604	BTB	C6-C5-N	2.07	119.66	111.59

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	F3P	C2-C3-C4-C5
3	A	600	F3P	C10-C3-C4-C5
3	B	1600	F3P	C3-C4-C5-C6
4	A	605	BTB	O1-C1-C2-C4
4	A	605	BTB	O1-C1-C2-N
4	A	605	BTB	C4-C2-C3-O3
4	A	605	BTB	N-C2-C3-O3
4	A	605	BTB	C1-C2-C4-O4
4	A	605	BTB	N-C2-C4-O4
4	A	605	BTB	C6-C5-N-C2
4	B	1604	BTB	O1-C1-C2-C4
4	B	1604	BTB	O1-C1-C2-N
4	B	1604	BTB	C4-C2-C3-O3
4	B	1604	BTB	N-C2-C3-O3
4	B	1604	BTB	C1-C2-C4-O4
4	B	1604	BTB	N-C2-C4-O4
4	B	1604	BTB	C6-C5-N-C2
4	B	1604	BTB	C8-C7-N-C5
4	B	1605	BTB	O1-C1-C2-C4
4	B	1605	BTB	O1-C1-C2-N
4	B	1605	BTB	C4-C2-C3-O3
4	B	1605	BTB	N-C2-C3-O3
4	B	1605	BTB	C1-C2-C4-O4
4	B	1605	BTB	N-C2-C4-O4
4	B	1605	BTB	C6-C5-N-C2
4	A	604	BTB	N-C5-C6-O6
4	B	1605	BTB	N-C7-C8-O8
4	A	605	BTB	N-C5-C6-O6
4	A	605	BTB	N-C7-C8-O8
4	B	1604	BTB	N-C7-C8-O8

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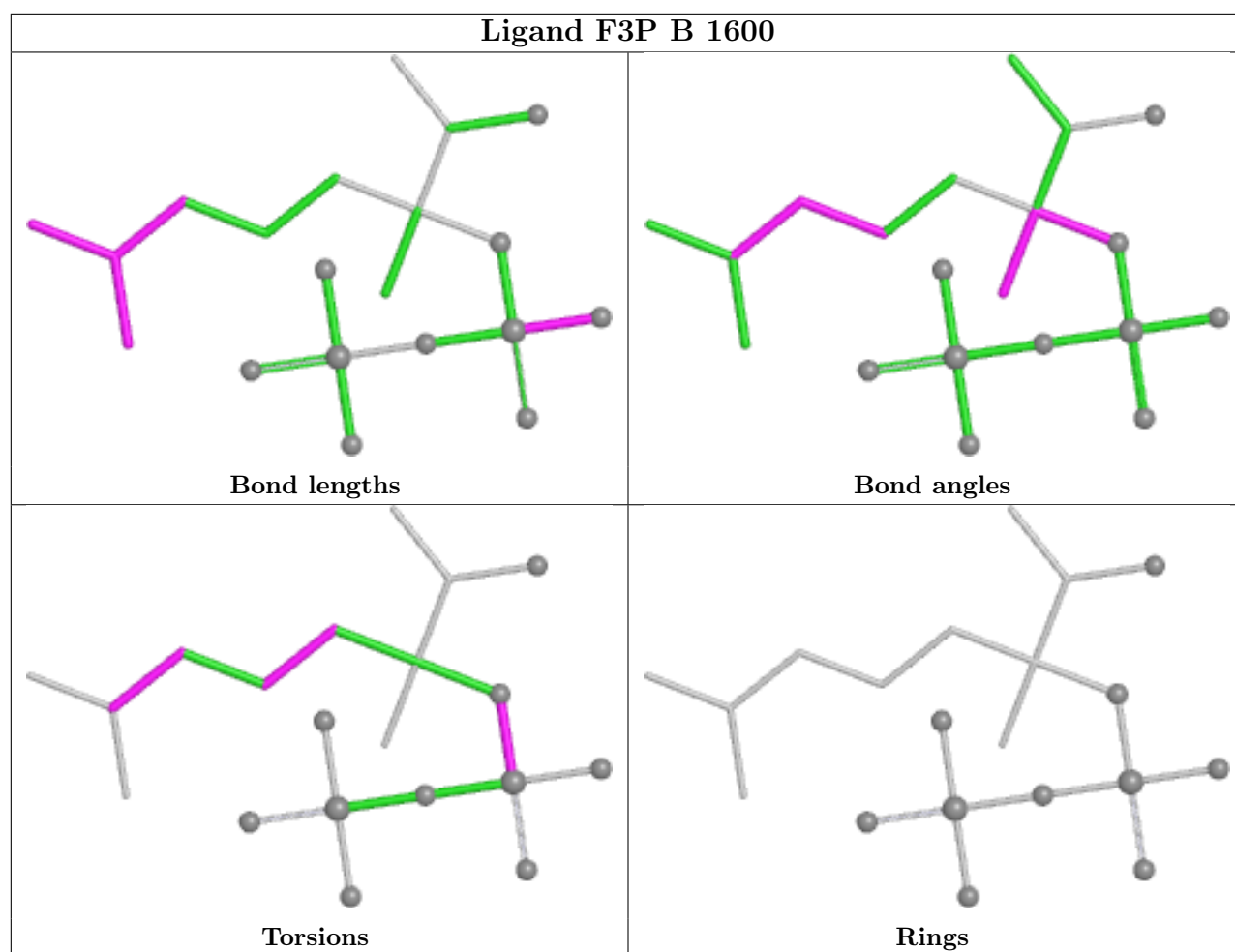
Mol	Chain	Res	Type	Atoms
4	A	604	BTB	C6-C5-N-C2
4	B	1604	BTB	C4-C2-N-C7
3	A	600	F3P	O1-C3-C4-C5
3	A	600	F3P	C5-C6-C7-C8
3	B	1600	F3P	C5-C6-C7-C8
3	B	1600	F3P	C3-O1-PA-O3A
4	A	605	BTB	C3-C2-N-C5
4	A	605	BTB	C3-C2-N-C7
4	A	605	BTB	C4-C2-N-C5
4	B	1604	BTB	C1-C2-N-C7

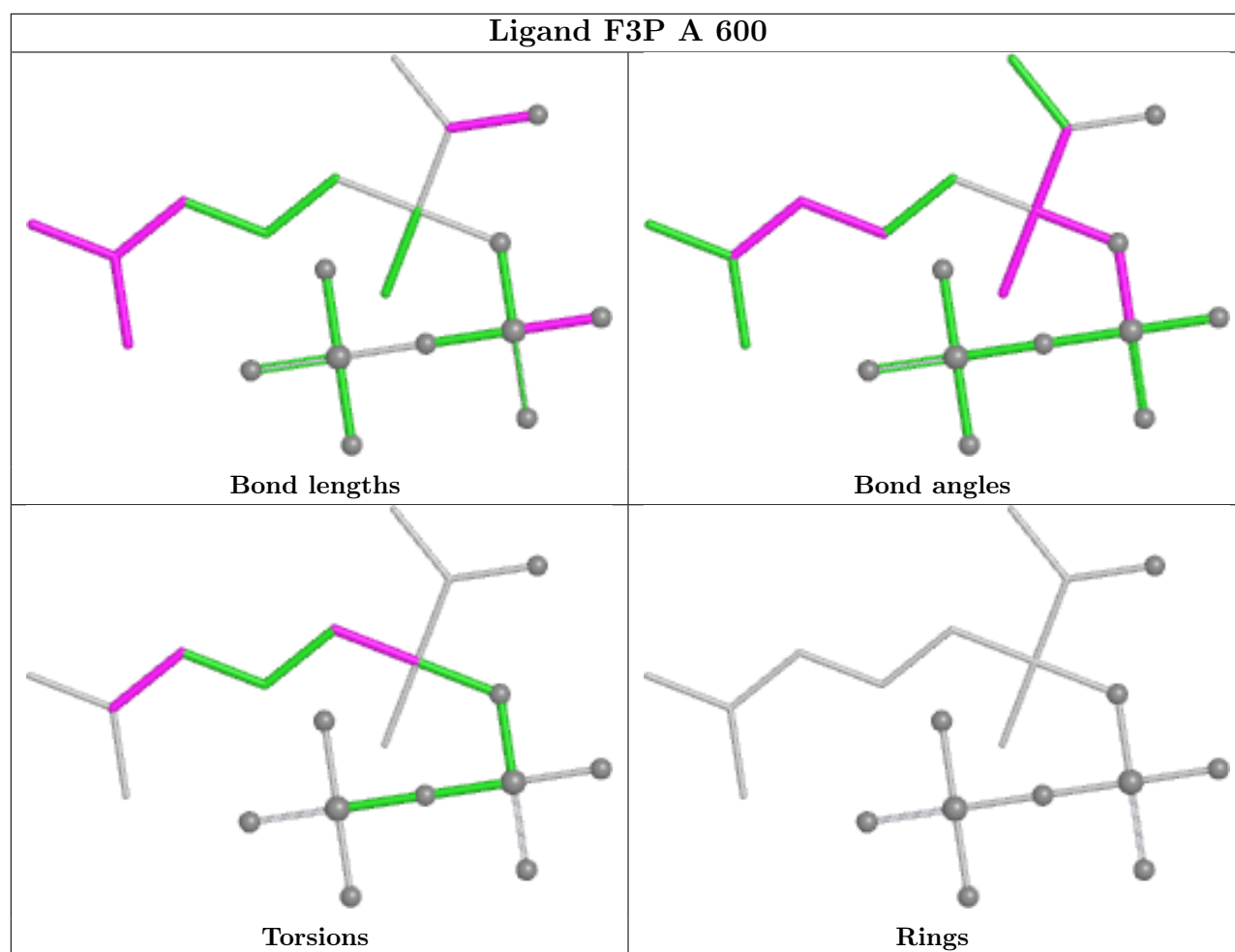
There are no ring outliers.

6 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1604	BTB	19	0
3	B	1600	F3P	13	0
3	A	600	F3P	9	0
4	A	604	BTB	3	0
4	B	1605	BTB	21	0
4	A	605	BTB	18	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/543 (100%)	-1.59	0 100 100	18, 46, 94, 100	0
1	B	543/543 (100%)	-1.59	0 100 100	16, 46, 96, 100	0
All	All	1086/1086 (100%)	-1.59	0 100 100	16, 46, 95, 100	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BTB	A	605	14/14	0.98	0.05	98,100,100,100	0
4	BTB	A	604	14/14	0.99	0.07	83,90,96,100	0
4	BTB	B	1604	14/14	0.99	0.05	67,89,100,100	0
4	BTB	B	1605	14/14	0.99	0.04	93,100,100,100	0
2	MN	B	1602	1/1	1.00	0.02	49,49,49,49	0
2	MN	B	1603	1/1	1.00	0.01	44,44,44,44	0
3	F3P	A	600	20/20	1.00	0.05	54,69,76,82	0

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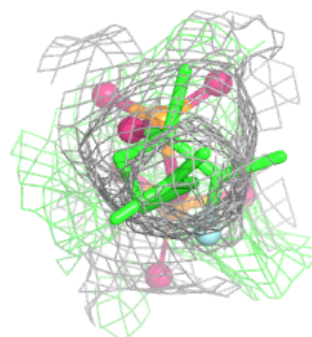
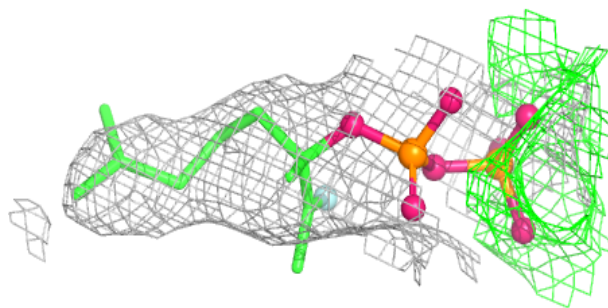
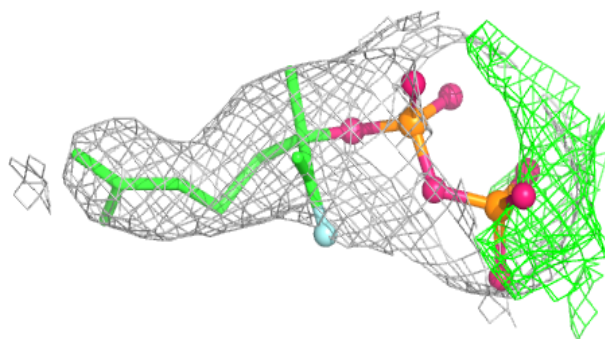
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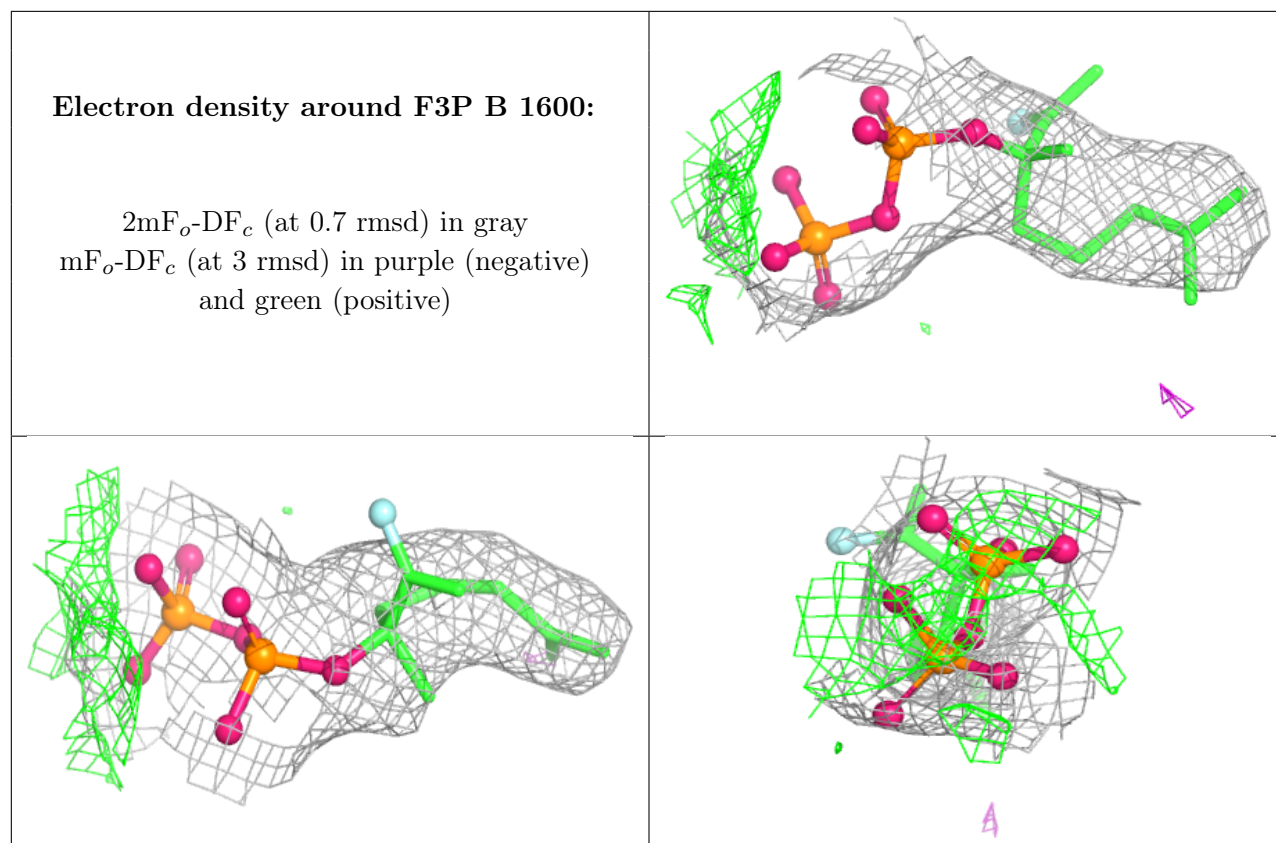
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	F3P	B	1600	20/20	1.00	0.04	44,71,100,100	0
2	MN	A	601	1/1	1.00	0.04	52,52,52,52	0
2	MN	A	602	1/1	1.00	0.03	41,41,41,41	0
2	MN	A	603	1/1	1.00	0.03	43,43,43,43	0
2	MN	B	1601	1/1	1.00	0.04	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F3P A 600:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.