Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:37 AM GMT

PDB ID	:	2RG0
Title	:	Crystal structure of cellobiohydrolase from Melanocarpus albomyces complexed with cellotetraose
Authors	:	Parkkinen, T.; Koivula, A.; Vehmaanper, J.; Rouvinen, J.
Deposited on	:	2007-10-02
Resolution	:	2.10 Å(reported)

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

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

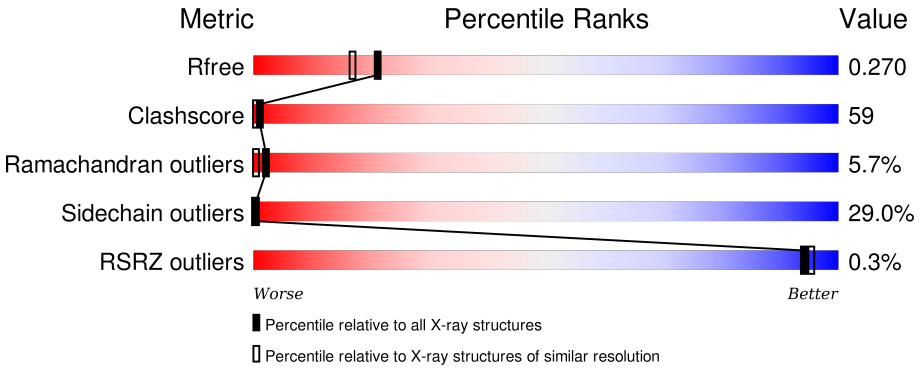
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	22% 55% 21%
1	B	430	21% 55% 22%
1	C	430	20% 59% 20%
1	D	430	23% 56% 19%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PCA	A	1	-	-	X	-
1	PCA	B	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13956 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.

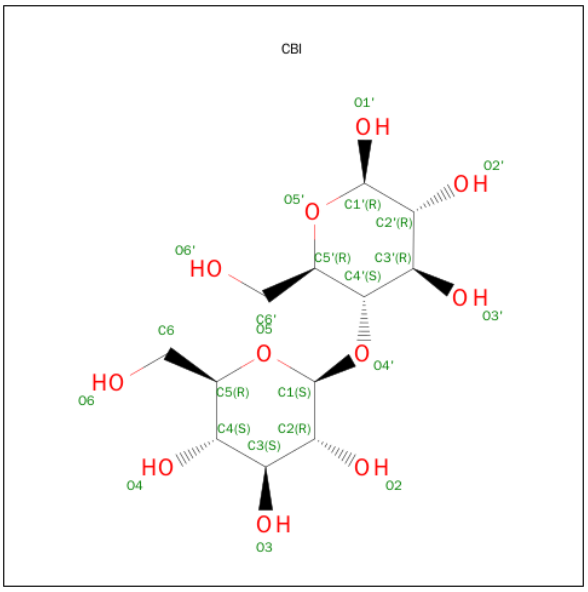
- Molecule 1 is a protein called Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	B	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	C	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	D	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			

There are 4 discrepancies between the modelled and reference sequences:

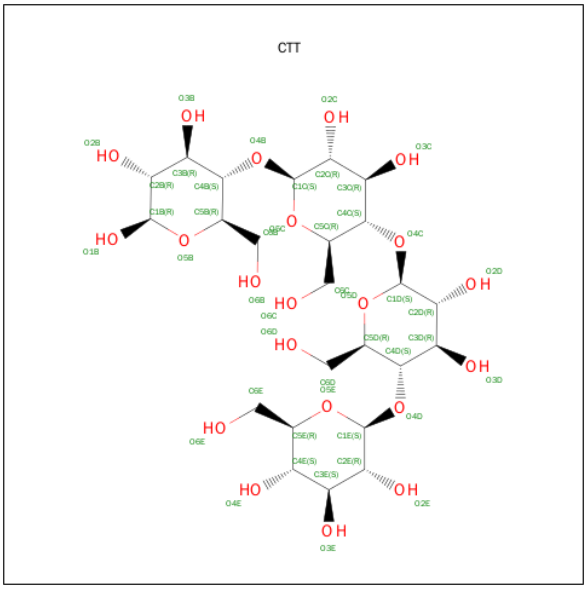
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
B	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
C	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
D	1	PCA	GLN	ENGINEERED	UNP Q8J0K6

- Molecule 2 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 12 11	0	0
2	A	1	Total C O 23 12 11	0	0
2	C	1	Total C O 23 12 11	0	0
2	D	1	Total C O 23 12 11	0	0
2	D	1	Total C O 23 12 11	0	0

- Molecule 3 is CELLOTETRAOSE (three-letter code: CTT) (formula: $C_{24}H_{42}O_{21}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			45	24	21		

- Molecule 4 is water.

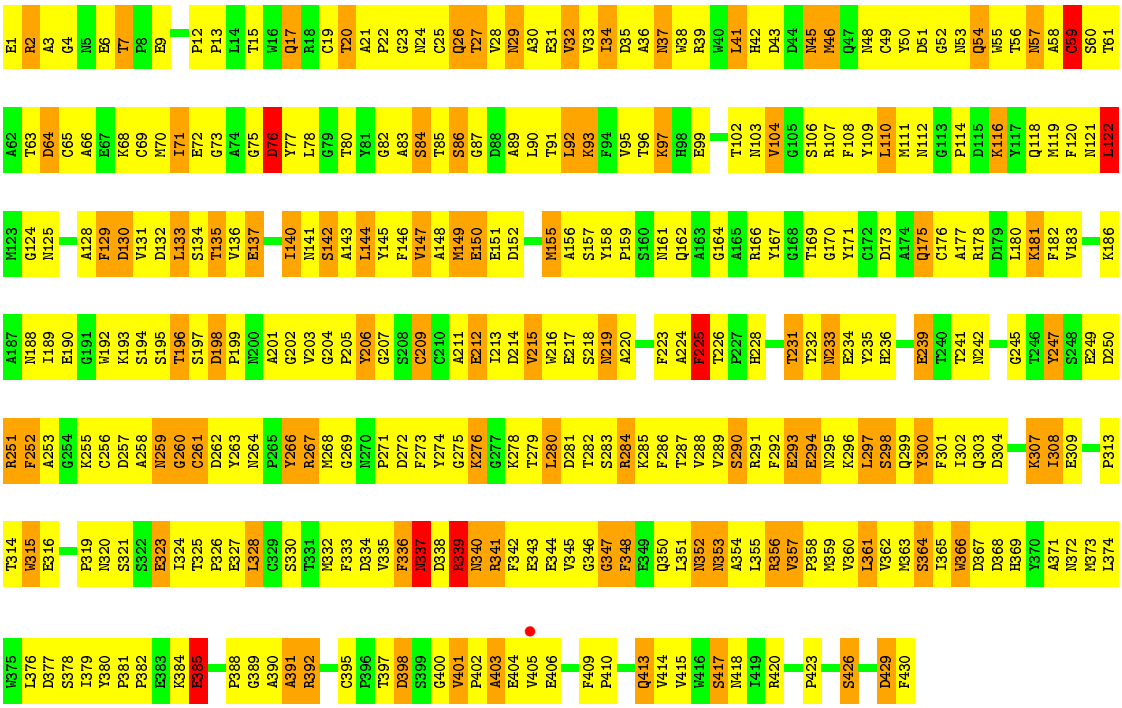
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	109	Total	O	0	0
			109	109		
4	C	122	Total	O	0	0
			122	122		
4	D	132	Total	O	0	0
			132	132		

3 Residue-property plots (i)

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

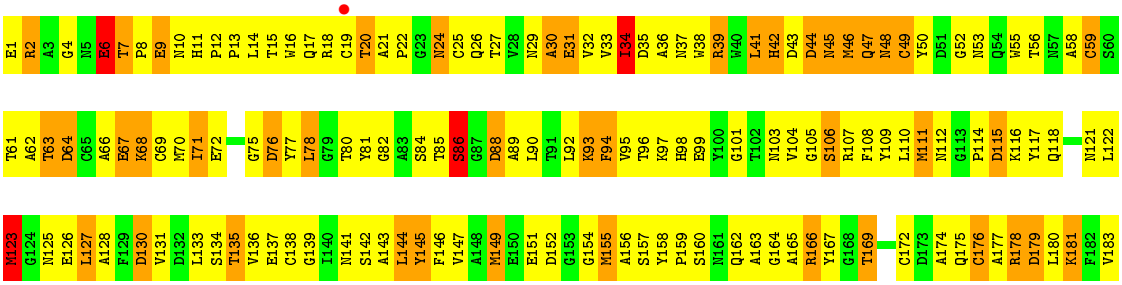
- Molecule 1: Cellulose 1,4-beta-cellobiosidase

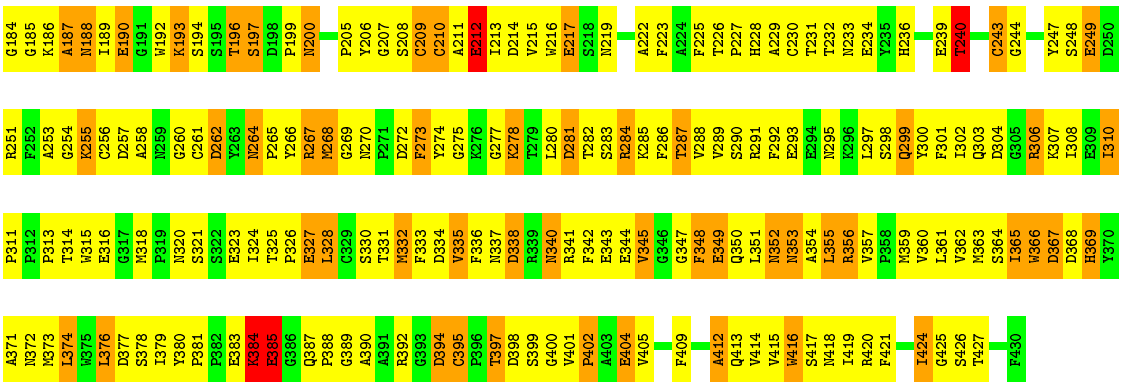
Chain A:



- Molecule 1: Cellulose 1,4-beta-cellobiosidase

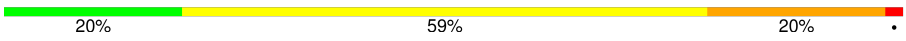
Chain B:

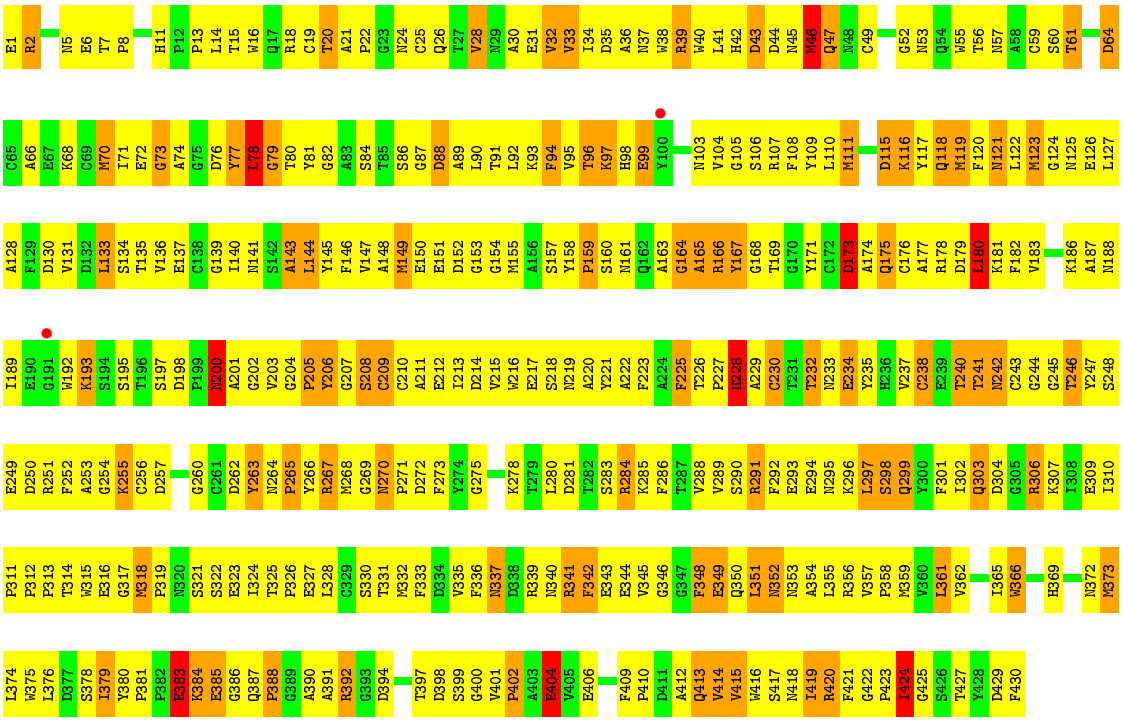




• Molecule 1: Cellulose 1,4-beta-cellobiosidase

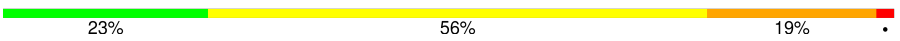
Chain C:

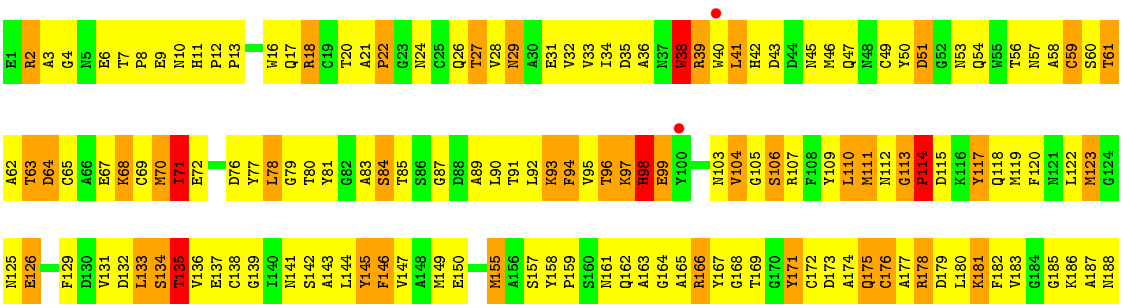


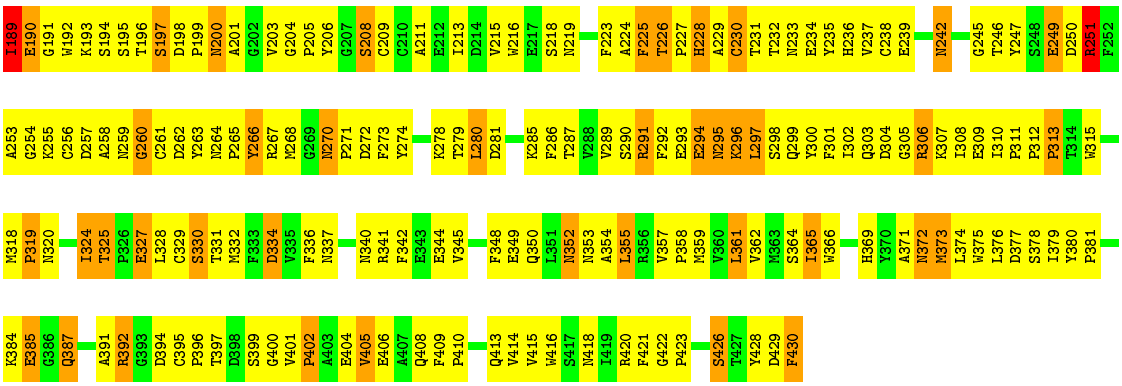


• Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain D:






I189 E190 G191 W192 K193 S194 S195 T196 S197 D198 P199 N200 A201 G202 V203 G204 P205 Y206 G207 S208 C209 C210 A211 E212 I213 D214 V215 W216 E217 S218 N219 F223 A224 F225 T226 P227 H228 A229 C230 T231 T232 N233 E234 Y235 H236 V237 C238 E239 N242 G245 T246 Y247 S248 E249 D250 R251 F252
A253 G254 K255 C256 D257 A258 N259 G260 C261 D262 Y263 N264 P265 Y266 R267 M268 G269 N270 P271 D272 F273 Y274 K278 T279 L280 D281 K285 F286 T287 V288 V289 S290 R291 F292 E293 E294 N295 K296 L297 S298 Q299 Y300 F301 I302 Q303 D304 G305 R306 K307 I308 E309 I310 P311 P312 P313 T314 W315
M318 P319 N320 I324 T325 P326 E327 L328 C329 S330 T331 M332 F333 D334 V335 F336 N337 N340 R341 F342 E343 E344 V345 F348 E349 Q350 L351 N352 N353 A354 L355 R356 V357 P358 M359 V360 L361 V362 M363 S364 I365 W366 H369 Y370 A371 N372 M373 L374 W375 L376 D377 S378 I379 Y380 P381
K384 E385 G386 Q387 A391 R392 G393 D394 C395 P396 T397 D398 S399 G400 V401 P402 A403 E404 V405 E406 A407 Q408 F409 P410 Q413 V414 V415 W416 S417 N418 I419 R420 F421 G422 P423 S426 Y427 Y428 D429 F430

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.98Å 94.81Å 190.43Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 24.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.10) 98.1 (24.62-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.211 , 0.282 0.211 , 0.270	Depositor DCC
R_{free} test set	5188 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	9.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 68.3	EDS
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 105275 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	13956	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTT, PCA, CBI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/3416	0.95	3/4648 (0.1%)
1	B	0.33	0/3416	0.98	5/4648 (0.1%)
1	C	0.32	0/3416	0.93	2/4648 (0.0%)
1	D	0.33	0/3416	0.99	6/4648 (0.1%)
All	All	0.33	0/13664	0.96	16/18592 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	251	ARG	CD-NE-CZ	8.88	136.04	123.60
1	B	366	TRP	C-N-CA	8.45	142.81	121.70
1	D	18	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	C	228	HIS	CA-CB-CG	6.30	124.31	113.60
1	B	42	HIS	C-N-CA	6.11	136.98	121.70
1	A	216	TRP	C-N-CA	5.87	136.38	121.70
1	A	339	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	D	26	GLN	C-N-CA	5.69	135.92	121.70
1	B	34	ILE	C-N-CA	5.47	135.37	121.70
1	A	225	PHE	CB-CG-CD2	5.33	124.53	120.80
1	B	39	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	C	143	ALA	C-N-CA	5.26	134.86	121.70
1	D	38	TRP	CA-CB-CG	5.23	123.64	113.70
1	D	189	ILE	C-N-CA	5.17	134.62	121.70
1	D	266	TYR	CB-CG-CD1	5.04	124.03	121.00
1	B	384	LYS	C-N-CA	5.02	134.26	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3028	376	0
1	B	3333	0	3027	401	0
1	C	3333	0	3028	399	0
1	D	3333	0	3028	360	0
2	A	46	0	44	11	0
2	C	23	0	22	3	0
2	D	46	0	44	11	0
3	B	45	0	42	9	0
4	A	101	0	0	12	0
4	B	109	0	0	11	0
4	C	122	0	0	12	0
4	D	132	0	0	12	0
All	All	13956	0	12263	1514	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 59.

All (1514) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HE3	1:D:6:GLU:HB3	1.39	1.04
1:B:37:ASN:HA	1:B:181:LYS:HE2	1.38	1.02
1:D:21:ALA:HB3	1:D:24:ASN:HD22	1.18	1.01
1:C:250:ASP:HB3	1:C:253:ALA:HB2	1.42	1.01
1:B:2:ARG:HA	1:B:162:GLN:HB2	1.40	0.99
1:A:296:LYS:HE3	1:A:323:GLU:HB3	1.44	0.98
1:B:32:VAL:HG11	1:B:90:LEU:HD22	1.46	0.97
1:A:297:LEU:HB2	1:A:324:ILE:HB	1.47	0.94
1:C:155:MET:HA	1:C:161:ASN:HB3	1.49	0.94
1:D:77:TYR:HB3	1:D:83:ALA:HB3	1.48	0.94
1:D:373:MET:HG3	1:D:376:LEU:HB3	1.49	0.94
1:C:39:ARG:HH22	1:C:74:ALA:HB2	1.31	0.93
1:B:111:MET:HA	1:B:118:GLN:H	1.36	0.91
1:C:267:ARG:HG3	1:C:392:ARG:HG3	1.51	0.88
1:B:230:CYS:HA	1:B:256:CYS:HA	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ASN:HB3	1:C:400:GLY:HA3	1.55	0.87
1:A:146:PHE:HB3	1:A:359:MET:HB3	1.55	0.86
1:D:291:ARG:HG3	1:D:298:SER:HB3	1.58	0.84
1:B:105:GLY:HA2	1:B:365:ILE:HG22	1.60	0.82
1:D:250:ASP:HB3	1:D:253:ALA:HB2	1.62	0.82
1:C:32:VAL:HG13	1:C:110:LEU:HD13	1.61	0.82
1:C:139:GLY:HA3	1:C:400:GLY:HA2	1.58	0.81
1:D:226:THR:HG23	1:D:262:ASP:HB3	1.61	0.81
1:D:297:LEU:HD11	1:D:355:LEU:HD11	1.62	0.81
1:D:408:GLN:HG3	1:D:409:PHE:HD1	1.46	0.81
1:D:135:THR:HB	1:D:413:GLN:H	1.45	0.81
1:D:110:LEU:HD12	1:D:111:MET:H	1.46	0.80
1:A:128:ALA:HB3	1:A:420:ARG:HB2	1.64	0.80
1:D:228:HIS:HB3	1:D:257:ASP:HB3	1.61	0.80
1:B:123:MET:HE1	1:B:356:ARG:HE	1.46	0.80
1:B:147:VAL:HG12	1:B:212:GLU:HB2	1.64	0.80
1:B:227:PRO:HG3	1:B:324:ILE:HG21	1.64	0.80
1:B:146:PHE:HB3	1:B:359:MET:HB3	1.62	0.79
1:B:42:HIS:HA	1:B:49:CYS:HB2	1.65	0.79
1:D:36:ALA:HA	1:D:39:ARG:HD2	1.64	0.78
1:D:129:PHE:HA	1:D:418:ASN:O	1.83	0.78
1:D:16:TRP:O	1:D:28:VAL:HB	1.83	0.78
1:A:342:PHE:HD2	1:A:343:GLU:HG3	1.48	0.78
1:D:396:PRO:O	1:D:399:SER:HB3	1.84	0.78
1:C:254:GLY:HA3	4:C:500:HOH:O	1.83	0.78
1:C:306:ARG:HH21	1:D:305:GLY:H	1.28	0.78
1:D:91:THR:O	1:D:92:LEU:HD23	1.84	0.77
1:D:227:PRO:HD2	1:D:261:CYS:O	1.83	0.77
1:A:2:ARG:HG3	1:A:69:CYS:O	1.84	0.77
1:A:137:GLU:O	1:A:140:ILE:HG13	1.84	0.77
1:B:177:ALA:HB3	1:B:208:SER:OG	1.85	0.77
1:B:178:ARG:HA	1:B:206:TYR:O	1.84	0.77
1:C:175:GLN:OE1	1:C:246:THR:HB	1.84	0.77
1:C:176:CYS:O	1:C:178:ARG:HG2	1.85	0.77
1:C:265:PRO:HA	1:C:270:ASN:HD22	1.49	0.77
1:B:146:PHE:HA	1:B:360:VAL:O	1.83	0.77
1:A:17:GLN:HB2	1:A:27:THR:HA	1.65	0.77
1:A:175:GLN:OE1	1:A:258:ALA:HB1	1.85	0.77
1:C:263:TYR:HA	1:C:268:MET:HE3	1.67	0.76
1:A:293:GLU:HG2	1:A:296:LYS:O	1.84	0.76
1:B:97:LYS:HD2	1:C:6:GLU:OE2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:HA	1:A:341:ARG:HD3	1.66	0.76
1:A:341:ARG:O	1:A:345:VAL:HG22	1.86	0.76
1:B:420:ARG:HB2	1:B:427:THR:HG22	1.68	0.76
1:C:36:ALA:HA	1:C:39:ARG:HG3	1.65	0.76
1:B:269:GLY:HA3	1:B:314:THR:OG1	1.84	0.76
1:A:104:VAL:HG23	2:A:432:CBI:O6	1.86	0.76
1:B:379:ILE:HA	1:B:390:ALA:O	1.85	0.76
1:D:95:VAL:HG22	1:D:104:VAL:HG13	1.68	0.76
1:D:295:ASN:H	1:D:352:ASN:ND2	1.84	0.76
1:C:41:LEU:HA	1:C:70:MET:O	1.86	0.76
1:B:126:GLU:HB2	1:B:290:SER:O	1.86	0.76
1:B:274:TYR:HA	1:B:280:LEU:HB3	1.67	0.76
1:D:96:THR:OG1	1:D:103:ASN:HB3	1.85	0.76
1:D:104:VAL:HG21	1:D:406:GLU:OE1	1.86	0.76
1:C:127:LEU:HD12	1:C:420:ARG:O	1.86	0.76
1:A:343:GLU:HA	1:A:347:GLY:H	1.50	0.75
1:A:34:ILE:HB	1:A:77:TYR:OH	1.86	0.75
1:B:147:VAL:O	1:B:360:VAL:HG23	1.86	0.75
1:A:267:ARG:HG3	1:A:392:ARG:HG3	1.67	0.75
1:D:125:ASN:HD22	1:D:423:PRO:HA	1.51	0.75
1:D:175:GLN:O	1:D:245:GLY:HA3	1.85	0.75
1:C:111:MET:HA	1:C:117:TYR:HA	1.69	0.75
1:C:41:LEU:HD23	1:C:70:MET:O	1.86	0.75
1:D:158:TYR:HB3	1:D:185:GLY:HA3	1.68	0.75
1:C:188:ASN:HB3	1:C:204:GLY:HA3	1.67	0.75
1:B:88:ASP:O	1:B:417:SER:HA	1.87	0.75
1:B:134:SER:HB3	4:B:510:HOH:O	1.86	0.75
1:B:292:PHE:HB3	1:B:355:LEU:HD11	1.68	0.74
1:C:226:THR:HG23	1:C:262:ASP:HB3	1.68	0.74
1:A:251:ARG:HH22	2:A:431:CBI:H2	1.52	0.74
1:A:276:LYS:HG3	1:A:283:SER:HB3	1.69	0.74
1:B:325:THR:OG1	1:B:328:LEU:HB2	1.88	0.74
1:B:41:LEU:HD23	1:B:71:ILE:HG23	1.69	0.74
1:C:379:ILE:HA	1:C:390:ALA:O	1.87	0.74
1:B:32:VAL:HA	1:B:109:TYR:O	1.88	0.74
1:B:268:MET:HA	1:B:315:TRP:NE1	2.03	0.74
1:C:206:TYR:HA	1:C:238:CYS:O	1.88	0.74
1:D:349:GLU:HA	1:D:352:ASN:OD1	1.88	0.73
1:A:89:ALA:HA	1:A:417:SER:HB3	1.70	0.73
1:A:356:ARG:HB2	1:A:356:ARG:HH11	1.53	0.73
1:A:107:ARG:HG3	1:A:364:SER:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:THR:HG23	1:D:29:ASN:HD21	1.53	0.73
1:B:229:ALA:O	1:B:345:VAL:HG21	1.88	0.73
1:D:120:PHE:O	1:D:358:PRO:HA	1.88	0.73
1:B:277:GLY:HA2	1:B:281:ASP:OD1	1.88	0.73
1:D:231:THR:OG1	1:D:255:LYS:HB3	1.88	0.73
1:D:354:ALA:O	1:D:357:VAL:HG23	1.88	0.73
1:D:264:ASN:HD21	1:D:266:TYR:HB3	1.52	0.73
1:D:92:LEU:HB2	1:D:414:VAL:HG12	1.71	0.73
1:A:17:GLN:OE1	1:A:420:ARG:HD3	1.89	0.73
1:D:211:ALA:HB2	1:D:233:ASN:HB3	1.69	0.73
1:D:122:LEU:O	1:D:292:PHE:HB2	1.89	0.73
1:A:110:LEU:HB3	1:A:118:GLN:HB3	1.71	0.73
1:B:240:THR:O	1:B:243:CYS:HB2	1.89	0.72
1:A:296:LYS:HA	1:A:324:ILE:O	1.88	0.72
1:A:296:LYS:HG3	1:A:325:THR:HG22	1.72	0.72
1:B:59:CYS:HB3	1:B:189:ILE:HD13	1.70	0.72
1:B:127:LEU:HD11	1:B:419:ILE:HG23	1.70	0.72
1:A:266:TYR:HB3	1:A:392:ARG:O	1.89	0.72
1:D:254:GLY:HA3	4:D:491:HOH:O	1.89	0.72
1:A:335:VAL:HG23	4:A:467:HOH:O	1.88	0.72
1:B:175:GLN:NE2	3:B:431:CTT:H4C	2.05	0.72
1:D:105:GLY:HA2	1:D:365:ILE:HG23	1.71	0.72
1:A:354:ALA:O	1:A:357:VAL:HG23	1.90	0.72
1:A:19:CYS:HB3	1:A:426:SER:O	1.89	0.72
1:B:117:TYR:O	1:B:151:GLU:HG3	1.90	0.72
1:A:38:TRP:HD1	1:A:103:ASN:HD21	1.38	0.72
1:B:53:ASN:O	1:B:194:SER:HB3	1.89	0.72
1:B:222:ALA:HB3	1:B:376:LEU:O	1.89	0.72
1:D:53:ASN:HA	1:D:200:ASN:O	1.89	0.72
1:C:84:SER:O	1:C:90:LEU:HD12	1.90	0.72
1:D:34:ILE:HG22	1:D:39:ARG:NH2	2.05	0.72
1:B:374:LEU:HD23	1:B:378:SER:HB3	1.70	0.71
1:D:39:ARG:HB3	1:D:71:ILE:HG22	1.71	0.71
1:D:41:LEU:HD13	1:D:49:CYS:HB2	1.71	0.71
1:A:149:MET:HE2	1:A:360:VAL:HG21	1.72	0.71
1:A:32:VAL:HG12	1:A:109:TYR:O	1.90	0.71
1:C:293:GLU:OE1	1:C:296:LYS:HE3	1.89	0.71
1:B:212:GLU:O	1:B:228:HIS:HB2	1.90	0.71
1:A:356:ARG:HD3	1:B:20:THR:HB	1.71	0.71
1:C:19:CYS:HA	1:C:25:CYS:HA	1.72	0.71
1:C:318:MET:HE2	1:C:332:MET:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:MET:HB2	1:B:116:LYS:O	1.89	0.71
1:A:292:PHE:HA	1:A:297:LEU:HD12	1.73	0.71
1:B:101:GLY:HA3	4:B:513:HOH:O	1.90	0.71
1:A:379:ILE:HG21	1:A:385:GLU:HB2	1.72	0.71
1:D:319:PRO:HD3	1:D:331:THR:OG1	1.91	0.71
1:D:401:VAL:HB	1:D:404:GLU:HB2	1.71	0.71
1:B:75:GLY:HA2	1:C:78:LEU:HD12	1.73	0.70
1:D:350:GLN:O	1:D:353:ASN:HB2	1.91	0.70
1:A:275:GLY:O	1:A:281:ASP:HA	1.90	0.70
1:D:189:ILE:HG23	1:D:190:GLU:H	1.56	0.70
1:D:39:ARG:HA	4:D:583:HOH:O	1.91	0.70
1:C:1:PCA:HA	1:C:66:ALA:O	1.91	0.70
1:A:295:ASN:H	1:A:352:ASN:HD21	1.37	0.70
1:D:177:ALA:O	1:D:180:LEU:HG	1.90	0.70
1:D:111:MET:HE1	1:D:114:PRO:HA	1.73	0.70
1:A:104:VAL:HG23	2:A:432:CBI:HO6	1.56	0.70
1:B:22:PRO:HD3	1:B:426:SER:HA	1.73	0.70
1:B:144:LEU:HD21	1:B:361:LEU:HG	1.74	0.70
1:A:59:CYS:HA	1:A:68:LYS:HD3	1.74	0.70
1:B:384:LYS:HD2	1:B:387:GLN:HB2	1.74	0.70
1:B:281:ASP:HB3	1:B:284:ARG:HG3	1.73	0.70
1:D:192:TRP:HA	1:D:203:VAL:O	1.91	0.70
1:C:149:MET:SD	1:C:171:TYR:HA	2.32	0.70
1:D:79:GLY:O	1:D:98:HIS:HB3	1.92	0.70
1:D:249:GLU:HG2	4:D:490:HOH:O	1.90	0.70
1:B:6:GLU:OE1	1:C:97:LYS:HG3	1.92	0.69
1:A:173:ASP:HB2	1:A:212:GLU:OE1	1.92	0.69
1:D:96:THR:HG23	1:D:103:ASN:O	1.91	0.69
1:A:49:CYS:HA	1:A:58:ALA:O	1.92	0.69
1:A:295:ASN:OD1	1:A:348:PHE:HB3	1.92	0.69
1:C:39:ARG:NH2	1:C:74:ALA:HB2	2.06	0.69
1:C:292:PHE:HB3	1:C:355:LEU:HD22	1.74	0.69
1:C:137:GLU:H	1:C:140:ILE:HD12	1.57	0.69
1:C:49:CYS:HA	1:C:56:THR:OG1	1.92	0.69
1:D:372:ASN:HB3	1:D:400:GLY:HA3	1.74	0.69
1:D:62:ALA:HA	1:D:187:ALA:HB3	1.74	0.69
1:D:239:GLU:H	1:D:242:ASN:ND2	1.91	0.69
1:B:372:ASN:HB2	1:B:374:LEU:HD12	1.75	0.69
1:B:156:ALA:O	1:B:159:PRO:HD3	1.93	0.69
1:C:141:ASN:O	1:C:365:ILE:HA	1.93	0.69
1:A:295:ASN:H	1:A:352:ASN:ND2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASN:HD22	2:A:432:CBI:H6'2	1.56	0.68
1:D:251:ARG:NH1	1:D:258:ALA:HB1	2.08	0.68
1:A:269:GLY:O	1:A:271:PRO:HD3	1.92	0.68
1:A:84:SER:O	1:A:90:LEU:HD12	1.93	0.68
1:A:319:PRO:HG3	1:A:327:GLU:HG3	1.75	0.68
1:C:32:VAL:HG12	1:C:109:TYR:O	1.93	0.68
1:B:34:ILE:HD13	1:B:35:ASP:H	1.59	0.68
1:D:163:ALA:HB1	1:D:167:TYR:HB2	1.75	0.68
1:C:345:VAL:O	1:C:350:GLN:HG2	1.94	0.68
1:B:110:LEU:O	1:B:118:GLN:HB3	1.94	0.68
1:B:111:MET:HA	1:B:118:GLN:N	2.09	0.68
1:C:150:GLU:OE2	1:C:157:SER:HB3	1.93	0.68
1:C:61:THR:OG1	1:C:64:ASP:HB3	1.92	0.68
1:C:143:ALA:HB2	1:C:217:GLU:HA	1.76	0.68
1:D:273:PHE:O	1:D:279:THR:HB	1.94	0.68
1:B:12:PRO:HB3	1:B:85:THR:HG21	1.76	0.68
1:B:267:ARG:HB3	1:B:268:MET:HE2	1.74	0.68
1:D:280:LEU:HD22	1:D:303:GLN:OE1	1.94	0.68
1:A:177:ALA:O	1:A:207:GLY:HA2	1.93	0.68
1:A:289:VAL:O	1:A:299:GLN:HA	1.94	0.68
1:C:373:MET:HA	1:C:375:TRP:NE1	2.08	0.67
1:C:31:GLU:O	1:C:111:MET:HB2	1.93	0.67
1:C:183:VAL:HG13	1:C:235:TYR:OH	1.95	0.67
1:C:148:ALA:HB2	1:C:359:MET:HG2	1.76	0.67
1:A:7:THR:HG21	1:A:73:GLY:O	1.95	0.67
1:A:132:ASP:HB3	1:A:415:VAL:HG22	1.76	0.67
1:D:267:ARG:HA	1:D:391:ALA:O	1.94	0.67
1:D:176:CYS:HA	1:D:208:SER:O	1.94	0.67
1:C:302:ILE:HA	1:C:306:ARG:O	1.95	0.67
1:B:372:ASN:O	1:B:400:GLY:HA3	1.93	0.67
1:A:224:ALA:HA	1:A:263:TYR:O	1.94	0.67
1:C:131:VAL:O	1:C:285:LYS:HA	1.94	0.67
1:C:37:ASN:HD21	1:C:180:LEU:HA	1.60	0.67
1:A:340:ASN:HD21	1:A:342:PHE:HB3	1.59	0.67
1:B:368:ASP:OD2	1:B:371:ALA:HB3	1.95	0.67
1:A:68:LYS:HG3	1:A:69:CYS:SG	2.35	0.67
1:B:155:MET:HG3	1:B:164:GLY:HA3	1.77	0.67
1:B:374:LEU:O	1:B:380:TYR:HB2	1.94	0.67
1:D:35:ASP:HB2	1:D:109:TYR:OH	1.96	0.66
1:B:36:ALA:HA	1:B:39:ARG:HG3	1.74	0.66
1:A:325:THR:OG1	1:A:327:GLU:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ILE:HD12	1:D:167:TYR:HB3	1.76	0.66
1:A:122:LEU:HG	1:A:359:MET:HG3	1.76	0.66
1:C:207:GLY:O	1:C:237:VAL:HG13	1.95	0.66
1:D:251:ARG:HH11	1:D:251:ARG:HG3	1.60	0.66
1:B:36:ALA:HB2	1:B:169:THR:HG22	1.77	0.66
1:A:83:ALA:HA	1:A:91:THR:O	1.96	0.66
1:D:401:VAL:O	1:D:405:VAL:HG22	1.95	0.66
1:A:196:THR:HG23	4:A:511:HOH:O	1.94	0.66
1:C:384:LYS:HE3	1:C:387:GLN:HE22	1.60	0.66
1:A:64:ASP:O	1:A:68:LYS:HG2	1.96	0.66
1:D:264:ASN:ND2	1:D:267:ARG:H	1.94	0.66
1:B:154:GLY:HA2	1:B:157:SER:OG	1.96	0.66
1:B:94:PHE:HA	1:B:365:ILE:HG21	1.77	0.66
1:D:268:MET:O	1:D:313:PRO:HA	1.96	0.66
1:D:149:MET:HG2	1:D:171:TYR:HA	1.77	0.66
1:C:173:ASP:HB2	1:C:212:GLU:OE1	1.96	0.66
1:B:401:VAL:HG12	1:B:404:GLU:HB2	1.78	0.66
1:B:376:LEU:HG	1:B:376:LEU:O	1.95	0.65
1:B:350:GLN:HA	1:B:353:ASN:OD1	1.95	0.65
1:D:166:ARG:HD2	1:D:167:TYR:HE2	1.61	0.65
1:C:380:TYR:HE2	2:C:431:CBI:HO2'	1.44	0.65
1:B:401:VAL:HG11	1:B:404:GLU:OE2	1.96	0.65
1:C:349:GLU:O	1:C:352:ASN:HB2	1.95	0.65
1:D:230:CYS:HB2	1:D:232:THR:O	1.96	0.65
1:D:155:MET:SD	1:D:164:GLY:HA2	2.36	0.65
1:A:57:ASN:HB2	4:A:457:HOH:O	1.97	0.65
1:D:110:LEU:HD12	1:D:111:MET:N	2.12	0.65
1:D:64:ASP:OD1	1:D:68:LYS:HD2	1.97	0.65
1:A:2:ARG:HA	1:A:162:GLN:OE1	1.96	0.65
1:B:134:SER:OG	1:B:283:SER:HA	1.96	0.65
1:B:111:MET:HE2	1:B:116:LYS:O	1.97	0.64
1:C:39:ARG:HA	1:C:39:ARG:HH11	1.62	0.64
1:A:257:ASP:OD2	1:A:260:GLY:HA2	1.96	0.64
1:D:134:SER:O	1:D:135:THR:HG23	1.98	0.64
1:A:378:SER:O	1:A:392:ARG:HB2	1.97	0.64
1:C:307:LYS:HD3	1:D:304:ASP:HB3	1.79	0.64
1:B:141:ASN:HB3	1:B:366:TRP:NE1	2.12	0.64
1:C:306:ARG:HH21	1:D:305:GLY:N	1.94	0.64
1:A:146:PHE:HA	1:A:360:VAL:O	1.98	0.64
1:C:182:PHE:HA	1:C:186:LYS:O	1.97	0.64
1:B:76:ASP:OD1	1:C:76:ASP:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:THR:OG1	1:C:415:VAL:HB	1.97	0.64
1:B:275:GLY:HA3	1:B:278:LYS:HD2	1.80	0.64
1:D:263:TYR:OH	1:D:313:PRO:HD3	1.97	0.64
1:B:81:TYR:HA	1:B:103:ASN:ND2	2.12	0.64
1:D:49:CYS:HA	1:D:58:ALA:HB3	1.79	0.64
1:A:340:ASN:O	1:A:344:GLU:HB2	1.97	0.64
1:C:40:TRP:O	1:C:71:ILE:HA	1.98	0.64
1:A:257:ASP:OD1	1:A:341:ARG:HB3	1.98	0.64
1:D:13:PRO:O	1:D:85:THR:HG21	1.98	0.64
1:A:133:LEU:HD11	1:A:286:PHE:HZ	1.63	0.64
1:B:230:CYS:HB3	1:B:255:LYS:O	1.97	0.64
1:D:264:ASN:HB3	1:D:267:ARG:HB3	1.80	0.64
1:D:147:VAL:O	1:D:359:MET:HB3	1.98	0.64
1:B:205:PRO:HA	1:B:240:THR:HG23	1.80	0.63
1:C:39:ARG:HD2	1:C:167:TYR:HB3	1.80	0.63
1:B:227:PRO:HB2	1:B:351:LEU:HD11	1.80	0.63
1:A:61:THR:HB	1:A:190:GLU:OE1	1.98	0.63
1:B:183:VAL:HG21	1:B:206:TYR:O	1.98	0.63
1:B:48:ASN:OD1	1:C:99:GLU:HG3	1.98	0.63
1:B:21:ALA:HA	1:B:426:SER:HB3	1.81	0.63
1:C:130:ASP:HA	1:C:286:PHE:O	1.98	0.63
1:B:117:TYR:HB2	1:B:151:GLU:HA	1.79	0.63
1:A:146:PHE:O	1:A:147:VAL:HG13	1.98	0.63
1:D:295:ASN:H	1:D:352:ASN:HD21	1.46	0.63
1:C:95:VAL:HG22	1:C:104:VAL:HG22	1.79	0.63
1:C:353:ASN:O	1:C:357:VAL:HG23	1.98	0.63
1:B:31:GLU:O	1:B:31:GLU:HG2	1.99	0.63
1:D:329:CYS:O	1:D:332:MET:HB3	1.98	0.63
1:C:153:GLY:HA3	1:C:165:ALA:N	2.14	0.63
1:A:215:VAL:HA	1:A:225:PHE:CD2	2.33	0.62
1:B:64:ASP:O	1:B:68:LYS:HB3	1.99	0.62
1:A:295:ASN:HA	1:A:348:PHE:CD2	2.34	0.62
1:C:288:VAL:HG13	1:C:299:GLN:NE2	2.14	0.62
1:B:88:ASP:HB2	1:B:418:ASN:H	1.63	0.62
1:C:35:ASP:OD2	1:C:37:ASN:HB2	1.99	0.62
1:D:149:MET:SD	1:D:171:TYR:HA	2.39	0.62
1:A:164:GLY:O	1:A:169:THR:HG23	1.99	0.62
1:C:317:GLY:O	1:C:331:THR:HB	2.00	0.62
1:C:198:ASP:HB2	1:C:369:HIS:CD2	2.34	0.62
1:A:151:GLU:HB2	4:A:439:HOH:O	1.98	0.62
1:B:384:LYS:HD3	1:B:385:GLU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLU:HA	4:B:507:HOH:O	1.98	0.62
1:C:195:SER:HB3	1:C:201:ALA:O	2.00	0.62
1:D:31:GLU:HG3	1:D:111:MET:HB2	1.81	0.62
1:C:366:TRP:HB3	4:C:493:HOH:O	1.98	0.62
1:A:37:ASN:OD1	1:A:181:LYS:HD3	1.99	0.62
1:C:115:ASP:HA	1:C:166:ARG:HG2	1.82	0.62
1:B:286:PHE:HB3	1:B:303:GLN:NE2	2.14	0.62
1:C:141:ASN:HB2	1:C:373:MET:SD	2.40	0.61
1:A:144:LEU:HD21	1:A:361:LEU:HD11	1.80	0.61
1:A:343:GLU:HG2	1:A:347:GLY:HA2	1.81	0.61
1:C:265:PRO:HG3	1:C:310:ILE:HG23	1.80	0.61
1:D:203:VAL:HG12	1:D:204:GLY:O	2.00	0.61
1:C:136:VAL:HG22	1:C:413:GLN:O	2.00	0.61
1:C:95:VAL:HA	1:C:103:ASN:O	2.00	0.61
1:C:420:ARG:HD2	1:C:427:THR:HB	1.82	0.61
1:A:141:ASN:O	1:A:365:ILE:HA	1.99	0.61
1:A:286:PHE:HB3	1:A:303:GLN:NE2	2.15	0.61
1:A:4:GLY:HA2	1:A:70:MET:SD	2.40	0.61
1:C:18:ARG:HB3	1:C:26:GLN:HG2	1.82	0.61
1:C:232:THR:HG22	1:C:234:GLU:HG2	1.83	0.61
1:D:34:ILE:HG23	1:D:35:ASP:O	2.00	0.61
1:A:84:SER:O	1:A:90:LEU:HA	2.01	0.61
1:D:179:ASP:HB3	1:D:247:TYR:CE1	2.36	0.61
1:D:163:ALA:HB3	1:D:169:THR:HG21	1.82	0.61
1:A:141:ASN:HB3	1:A:366:TRP:NE1	2.15	0.61
1:A:264:ASN:HB3	1:A:267:ARG:HB2	1.83	0.61
1:C:92:LEU:O	1:C:413:GLN:HA	2.00	0.61
1:D:396:PRO:HD2	1:D:399:SER:HB2	1.82	0.61
1:D:50:TYR:O	1:D:51:ASP:HB2	2.01	0.61
1:A:42:HIS:HA	1:A:48:ASN:HA	1.83	0.61
1:C:89:ALA:HB2	1:C:417:SER:HB3	1.81	0.61
1:A:114:PRO:O	1:A:166:ARG:HB2	2.00	0.60
1:B:315:TRP:CH2	1:B:388:PRO:HB3	2.37	0.60
1:C:346:GLY:HA3	1:C:350:GLN:HB2	1.83	0.60
1:C:22:PRO:HG3	1:C:425:GLY:O	2.00	0.60
1:A:377:ASP:HB2	1:A:395:CYS:SG	2.41	0.60
1:B:126:GLU:OE1	1:B:291:ARG:HG2	2.01	0.60
1:D:239:GLU:H	1:D:242:ASN:HD22	1.46	0.60
1:B:267:ARG:HG2	1:B:389:GLY:HA2	1.83	0.60
1:C:34:ILE:HG22	1:C:77:TYR:OH	2.02	0.60
1:A:50:TYR:HA	1:A:55:TRP:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:TYR:CD1	1:A:382:PRO:HD3	2.36	0.60
1:D:206:TYR:CD2	1:D:239:GLU:HG3	2.36	0.60
1:A:73:GLY:O	1:D:99:GLU:HG3	2.01	0.60
1:A:336:PHE:CD1	1:A:388:PRO:HB2	2.37	0.60
1:A:188:ASN:OD1	1:A:206:TYR:HB2	2.01	0.60
1:C:41:LEU:HG	1:C:71:ILE:HG22	1.84	0.60
1:C:155:MET:HG3	1:C:161:ASN:O	2.02	0.60
1:C:264:ASN:O	1:C:268:MET:HG2	2.02	0.60
1:A:55:TRP:HB3	1:A:189:ILE:HD12	1.84	0.60
1:A:1:PCA:HG2	1:A:71:ILE:HD11	1.84	0.60
1:A:110:LEU:HD12	1:A:111:MET:H	1.67	0.60
1:B:255:LYS:HG2	4:B:578:HOH:O	2.01	0.59
1:A:357:VAL:HG12	1:A:358:PRO:HD2	1.83	0.59
1:C:133:LEU:HD11	1:C:286:PHE:CZ	2.37	0.59
1:C:106:SER:HG	1:C:108:PHE:HE1	1.50	0.59
1:D:125:ASN:HB3	1:D:422:GLY:O	2.02	0.59
1:D:182:PHE:O	1:D:183:VAL:HG23	2.01	0.59
1:B:301:PHE:O	1:B:307:LYS:HG2	2.02	0.59
1:B:144:LEU:HD23	1:B:362:VAL:O	2.02	0.59
1:B:42:HIS:ND1	1:B:46:MET:HA	2.17	0.59
1:A:377:ASP:O	1:A:395:CYS:HB2	2.02	0.59
1:D:375:TRP:CH2	2:D:431:CBI:H5	2.37	0.59
1:D:385:GLU:O	1:D:387:GLN:HG3	2.02	0.59
1:D:107:ARG:HH11	2:D:432:CBI:H2'	1.67	0.59
1:A:119:MET:HA	1:A:359:MET:O	2.02	0.59
1:C:183:VAL:HG13	1:C:208:SER:OG	2.03	0.59
1:B:35:ASP:O	1:B:38:TRP:HB2	2.02	0.59
1:C:225:PHE:O	1:C:262:ASP:HA	2.03	0.59
1:A:34:ILE:HG23	1:A:35:ASP:O	2.02	0.59
1:C:183:VAL:O	1:C:186:LYS:HG2	2.03	0.59
1:C:122:LEU:HD23	1:C:292:PHE:CD2	2.38	0.59
1:C:307:LYS:HB2	1:C:430:PHE:CE2	2.38	0.59
1:B:179:ASP:HB3	1:B:247:TYR:CE2	2.38	0.59
1:D:17:GLN:O	1:D:420:ARG:HA	2.03	0.59
1:A:1:PCA:HA	1:A:66:ALA:O	2.02	0.58
1:B:11:HIS:HB3	1:B:31:GLU:HG3	1.83	0.58
1:A:231:THR:HG21	4:A:480:HOH:O	2.02	0.58
1:B:122:LEU:HD11	1:B:146:PHE:CE1	2.37	0.58
1:A:288:VAL:HG22	1:A:301:PHE:HE2	1.67	0.58
1:B:213:ILE:HG21	1:B:292:PHE:HE2	1.68	0.58
1:A:147:VAL:HG12	1:A:212:GLU:HA	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLU:OE1	1:C:424:ILE:HA	2.04	0.58
1:D:47:GLN:HG2	1:D:58:ALA:HB2	1.86	0.58
1:B:353:ASN:HA	1:B:356:ARG:HG3	1.85	0.58
1:B:265:PRO:O	1:B:270:ASN:HB2	2.02	0.58
1:D:366:TRP:CD1	2:D:432:CBI:H3'	2.39	0.58
1:B:30:ALA:HB1	1:B:111:MET:O	2.03	0.58
1:B:291:ARG:HD3	1:B:424:ILE:HG23	1.86	0.58
1:C:209:CYS:O	1:C:235:TYR:HA	2.04	0.58
1:C:381:PRO:HD3	4:C:433:HOH:O	2.02	0.58
1:B:374:LEU:HD23	1:B:378:SER:CB	2.34	0.58
1:C:402:PRO:O	1:C:406:GLU:HG3	2.04	0.58
1:A:296:LYS:O	1:A:297:LEU:HD13	2.03	0.58
1:D:111:MET:HA	1:D:117:TYR:HA	1.86	0.58
1:A:142:SER:HA	1:A:364:SER:O	2.03	0.58
1:C:33:VAL:O	1:C:108:PHE:HA	2.03	0.58
1:D:132:ASP:OD1	1:D:134:SER:HB3	2.03	0.58
1:D:155:MET:CE	1:D:164:GLY:HA2	2.34	0.58
1:B:209:CYS:HB2	1:B:236:HIS:NE2	2.18	0.58
1:B:111:MET:HE1	1:B:165:ALA:HB1	1.86	0.58
1:C:306:ARG:NH2	1:D:305:GLY:H	2.00	0.58
1:A:251:ARG:NH2	2:A:431:CBI:H2	2.17	0.58
1:B:231:THR:HG23	1:B:345:VAL:HB	1.85	0.58
1:C:341:ARG:HG3	1:C:341:ARG:O	2.04	0.58
1:D:155:MET:HG3	1:D:161:ASN:O	2.03	0.58
1:D:144:LEU:O	1:D:144:LEU:HD23	2.04	0.58
1:D:31:GLU:OE2	1:D:114:PRO:HD3	2.04	0.57
1:B:225:PHE:CZ	1:B:297:LEU:HD23	2.39	0.57
1:B:368:ASP:CB	1:B:373:MET:HE2	2.34	0.57
1:A:250:ASP:HB3	1:A:253:ALA:HB2	1.85	0.57
1:C:211:ALA:HB2	1:C:233:ASN:OD1	2.04	0.57
1:C:143:ALA:CB	1:C:217:GLU:HA	2.33	0.57
1:A:183:VAL:HG21	1:A:206:TYR:O	2.04	0.57
1:A:295:ASN:N	1:A:352:ASN:HD21	2.02	0.57
1:D:163:ALA:HB1	1:D:167:TYR:CB	2.34	0.57
1:B:122:LEU:HD21	1:B:146:PHE:CD1	2.39	0.57
1:B:149:MET:HB2	1:B:360:VAL:HG21	1.85	0.57
1:B:128:ALA:CB	1:B:289:VAL:HG22	2.35	0.57
1:A:90:LEU:HD12	1:A:91:THR:H	1.69	0.57
1:B:327:GLU:O	1:B:331:THR:HG23	2.04	0.57
1:A:307:LYS:HD3	1:A:430:PHE:HB3	1.86	0.57
1:A:29:ASN:HD22	1:A:29:ASN:N	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLU:O	1:B:151:GLU:HG2	2.04	0.57
1:B:105:GLY:HA2	1:B:365:ILE:CG2	2.34	0.57
1:C:325:THR:HG21	4:C:453:HOH:O	2.04	0.57
1:D:35:ASP:HB2	1:D:109:TYR:CZ	2.39	0.57
1:C:127:LEU:HG	1:C:128:ALA:H	1.69	0.57
1:B:335:VAL:HG12	1:B:336:PHE:HD1	1.70	0.57
1:C:381:PRO:HB2	1:C:383:GLU:OE2	2.05	0.57
1:A:351:LEU:O	1:A:355:LEU:HG	2.05	0.57
1:A:177:ALA:HB1	1:A:180:LEU:HG	1.85	0.57
1:C:121:ASN:O	1:C:421:PHE:HZ	1.88	0.57
1:D:264:ASN:ND2	1:D:266:TYR:HB3	2.18	0.57
1:C:296:LYS:HD2	1:C:323:GLU:OE2	2.05	0.57
1:B:335:VAL:HG12	1:B:336:PHE:CD1	2.39	0.57
1:C:401:VAL:CG1	1:C:404:GLU:HB2	2.35	0.57
1:A:77:TYR:HB3	1:A:83:ALA:HB3	1.86	0.56
1:C:295:ASN:H	1:C:352:ASN:HD21	1.52	0.56
1:A:202:GLY:O	1:A:203:VAL:HG23	2.04	0.56
1:A:280:LEU:HD22	1:A:308:ILE:HG21	1.87	0.56
1:B:295:ASN:HA	1:B:348:PHE:CE2	2.40	0.56
1:B:217:GLU:O	1:B:376:LEU:HD11	2.04	0.56
1:D:3:ALA:HB1	1:D:167:TYR:OH	2.04	0.56
1:B:144:LEU:HA	1:B:362:VAL:O	2.04	0.56
1:B:213:ILE:HG21	1:B:292:PHE:CE2	2.41	0.56
1:B:292:PHE:CB	1:B:355:LEU:HD11	2.35	0.56
1:A:257:ASP:CB	1:A:341:ARG:HG2	2.35	0.56
1:A:39:ARG:HA	1:D:99:GLU:OE2	2.05	0.56
1:B:301:PHE:HB2	1:B:308:ILE:HB	1.87	0.56
1:A:112:ASN:O	1:A:116:LYS:HD2	2.05	0.56
1:B:42:HIS:HB2	1:B:47:GLN:O	2.04	0.56
1:B:71:ILE:HD11	1:B:163:ALA:CB	2.35	0.56
1:A:155:MET:HG3	1:A:161:ASN:O	2.06	0.56
1:D:111:MET:CE	1:D:114:PRO:HA	2.35	0.56
1:D:423:PRO:HD2	1:D:426:SER:OG	2.04	0.56
1:D:81:TYR:O	1:D:96:THR:HG21	2.06	0.56
1:D:18:ARG:HA	1:D:421:PHE:O	2.05	0.56
1:D:265:PRO:HA	1:D:268:MET:HB2	1.87	0.56
1:D:195:SER:HB3	1:D:198:ASP:HB3	1.87	0.56
1:B:350:GLN:O	1:B:350:GLN:HG3	2.05	0.56
1:D:372:ASN:HD22	1:D:402:PRO:HD3	1.71	0.56
1:D:125:ASN:HD22	1:D:423:PRO:CA	2.19	0.56
1:A:178:ARG:HB2	1:A:247:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:THR:HG22	1:D:190:GLU:OE1	2.06	0.56
1:A:233:ASN:N	1:A:233:ASN:HD22	2.04	0.56
1:D:215:VAL:HG22	1:D:225:PHE:CE2	2.40	0.56
1:D:2:ARG:HE	1:D:67:GLU:HA	1.71	0.56
1:B:42:HIS:CE1	1:B:46:MET:HA	2.41	0.56
1:B:368:ASP:O	1:B:372:ASN:HA	2.06	0.56
1:B:9:GLU:HA	1:B:9:GLU:OE2	2.05	0.56
1:A:133:LEU:HD11	1:A:286:PHE:CZ	2.40	0.56
1:A:288:VAL:HG22	1:A:301:PHE:CE2	2.40	0.56
1:C:122:LEU:HB3	1:C:292:PHE:CG	2.41	0.55
1:D:132:ASP:HB3	1:D:415:VAL:CG1	2.37	0.55
1:A:281:ASP:OD2	1:A:284:ARG:HD2	2.06	0.55
1:B:301:PHE:O	1:B:307:LYS:HA	2.06	0.55
1:A:353:ASN:N	1:A:353:ASN:HD22	2.03	0.55
1:C:125:ASN:HB3	1:C:422:GLY:O	2.06	0.55
1:A:170:GLY:O	1:A:235:TYR:HE1	1.88	0.55
1:B:135:THR:O	1:B:412:ALA:HB1	2.05	0.55
1:D:141:ASN:O	1:D:365:ILE:HA	2.06	0.55
1:A:106:SER:HG	1:A:108:PHE:HE1	1.52	0.55
1:A:1:PCA:HG3	1:A:182:PHE:CE1	2.42	0.55
1:D:391:ALA:HB3	4:D:549:HOH:O	2.06	0.55
1:C:182:PHE:CE1	1:C:187:ALA:HB2	2.42	0.55
1:B:130:ASP:HA	1:B:286:PHE:O	2.06	0.55
1:C:110:LEU:HD23	1:C:361:LEU:O	2.06	0.55
1:C:265:PRO:CA	1:C:270:ASN:HD22	2.17	0.55
1:A:252:PHE:HB3	1:A:341:ARG:HH11	1.72	0.55
1:C:66:ALA:HB1	1:C:160:SER:OG	2.07	0.55
1:A:289:VAL:HG21	1:A:300:TYR:CE1	2.41	0.55
1:C:233:ASN:OD1	1:C:354:ALA:HB2	2.06	0.55
1:C:95:VAL:CG2	1:C:104:VAL:HG22	2.36	0.55
1:B:163:ALA:O	1:B:166:ARG:HD2	2.07	0.55
1:C:340:ASN:OD1	1:C:343:GLU:HB2	2.07	0.55
1:D:21:ALA:HB3	1:D:24:ASN:ND2	2.04	0.55
1:D:342:PHE:CZ	1:D:348:PHE:HA	2.41	0.55
1:B:379:ILE:HB	1:B:397:THR:CG2	2.37	0.55
1:B:401:VAL:CG1	1:B:404:GLU:HB2	2.35	0.55
1:A:367:ASP:OD2	1:A:402:PRO:HB3	2.07	0.55
1:B:175:GLN:HE22	3:B:431:CTT:H4C	1.72	0.55
1:A:324:ILE:HG22	1:A:348:PHE:CZ	2.42	0.55
1:D:109:TYR:CD1	1:D:362:VAL:HG22	2.42	0.55
1:D:95:VAL:CG1	1:D:97:LYS:HE2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASN:HB2	1:B:357:VAL:HG21	1.88	0.55
1:B:297:LEU:HB2	1:B:324:ILE:HB	1.88	0.55
1:A:37:ASN:ND2	2:A:432:CBI:H6'2	2.22	0.55
1:D:377:ASP:HB2	1:D:395:CYS:SG	2.47	0.55
1:C:263:TYR:CZ	1:C:322:SER:HA	2.41	0.54
1:D:267:ARG:HG2	1:D:267:ARG:O	2.06	0.54
1:C:318:MET:CE	1:C:332:MET:HA	2.37	0.54
1:C:292:PHE:HB3	1:C:355:LEU:CD2	2.37	0.54
1:B:175:GLN:OE1	1:B:258:ALA:HB1	2.07	0.54
1:B:267:ARG:HB3	1:B:268:MET:CE	2.37	0.54
1:B:374:LEU:HD21	1:B:397:THR:HA	1.88	0.54
1:D:206:TYR:CE2	1:D:239:GLU:HG3	2.42	0.54
1:B:13:PRO:HA	1:B:31:GLU:CB	2.37	0.54
1:A:350:GLN:O	1:A:353:ASN:HB2	2.07	0.54
1:B:223:PHE:O	1:B:264:ASN:HB2	2.07	0.54
1:A:55:TRP:CE3	1:A:189:ILE:HD12	2.43	0.54
1:B:50:TYR:HD1	1:B:55:TRP:HA	1.72	0.54
1:B:122:LEU:CD2	1:B:213:ILE:HD13	2.38	0.54
1:C:306:ARG:HE	1:D:305:GLY:N	2.05	0.54
1:C:128:ALA:HA	1:C:288:VAL:O	2.07	0.54
1:C:369:HIS:HA	1:C:402:PRO:HG3	1.90	0.54
1:C:94:PHE:CE2	1:C:95:VAL:HG23	2.42	0.54
1:C:109:TYR:CD1	1:C:362:VAL:HG13	2.42	0.54
1:C:229:ALA:HB1	1:C:233:ASN:OD1	2.08	0.54
1:B:59:CYS:HB3	1:B:189:ILE:CD1	2.36	0.54
1:D:291:ARG:CG	1:D:298:SER:HB3	2.34	0.54
1:A:333:PHE:CE2	1:A:340:ASN:HA	2.43	0.54
1:A:141:ASN:OD1	1:A:143:ALA:HB2	2.08	0.54
1:D:198:ASP:OD1	1:D:201:ALA:HB3	2.08	0.54
1:D:289:VAL:HB	1:D:300:TYR:CE2	2.43	0.54
1:C:14:LEU:HD12	1:C:15:THR:H	1.73	0.54
1:A:17:GLN:HG2	1:A:17:GLN:O	2.07	0.54
1:A:41:LEU:HD12	1:A:49:CYS:HB2	1.89	0.54
1:C:230:CYS:HB3	1:C:256:CYS:HA	1.90	0.54
1:C:6:GLU:HB3	1:C:72:GLU:OE2	2.08	0.54
1:B:175:GLN:HE21	3:B:431:CTT:H1D	1.72	0.54
1:C:198:ASP:HB2	1:C:369:HIS:NE2	2.23	0.54
1:B:82:GLY:HA3	1:B:93:LYS:HB3	1.88	0.54
1:B:112:ASN:HB2	1:B:118:GLN:OE1	2.07	0.54
1:B:95:VAL:HG22	1:B:104:VAL:HG22	1.89	0.54
1:A:65:CYS:HA	1:A:68:LYS:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:SER:O	1:A:199:PRO:HD3	2.08	0.54
1:D:107:ARG:HA	1:D:364:SER:HB3	1.90	0.53
1:A:82:GLY:O	1:A:93:LYS:HG3	2.08	0.53
1:D:27:THR:HG23	1:D:29:ASN:ND2	2.21	0.53
1:B:92:LEU:HD22	1:B:106:SER:HB3	1.90	0.53
1:A:36:ALA:HA	1:A:39:ARG:HD2	1.88	0.53
1:B:333:PHE:CD2	1:B:340:ASN:HA	2.43	0.53
1:A:217:GLU:O	1:A:223:PHE:HB2	2.09	0.53
1:D:272:ASP:HA	1:D:278:LYS:HD3	1.88	0.53
1:B:287:THR:HB	1:B:302:ILE:HB	1.90	0.53
1:A:319:PRO:CG	1:A:327:GLU:HG3	2.38	0.53
1:C:31:GLU:HG3	1:C:111:MET:CE	2.38	0.53
1:B:19:CYS:HA	1:B:25:CYS:HA	1.88	0.53
1:D:11:HIS:CD2	1:D:33:VAL:HB	2.44	0.53
1:B:384:LYS:HA	1:B:384:LYS:HE2	1.90	0.53
1:B:123:MET:HE3	1:B:356:ARG:HH21	1.73	0.53
1:B:127:LEU:HD12	1:B:420:ARG:O	2.08	0.53
1:A:372:ASN:HB3	1:A:400:GLY:HA3	1.91	0.53
1:D:58:ALA:O	1:D:68:LYS:HD3	2.08	0.53
1:A:92:LEU:HD22	1:A:108:PHE:CE1	2.44	0.53
1:A:111:MET:HE1	1:A:166:ARG:HA	1.90	0.53
1:B:34:ILE:HG12	1:B:108:PHE:CE1	2.43	0.53
1:D:149:MET:CG	1:D:171:TYR:HA	2.39	0.53
1:C:135:THR:HG22	1:C:412:ALA:HA	1.90	0.53
1:A:82:GLY:O	1:A:93:LYS:HD2	2.08	0.53
1:A:372:ASN:O	1:A:400:GLY:HA3	2.08	0.53
1:B:178:ARG:HB3	1:B:178:ARG:HH11	1.73	0.53
1:D:77:TYR:O	1:D:81:TYR:HB2	2.08	0.53
1:D:377:ASP:O	1:D:395:CYS:HB2	2.07	0.53
1:A:46:MET:HB3	4:A:526:HOH:O	2.08	0.53
1:B:142:SER:HB2	1:B:414:VAL:HG11	1.90	0.53
1:D:297:LEU:HB2	1:D:324:ILE:HB	1.89	0.53
1:A:37:ASN:O	2:A:432:CBI:H3	2.09	0.53
1:D:65:CYS:HB3	1:D:182:PHE:CZ	2.44	0.53
1:B:22:PRO:CD	1:B:426:SER:HA	2.38	0.53
1:B:68:LYS:O	1:B:68:LYS:HG3	2.09	0.53
1:A:99:GLU:HG3	1:D:40:TRP:CD1	2.42	0.53
1:C:319:PRO:CG	1:C:328:LEU:HD23	2.39	0.53
1:C:286:PHE:HB3	1:C:303:GLN:HG3	1.90	0.53
1:D:40:TRP:O	1:D:72:GLU:HG2	2.09	0.53
1:D:20:THR:OG1	1:D:24:ASN:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:LYS:CE	1:C:387:GLN:HE22	2.21	0.53
1:A:233:ASN:H	1:A:233:ASN:HD22	1.56	0.53
1:C:130:ASP:OD2	1:C:418:ASN:HB3	2.09	0.53
1:D:92:LEU:HB2	1:D:414:VAL:CG1	2.38	0.53
1:C:188:ASN:O	1:C:192:TRP:HE3	1.92	0.53
1:A:38:TRP:CE2	2:A:432:CBI:H5	2.44	0.53
1:C:198:ASP:HB3	1:C:201:ALA:HB3	1.90	0.53
1:B:193:LYS:HA	4:B:501:HOH:O	2.09	0.53
1:C:193:LYS:HB2	1:C:203:VAL:HB	1.90	0.53
1:B:226:THR:OG1	1:B:262:ASP:HB2	2.09	0.53
1:C:384:LYS:CD	1:C:387:GLN:HE22	2.22	0.53
1:A:148:ALA:HB2	1:A:359:MET:HE2	1.90	0.53
1:C:13:PRO:HA	1:C:31:GLU:HB3	1.90	0.53
1:D:92:LEU:O	1:D:413:GLN:HB2	2.08	0.53
1:D:122:LEU:HD11	1:D:146:PHE:CD1	2.44	0.53
1:A:132:ASP:HB3	1:A:415:VAL:HG13	1.90	0.53
1:C:133:LEU:O	1:C:220:ALA:HB2	2.09	0.52
1:B:229:ALA:HB3	4:B:557:HOH:O	2.07	0.52
1:B:146:PHE:HE2	1:B:361:LEU:HB2	1.73	0.52
1:D:266:TYR:HB2	4:D:512:HOH:O	2.08	0.52
1:C:143:ALA:HA	1:C:216:TRP:O	2.09	0.52
1:C:341:ARG:O	1:C:344:GLU:HB3	2.09	0.52
1:C:369:HIS:CE1	1:C:402:PRO:HB3	2.43	0.52
1:A:336:PHE:HD1	1:A:388:PRO:HB2	1.75	0.52
1:A:195:SER:HB3	4:A:518:HOH:O	2.09	0.52
1:B:141:ASN:HD21	1:B:217:GLU:HB3	1.75	0.52
1:C:288:VAL:HG22	1:C:301:PHE:CE2	2.45	0.52
1:B:92:LEU:HD22	1:B:106:SER:CB	2.39	0.52
1:A:50:TYR:CA	1:A:56:THR:HG23	2.40	0.52
1:B:274:TYR:CD1	1:B:280:LEU:HD12	2.45	0.52
1:C:120:PHE:HB2	1:C:146:PHE:CE2	2.44	0.52
1:D:213:ILE:HG22	1:D:213:ILE:O	2.09	0.52
1:D:2:ARG:HB2	1:D:70:MET:HB3	1.90	0.52
1:A:86:SER:HB3	1:A:89:ALA:HB3	1.92	0.52
1:B:1:PCA:O	1:B:162:GLN:HG3	2.10	0.52
1:C:147:VAL:HG12	1:C:212:GLU:CB	2.40	0.52
1:C:144:LEU:HD11	1:C:361:LEU:HD21	1.90	0.52
1:B:379:ILE:HB	1:B:397:THR:HG21	1.91	0.52
1:A:356:ARG:HH11	1:A:356:ARG:CB	2.23	0.52
1:B:176:CYS:O	1:B:178:ARG:HG2	2.10	0.52
1:A:292:PHE:HA	1:A:297:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:VAL:HG11	1:D:97:LYS:HE2	1.90	0.52
1:A:226:THR:HG22	1:A:228:HIS:CD2	2.45	0.52
1:B:420:ARG:HB2	1:B:427:THR:CG2	2.38	0.52
1:D:12:PRO:HD2	1:D:32:VAL:O	2.10	0.52
1:A:41:LEU:O	1:A:48:ASN:HA	2.10	0.51
1:C:19:CYS:HB3	1:C:24:ASN:O	2.11	0.51
1:A:324:ILE:HG22	1:A:348:PHE:CE1	2.45	0.51
1:D:139:GLY:HA2	1:D:373:MET:HB3	1.92	0.51
1:D:41:LEU:O	1:D:42:HIS:HB3	2.10	0.51
1:C:34:ILE:HD12	1:C:108:PHE:CZ	2.46	0.51
1:B:345:VAL:HG23	1:B:345:VAL:O	2.10	0.51
1:B:10:ASN:O	1:B:77:TYR:HE1	1.93	0.51
1:A:132:ASP:HB3	1:A:415:VAL:CG2	2.40	0.51
1:A:287:THR:O	1:A:301:PHE:HA	2.09	0.51
1:B:172:CYS:HB2	1:B:209:CYS:O	2.10	0.51
1:A:20:THR:HG23	1:A:24:ASN:O	2.10	0.51
1:D:143:ALA:HA	1:D:216:TRP:O	2.09	0.51
1:D:299:GLN:HG2	1:D:299:GLN:O	2.09	0.51
1:C:131:VAL:HG22	1:C:133:LEU:HG	1.92	0.51
1:D:211:ALA:CB	1:D:233:ASN:HB3	2.39	0.51
1:A:198:ASP:HB3	1:A:201:ALA:HB3	1.91	0.51
1:C:193:LYS:HD2	1:C:203:VAL:CG1	2.40	0.51
1:C:31:GLU:HG3	1:C:111:MET:HE3	1.91	0.51
1:D:80:THR:HG23	1:D:98:HIS:CD2	2.45	0.51
1:D:4:GLY:HA3	1:D:72:GLU:OE2	2.10	0.51
1:D:166:ARG:HD2	1:D:167:TYR:CE2	2.45	0.51
1:D:47:GLN:CG	1:D:58:ALA:HB2	2.40	0.51
1:B:368:ASP:HB2	1:B:373:MET:HE2	1.92	0.51
1:B:325:THR:HB	1:B:326:PRO:HD2	1.92	0.51
1:C:147:VAL:HG23	1:C:149:MET:CG	2.40	0.51
1:C:163:ALA:HB1	1:C:167:TYR:CD2	2.45	0.51
1:C:319:PRO:HG3	1:C:328:LEU:HA	1.92	0.51
1:A:256:CYS:O	1:A:341:ARG:HD3	2.10	0.51
1:C:92:LEU:HD22	4:C:490:HOH:O	2.09	0.51
1:D:310:ILE:HG23	1:D:311:PRO:HD2	1.93	0.51
1:C:373:MET:HG2	1:C:376:LEU:HD22	1.93	0.51
1:D:396:PRO:HD2	1:D:399:SER:CB	2.41	0.51
1:C:80:THR:HB	1:C:81:TYR:CD2	2.46	0.51
1:B:377:ASP:HB2	1:B:395:CYS:SG	2.50	0.51
1:B:232:THR:HG22	1:B:232:THR:O	2.11	0.51
1:C:153:GLY:HA3	1:C:165:ALA:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HD21	1:B:146:PHE:HD1	1.76	0.51
1:B:136:VAL:HG23	1:B:413:GLN:O	2.11	0.51
1:B:366:TRP:CG	3:B:431:CTT:H3E	2.46	0.51
1:D:107:ARG:HD3	2:D:432:CBI:H2'	1.93	0.51
1:C:385:GLU:HG3	1:C:386:GLY:N	2.26	0.51
1:C:37:ASN:ND2	1:C:180:LEU:HA	2.25	0.51
1:C:178:ARG:HD3	1:C:248:SER:OG	2.11	0.51
1:D:379:ILE:O	1:D:379:ILE:HG22	2.10	0.51
1:B:315:TRP:CZ2	1:B:388:PRO:HB3	2.46	0.50
1:A:225:PHE:CE1	1:A:297:LEU:HB3	2.46	0.50
1:A:319:PRO:CB	1:A:327:GLU:HG3	2.41	0.50
1:B:16:TRP:CD1	1:B:30:ALA:HB3	2.46	0.50
1:A:144:LEU:HD21	1:A:361:LEU:CD1	2.40	0.50
1:C:14:LEU:HB3	1:C:32:VAL:HG22	1.93	0.50
1:B:379:ILE:HG22	1:B:379:ILE:O	2.10	0.50
1:B:21:ALA:HB1	1:B:22:PRO:HD2	1.92	0.50
1:C:295:ASN:HA	1:C:348:PHE:CE2	2.46	0.50
1:D:17:GLN:CG	1:D:420:ARG:HG2	2.40	0.50
1:C:125:ASN:HD22	1:C:422:GLY:C	2.15	0.50
1:B:107:ARG:HA	1:B:363:MET:O	2.10	0.50
1:B:341:ARG:HB3	4:B:498:HOH:O	2.10	0.50
1:A:122:LEU:O	1:A:125:ASN:HB2	2.11	0.50
1:B:94:PHE:CD2	1:B:95:VAL:HG23	2.46	0.50
1:B:7:THR:O	1:B:72:GLU:OE1	2.30	0.50
1:C:232:THR:HG22	1:C:234:GLU:CG	2.41	0.50
1:D:209:CYS:SG	1:D:238:CYS:HB3	2.52	0.50
1:B:268:MET:HA	1:B:315:TRP:CD1	2.47	0.50
1:A:173:ASP:HB2	1:A:212:GLU:HG3	1.93	0.50
1:B:233:ASN:O	1:B:357:VAL:HG11	2.11	0.50
1:C:34:ILE:HA	1:C:107:ARG:O	2.10	0.50
1:C:133:LEU:HD11	1:C:286:PHE:HZ	1.76	0.50
1:A:129:PHE:O	1:A:130:ASP:OD1	2.30	0.50
1:A:23:GLY:HA2	4:A:487:HOH:O	2.11	0.50
1:B:186:LYS:O	1:B:187:ALA:O	2.30	0.50
1:C:242:ASN:O	1:C:254:GLY:HA2	2.12	0.50
1:B:289:VAL:O	1:B:299:GLN:HB2	2.12	0.50
1:A:220:ALA:HB1	1:A:276:LYS:CE	2.41	0.50
1:D:401:VAL:HB	1:D:404:GLU:CB	2.40	0.50
1:B:287:THR:HG22	1:B:287:THR:O	2.10	0.50
1:B:262:ASP:OD1	1:B:262:ASP:O	2.30	0.50
1:A:209:CYS:HB2	1:A:236:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:OE1	1:A:352:ASN:OD1	2.30	0.50
1:D:59:CYS:HA	1:D:68:LYS:HD3	1.93	0.50
1:C:35:ASP:OD1	1:C:109:TYR:OH	2.30	0.50
1:B:43:ASP:HB2	1:B:47:GLN:O	2.11	0.50
1:A:346:GLY:O	1:A:347:GLY:O	2.30	0.50
1:D:133:LEU:HD21	1:D:216:TRP:HZ2	1.77	0.50
1:B:143:ALA:HB1	1:B:216:TRP:O	2.11	0.50
1:D:112:ASN:O	1:D:113:GLY:O	2.30	0.50
1:C:96:THR:HG23	4:C:529:HOH:O	2.11	0.50
1:B:197:SER:HB3	1:B:369:HIS:HB2	1.93	0.50
1:A:401:VAL:O	1:A:405:VAL:HG22	2.11	0.50
1:B:243:CYS:O	1:B:253:ALA:HB3	2.12	0.50
1:B:315:TRP:HB2	1:B:318:MET:SD	2.52	0.50
1:C:110:LEU:HD23	1:C:361:LEU:HB3	1.94	0.50
1:A:261:CYS:HB2	1:A:342:PHE:CD1	2.47	0.50
1:C:188:ASN:HB2	1:C:192:TRP:HZ3	1.76	0.50
1:C:265:PRO:HA	1:C:270:ASN:ND2	2.21	0.50
1:C:289:VAL:O	1:C:289:VAL:HG12	2.11	0.50
1:C:349:GLU:OE2	1:C:352:ASN:OD1	2.30	0.50
1:B:13:PRO:HA	1:B:31:GLU:HB2	1.93	0.50
1:B:121:ASN:O	1:B:125:ASN:OD1	2.30	0.50
1:C:264:ASN:HB3	1:C:267:ARG:HB2	1.94	0.50
1:A:182:PHE:HB3	1:A:186:LYS:O	2.12	0.50
1:B:379:ILE:HD12	1:B:397:THR:HG23	1.94	0.50
1:B:20:THR:OG1	1:B:24:ASN:O	2.30	0.50
1:C:157:SER:HG	1:C:158:TYR:HD2	1.60	0.50
1:C:295:ASN:OD1	1:C:352:ASN:OD1	2.30	0.50
1:A:155:MET:O	1:A:158:TYR:O	2.30	0.50
1:A:218:SER:O	1:A:219:ASN:HB3	2.12	0.50
1:B:178:ARG:HB3	1:B:178:ARG:NH1	2.27	0.50
1:C:379:ILE:HD11	4:C:533:HOH:O	2.11	0.50
1:C:38:TRP:CZ2	1:C:106:SER:HA	2.47	0.50
1:B:354:ALA:HA	1:B:357:VAL:CG2	2.42	0.50
1:C:206:TYR:HB3	1:C:237:VAL:CG1	2.42	0.50
1:A:228:HIS:HB3	1:A:257:ASP:O	2.12	0.50
1:D:380:TYR:HE2	2:D:431:CBI:HO2'	1.56	0.50
1:D:237:VAL:HG12	1:D:237:VAL:O	2.11	0.50
1:B:29:ASN:O	1:B:30:ALA:O	2.30	0.49
1:C:216:TRP:HE1	1:C:218:SER:HG	1.59	0.49
1:B:123:MET:CE	1:B:356:ARG:HH21	2.25	0.49
1:A:65:CYS:HA	1:A:68:LYS:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:TYR:CD1	1:A:381:PRO:HA	2.46	0.49
1:D:251:ARG:O	1:D:251:ARG:HG2	2.12	0.49
1:D:245:GLY:O	1:D:251:ARG:HG3	2.12	0.49
1:B:41:LEU:HD23	1:B:71:ILE:CG2	2.41	0.49
1:A:19:CYS:O	1:A:426:SER:OG	2.30	0.49
1:A:268:MET:SD	1:A:313:PRO:HB3	2.52	0.49
1:B:179:ASP:HB3	1:B:247:TYR:CZ	2.47	0.49
1:D:17:GLN:HG3	1:D:420:ARG:HG2	1.94	0.49
1:C:193:LYS:CB	1:C:203:VAL:HB	2.42	0.49
1:A:59:CYS:HB3	1:A:189:ILE:CD1	2.42	0.49
1:B:380:TYR:HB3	1:B:392:ARG:CZ	2.41	0.49
1:A:276:LYS:HD3	1:A:276:LYS:N	2.27	0.49
1:D:259:ASN:O	1:D:260:GLY:O	2.29	0.49
1:A:135:THR:OG1	1:A:135:THR:O	2.30	0.49
1:D:35:ASP:HB3	1:D:38:TRP:CZ3	2.47	0.49
1:C:390:ALA:O	1:C:392:ARG:HD2	2.11	0.49
1:A:233:ASN:OD1	1:A:354:ALA:HB2	2.12	0.49
1:B:215:VAL:HA	1:B:225:PHE:CE2	2.47	0.49
1:B:378:SER:O	1:B:392:ARG:HD2	2.12	0.49
1:A:267:ARG:HE	1:A:389:GLY:HA2	1.78	0.49
1:A:273:PHE:HA	1:A:279:THR:HB	1.95	0.49
1:A:357:VAL:O	1:A:359:MET:HG2	2.12	0.49
1:D:302:ILE:HG23	1:D:306:ARG:O	2.11	0.49
1:C:204:GLY:O	1:C:205:PRO:O	2.30	0.49
1:B:126:GLU:O	1:B:421:PHE:HA	2.12	0.49
1:A:86:SER:CB	1:A:89:ALA:HB3	2.42	0.49
1:D:215:VAL:HG21	1:D:292:PHE:CZ	2.47	0.49
1:D:51:ASP:O	1:D:54:GLN:O	2.30	0.49
1:A:263:TYR:OH	1:A:313:PRO:HD3	2.12	0.49
1:A:295:ASN:H	1:A:352:ASN:CG	2.15	0.49
1:A:188:ASN:O	1:A:192:TRP:HE3	1.96	0.49
1:C:173:ASP:O	1:C:210:CYS:O	2.29	0.49
1:B:189:ILE:O	1:B:192:TRP:HB2	2.12	0.49
1:B:90:LEU:O	1:B:416:TRP:HD1	1.95	0.49
1:C:152:ASP:O	1:C:164:GLY:HA3	2.12	0.49
1:D:159:PRO:O	1:D:162:GLN:OE1	2.30	0.49
1:C:214:ASP:OD1	1:C:217:GLU:OE1	2.30	0.49
1:D:372:ASN:ND2	1:D:402:PRO:HD3	2.26	0.49
1:A:64:ASP:OD2	1:A:68:LYS:HD2	2.11	0.49
1:B:127:LEU:HG	1:B:128:ALA:N	2.26	0.49
1:B:424:ILE:O	1:B:424:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:THR:OG1	1:B:412:ALA:HA	2.13	0.49
1:A:400:GLY:O	1:A:402:PRO:HD3	2.12	0.49
1:B:199:PRO:HG2	1:B:200:ASN:OD1	2.12	0.49
1:B:4:GLY:HA2	1:B:70:MET:CE	2.42	0.49
1:D:64:ASP:O	1:D:68:LYS:HB2	2.12	0.49
1:C:373:MET:HG3	1:C:375:TRP:CZ2	2.48	0.49
1:C:226:THR:HG21	2:C:431:CBI:O2	2.12	0.49
1:C:293:GLU:HG3	1:C:296:LYS:HB3	1.95	0.49
1:C:18:ARG:HB2	1:C:28:VAL:HG21	1.93	0.49
1:C:325:THR:HB	1:C:326:PRO:HD2	1.95	0.49
1:D:366:TRP:HB3	4:D:599:HOH:O	2.11	0.49
1:A:145:TYR:HB2	1:A:213:ILE:O	2.12	0.49
1:A:290:SER:HB3	1:A:299:GLN:HG3	1.95	0.49
1:B:155:MET:O	1:B:158:TYR:O	2.30	0.49
1:B:187:ALA:O	1:B:188:ASN:HB2	2.13	0.49
1:D:34:ILE:HG22	1:D:39:ARG:HH21	1.76	0.49
1:A:109:TYR:CE1	1:A:362:VAL:HG13	2.48	0.49
1:A:48:ASN:O	1:A:58:ALA:HB3	2.12	0.49
1:C:206:TYR:HB3	1:C:237:VAL:HG11	1.94	0.49
1:C:122:LEU:O	1:C:292:PHE:HB2	2.13	0.49
1:C:55:TRP:CG	1:C:189:ILE:HG13	2.47	0.49
1:C:384:LYS:O	1:C:385:GLU:O	2.31	0.49
1:A:418:ASN:O	1:A:420:ARG:HG2	2.13	0.49
1:B:99:GLU:OE1	1:C:81:TYR:OH	2.30	0.49
1:C:1:PCA:HG3	1:C:182:PHE:CD2	2.47	0.49
1:C:148:ALA:HA	1:C:359:MET:HA	1.94	0.49
1:A:215:VAL:HA	1:A:225:PHE:HD2	1.78	0.48
1:D:373:MET:SD	1:D:376:LEU:HD23	2.52	0.48
1:D:49:CYS:O	1:D:56:THR:HG23	2.13	0.48
1:A:340:ASN:HD21	1:A:342:PHE:CB	2.24	0.48
1:B:128:ALA:HA	1:B:288:VAL:O	2.12	0.48
1:B:142:SER:OG	1:B:142:SER:O	2.30	0.48
1:B:180:LEU:HB2	1:B:183:VAL:HG23	1.96	0.48
1:B:188:ASN:HB3	1:B:192:TRP:CZ3	2.47	0.48
1:B:145:TYR:CD1	1:B:362:VAL:HB	2.49	0.48
1:B:353:ASN:O	1:B:357:VAL:HG23	2.12	0.48
1:C:40:TRP:HB3	1:C:72:GLU:HB2	1.94	0.48
1:C:126:GLU:CD	1:C:425:GLY:H	2.16	0.48
1:A:15:THR:HA	1:A:28:VAL:O	2.12	0.48
1:D:36:ALA:O	1:D:39:ARG:HB2	2.13	0.48
1:A:257:ASP:HB2	1:A:341:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:THR:O	1:D:27:THR:HG22	2.12	0.48
1:B:209:CYS:HB2	1:B:236:HIS:CD2	2.48	0.48
1:B:264:ASN:OD1	1:B:266:TYR:HB3	2.13	0.48
1:C:39:ARG:NH1	1:C:39:ARG:HA	2.25	0.48
1:C:384:LYS:HA	1:C:384:LYS:HD2	1.52	0.48
1:C:18:ARG:CB	1:C:26:GLN:HG2	2.43	0.48
1:D:327:GLU:O	1:D:331:THR:HG23	2.13	0.48
1:B:80:THR:HG22	1:B:81:TYR:CG	2.48	0.48
1:A:177:ALA:CB	1:A:180:LEU:HG	2.43	0.48
1:A:178:ARG:HE	1:A:205:PRO:HA	1.79	0.48
1:B:340:ASN:CG	1:B:343:GLU:HB2	2.34	0.48
1:D:2:ARG:HH21	1:D:68:LYS:N	2.11	0.48
1:B:14:LEU:HD23	1:B:110:LEU:HD11	1.95	0.48
1:C:139:GLY:CA	1:C:400:GLY:HA2	2.38	0.48
1:D:182:PHE:CD1	1:D:187:ALA:HA	2.49	0.48
1:D:80:THR:HG22	1:D:80:THR:O	2.13	0.48
1:C:327:GLU:O	1:C:330:SER:OG	2.30	0.48
1:B:244:GLY:HA3	1:B:254:GLY:H	1.78	0.48
1:C:264:ASN:H	1:C:268:MET:CE	2.26	0.48
1:D:93:LYS:HE3	1:D:413:GLN:OE1	2.12	0.48
1:D:129:PHE:HE2	1:D:131:VAL:HB	1.78	0.48
1:B:114:PRO:HG2	1:B:115:ASP:OD2	2.13	0.48
1:A:316:GLU:OE2	1:A:316:GLU:HA	2.14	0.48
1:A:391:ALA:O	1:A:392:ARG:HG3	2.13	0.48
1:B:48:ASN:O	1:B:56:THR:HG21	2.14	0.48
1:C:35:ASP:HB3	1:C:38:TRP:CZ3	2.48	0.48
1:D:414:VAL:HG21	1:D:416:TRP:CZ2	2.48	0.48
1:D:423:PRO:O	1:D:426:SER:HB3	2.13	0.48
1:C:14:LEU:H	1:C:31:GLU:HA	1.78	0.48
1:D:352:ASN:HA	1:D:355:LEU:HB2	1.95	0.48
1:D:93:LYS:HE2	4:D:530:HOH:O	2.13	0.48
1:A:50:TYR:N	1:A:56:THR:HG23	2.29	0.48
1:A:55:TRP:HB3	1:A:189:ILE:CD1	2.44	0.48
1:B:115:ASP:OD2	1:B:115:ASP:N	2.47	0.48
1:C:18:ARG:HD2	1:C:26:GLN:OE1	2.14	0.48
1:A:131:VAL:HA	1:A:415:VAL:O	2.14	0.48
1:A:280:LEU:HD21	1:A:301:PHE:CG	2.48	0.48
1:B:136:VAL:HG21	1:B:414:VAL:HB	1.95	0.48
1:D:330:SER:O	1:D:334:ASP:OD2	2.31	0.48
1:B:249:GLU:H	1:B:249:GLU:HG2	1.51	0.48
1:A:326:PRO:O	1:A:330:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD21	1:B:108:PHE:CD1	2.49	0.48
1:B:80:THR:OG1	1:C:76:ASP:HB2	2.13	0.48
1:C:94:PHE:CD2	1:C:95:VAL:HG23	2.49	0.48
1:B:41:LEU:HD13	1:B:69:CYS:HB3	1.96	0.47
1:D:215:VAL:HG22	1:D:225:PHE:HE2	1.78	0.47
1:B:10:ASN:O	1:B:12:PRO:HD3	2.14	0.47
1:C:119:MET:SD	1:C:151:GLU:HG3	2.54	0.47
1:B:183:VAL:HG11	1:B:206:TYR:HB3	1.95	0.47
1:A:164:GLY:HA2	1:A:169:THR:OG1	2.15	0.47
1:C:134:SER:HB2	1:C:283:SER:HA	1.95	0.47
1:C:387:GLN:O	1:C:390:ALA:HB3	2.13	0.47
1:C:106:SER:OG	1:C:108:PHE:HE1	1.96	0.47
1:B:135:THR:O	1:B:137:GLU:HG2	2.14	0.47
1:A:320:ASN:O	1:A:321:SER:HB3	2.14	0.47
1:B:126:GLU:OE1	1:B:424:ILE:HA	2.14	0.47
1:A:308:ILE:HG22	1:A:308:ILE:O	2.15	0.47
1:C:309:GLU:HG2	4:C:525:HOH:O	2.15	0.47
1:B:1:PCA:HA	1:B:66:ALA:O	2.15	0.47
1:D:2:ARG:H	1:D:2:ARG:HG2	1.34	0.47
1:B:128:ALA:HB1	1:B:289:VAL:HG22	1.95	0.47
1:A:389:GLY:HA3	4:A:495:HOH:O	2.15	0.47
1:B:130:ASP:CG	1:B:418:ASN:HD22	2.17	0.47
1:B:117:TYR:H	1:B:151:GLU:HG2	1.78	0.47
1:D:115:ASP:O	1:D:165:ALA:HB3	2.15	0.47
1:C:275:GLY:CA	1:C:278:LYS:HG3	2.45	0.47
1:C:7:THR:O	1:C:73:GLY:HA3	2.15	0.47
1:D:96:THR:HG1	1:D:103:ASN:HB3	1.79	0.47
1:D:374:LEU:HD21	1:D:399:SER:O	2.13	0.47
1:B:181:LYS:HE3	1:B:181:LYS:HB2	1.29	0.47
1:C:241:THR:O	1:C:253:ALA:HB1	2.15	0.47
1:D:107:ARG:HG2	1:D:109:TYR:CE1	2.50	0.47
1:D:189:ILE:HG23	1:D:190:GLU:HG3	1.95	0.47
1:C:375:TRP:O	1:C:392:ARG:HG2	2.14	0.47
1:A:173:ASP:HB2	1:A:212:GLU:CD	2.35	0.47
1:A:379:ILE:CG2	1:A:385:GLU:HB2	2.43	0.47
1:A:178:ARG:HG2	1:A:204:GLY:O	2.15	0.47
1:C:230:CYS:HB3	1:C:255:LYS:O	2.14	0.47
1:A:22:PRO:O	1:A:429:ASP:OD2	2.32	0.47
1:C:82:GLY:O	1:C:93:LYS:HB2	2.15	0.47
1:D:336:PHE:O	1:D:337:ASN:HB2	2.14	0.47
1:A:95:VAL:HG23	1:A:410:PRO:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:THR:CG2	1:D:29:ASN:HD21	2.23	0.47
1:C:257:ASP:CG	1:C:260:GLY:H	2.18	0.47
1:C:245:GLY:H	1:C:251:ARG:HA	1.79	0.47
1:A:319:PRO:HG2	1:A:328:LEU:HD23	1.97	0.47
1:C:117:TYR:OH	1:C:168:GLY:HA2	2.15	0.47
1:D:415:VAL:HG13	1:D:415:VAL:O	2.14	0.47
1:A:252:PHE:HE2	1:A:259:ASN:ND2	2.13	0.47
1:D:341:ARG:HD2	1:D:345:VAL:HG13	1.97	0.47
1:D:94:PHE:CD1	1:D:104:VAL:HG12	2.50	0.47
1:D:31:GLU:HG3	1:D:111:MET:CB	2.43	0.47
1:C:262:ASP:O	1:C:268:MET:HE3	2.14	0.47
1:C:263:TYR:OH	1:C:321:SER:O	2.33	0.47
1:B:231:THR:CG2	1:B:345:VAL:HB	2.44	0.47
1:D:266:TYR:CZ	1:D:271:PRO:HB3	2.50	0.47
1:C:147:VAL:HG23	1:C:149:MET:HG2	1.97	0.47
1:B:306:ARG:HB3	1:B:306:ARG:HE	1.56	0.47
1:B:175:GLN:O	1:B:176:CYS:HB2	2.15	0.46
1:C:155:MET:HA	1:C:161:ASN:CB	2.33	0.46
1:D:105:GLY:CA	1:D:365:ILE:HG23	2.42	0.46
1:A:343:GLU:HA	1:A:347:GLY:N	2.26	0.46
1:B:15:THR:HB	1:B:27:THR:CG2	2.45	0.46
1:C:32:VAL:HG12	1:C:109:TYR:C	2.35	0.46
1:D:136:VAL:HG11	1:D:142:SER:OG	2.15	0.46
1:B:196:THR:OG1	1:B:196:THR:O	2.30	0.46
1:D:35:ASP:HB2	1:D:109:TYR:CE2	2.51	0.46
1:C:312:PRO:HB3	1:C:321:SER:HA	1.97	0.46
1:D:280:LEU:HA	1:D:303:GLN:OE1	2.16	0.46
1:B:126:GLU:HB3	1:B:291:ARG:HG2	1.95	0.46
1:A:379:ILE:HA	1:A:391:ALA:HA	1.96	0.46
1:C:26:GLN:HG3	1:C:28:VAL:HG22	1.98	0.46
1:C:147:VAL:HG12	1:C:212:GLU:HB3	1.97	0.46
1:C:122:LEU:HB3	1:C:292:PHE:CB	2.45	0.46
1:B:82:GLY:O	1:B:93:LYS:HB2	2.14	0.46
1:C:193:LYS:HB2	1:C:203:VAL:O	2.16	0.46
1:D:45:ASN:O	1:D:46:MET:HB2	2.16	0.46
1:D:229:ALA:O	1:D:257:ASP:HB2	2.15	0.46
1:D:307:LYS:HD2	1:D:430:PHE:CD2	2.51	0.46
1:C:160:SER:OG	1:C:160:SER:O	2.30	0.46
1:B:39:ARG:HH21	1:B:167:TYR:C	2.18	0.46
1:D:223:PHE:O	1:D:224:ALA:HB2	2.15	0.46
1:A:293:GLU:OE1	1:A:298:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:HA	1:B:416:TRP:O	2.16	0.46
1:C:166:ARG:HB2	1:C:167:TYR:CD2	2.50	0.46
1:B:144:LEU:O	1:B:145:TYR:HB3	2.15	0.46
1:B:213:ILE:HG22	1:B:213:ILE:O	2.15	0.46
1:C:14:LEU:HD12	1:C:15:THR:N	2.31	0.46
1:D:174:ALA:HB1	1:D:257:ASP:O	2.16	0.46
1:D:400:GLY:O	1:D:402:PRO:HD3	2.14	0.46
1:A:297:LEU:O	1:A:323:GLU:HA	2.16	0.46
1:D:2:ARG:HA	1:D:162:GLN:HB2	1.98	0.46
1:C:392:ARG:N	1:C:392:ARG:HD2	2.31	0.46
1:C:392:ARG:HG2	1:C:392:ARG:HH11	1.79	0.46
1:D:126:GLU:HB2	1:D:291:ARG:HA	1.96	0.46
1:C:288:VAL:HG13	1:C:299:GLN:HE21	1.80	0.46
1:B:377:ASP:O	1:B:378:SER:HB2	2.16	0.46
1:A:380:TYR:HB3	1:A:392:ARG:CZ	2.46	0.46
1:C:146:PHE:O	1:C:212:GLU:HA	2.16	0.46
1:B:50:TYR:CD1	1:B:55:TRP:HA	2.51	0.46
1:C:121:ASN:ND2	1:C:121:ASN:H	2.14	0.46
1:C:221:TYR:O	1:C:222:ALA:HB2	2.16	0.46
1:C:227:PRO:HG3	1:C:297:LEU:CD2	2.45	0.46
1:D:7:THR:HA	1:D:8:PRO:HD3	1.67	0.46
1:C:263:TYR:OH	1:C:322:SER:HA	2.16	0.46
1:C:105:GLY:HA3	1:C:365:ILE:O	2.16	0.46
1:A:114:PRO:HB2	1:A:166:ARG:CZ	2.45	0.46
1:C:318:MET:HE1	1:C:336:PHE:CZ	2.51	0.46
1:D:113:GLY:O	1:D:115:ASP:N	2.49	0.46
1:C:164:GLY:HA2	1:C:169:THR:OG1	2.15	0.46
1:C:319:PRO:HD3	1:C:331:THR:OG1	2.15	0.46
1:A:149:MET:CE	1:A:360:VAL:HG21	2.45	0.46
1:A:96:THR:OG1	1:A:103:ASN:O	2.30	0.46
1:B:400:GLY:O	1:B:402:PRO:HD3	2.16	0.46
1:C:208:SER:OG	1:C:235:TYR:OH	2.30	0.46
1:B:48:ASN:O	1:B:56:THR:OG1	2.30	0.46
1:B:226:THR:HG23	1:B:261:CYS:C	2.36	0.46
1:C:269:GLY:O	1:C:314:THR:HG21	2.16	0.46
1:D:293:GLU:HB2	1:D:296:LYS:O	2.16	0.46
1:D:105:GLY:O	1:D:106:SER:HB3	2.16	0.46
1:D:141:ASN:HB2	1:D:373:MET:SD	2.56	0.46
1:D:157:SER:O	1:D:159:PRO:HD3	2.15	0.46
1:A:2:ARG:HH22	1:A:70:MET:CE	2.27	0.46
1:A:9:GLU:OE1	1:A:33:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:N	4:A:518:HOH:O	2.48	0.46
1:D:172:CYS:O	1:D:173:ASP:HB3	2.16	0.46
1:B:147:VAL:CG1	1:B:212:GLU:HB2	2.39	0.46
1:A:267:ARG:HE	1:A:389:GLY:CA	2.28	0.46
1:C:257:ASP:HA	1:C:341:ARG:HG2	1.98	0.46
1:A:39:ARG:NH1	1:A:73:GLY:HA2	2.30	0.46
1:A:132:ASP:HB3	1:A:415:VAL:CG1	2.46	0.46
1:B:341:ARG:NH1	1:B:344:GLU:OE1	2.49	0.46
1:B:15:THR:O	1:B:15:THR:OG1	2.30	0.46
1:A:211:ALA:HB2	1:A:233:ASN:HB3	1.99	0.45
1:D:408:GLN:HG3	1:D:409:PHE:CD1	2.38	0.45
1:B:354:ALA:HA	1:B:357:VAL:HG23	1.98	0.45
1:B:227:PRO:CG	1:B:324:ILE:HG21	2.41	0.45
1:C:94:PHE:CZ	1:C:104:VAL:HG13	2.52	0.45
1:C:266:TYR:CD2	1:C:271:PRO:HA	2.51	0.45
1:B:366:TRP:HE3	1:B:367:ASP:O	1.99	0.45
1:B:327:GLU:N	1:B:327:GLU:OE2	2.50	0.45
1:C:336:PHE:HA	1:C:388:PRO:HB2	1.98	0.45
1:B:76:ASP:OD1	1:B:76:ASP:O	2.34	0.45
1:C:324:ILE:HG22	1:C:324:ILE:O	2.16	0.45
1:A:225:PHE:CZ	1:A:297:LEU:HB3	2.50	0.45
1:D:2:ARG:O	1:D:71:ILE:N	2.50	0.45
1:C:78:LEU:O	1:C:80:THR:N	2.50	0.45
1:B:126:GLU:OE2	1:B:427:THR:OG1	2.30	0.45
1:B:291:ARG:HB3	1:B:424:ILE:HG12	1.98	0.45
1:B:152:ASP:OD2	1:B:155:MET:HB2	2.16	0.45
1:C:275:GLY:HA3	1:C:278:LYS:HG3	1.98	0.45
1:B:175:GLN:NE2	3:B:431:CTT:O2D	2.49	0.45
1:B:178:ARG:NE	1:B:248:SER:OG	2.49	0.45
1:B:384:LYS:HG3	1:B:387:GLN:HB2	1.98	0.45
1:B:1:PCA:O	1:B:162:GLN:N	2.50	0.45
1:C:264:ASN:O	1:C:267:ARG:N	2.50	0.45
1:B:227:PRO:HB2	1:B:351:LEU:CD1	2.46	0.45
1:B:299:GLN:HG3	1:B:300:TYR:N	2.31	0.45
1:D:264:ASN:O	1:D:268:MET:N	2.50	0.45
1:A:133:LEU:HD12	1:A:133:LEU:H	1.80	0.45
1:B:200:ASN:ND2	4:B:504:HOH:O	2.50	0.45
1:D:371:ALA:O	1:D:373:MET:N	2.50	0.45
1:D:38:TRP:HE3	1:D:38:TRP:H	1.64	0.45
1:C:32:VAL:CG1	1:C:110:LEU:HA	2.45	0.45
1:D:200:ASN:N	1:D:200:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:O	1:C:26:GLN:N	2.50	0.45
1:B:39:ARG:NH2	1:B:167:TYR:HA	2.32	0.45
1:A:39:ARG:NE	1:A:167:TYR:O	2.50	0.45
1:C:135:THR:HG22	1:C:135:THR:O	2.17	0.45
1:D:181:LYS:HB2	1:D:181:LYS:HE2	1.66	0.45
1:B:267:ARG:NH1	3:B:431:CTT:H6B	2.32	0.45
1:A:17:GLN:HE21	1:A:25:CYS:HB2	1.81	0.45
1:A:51:ASP:O	1:A:53:ASN:N	2.50	0.45
1:C:265:PRO:O	1:C:270:ASN:ND2	2.50	0.45
1:B:380:TYR:CG	1:B:381:PRO:HA	2.51	0.45
1:B:115:ASP:OD1	1:B:166:ARG:NH1	2.50	0.45
1:C:212:GLU:O	1:C:212:GLU:HG3	2.16	0.45
1:B:9:GLU:OE2	1:B:39:ARG:NH1	2.50	0.45
1:D:270:ASN:OD1	1:D:311:PRO:HB2	2.16	0.45
1:B:251:ARG:NH2	3:B:431:CTT:O6C	2.49	0.45
1:A:348:PHE:HD2	1:A:352:ASN:ND2	2.15	0.45
1:D:107:ARG:HD3	2:D:432:CBI:C2'	2.46	0.45
1:C:39:ARG:CA	1:C:39:ARG:HH11	2.29	0.45
1:B:112:ASN:ND2	1:B:118:GLN:OE1	2.50	0.45
1:C:188:ASN:HB2	1:C:192:TRP:CZ3	2.52	0.45
1:A:252:PHE:O	1:A:341:ARG:NH1	2.50	0.45
1:D:215:VAL:HG21	1:D:292:PHE:HZ	1.81	0.45
1:D:178:ARG:HB2	1:D:203:VAL:HG13	1.99	0.45
1:D:401:VAL:O	1:D:404:GLU:N	2.50	0.45
1:D:239:GLU:O	1:D:242:ASN:ND2	2.50	0.45
1:C:401:VAL:HG11	1:C:404:GLU:OE2	2.16	0.45
1:C:42:HIS:HB2	1:C:47:GLN:O	2.17	0.45
1:C:264:ASN:C	1:C:268:MET:HG2	2.37	0.45
1:D:409:PHE:N	1:D:410:PRO:HD3	2.32	0.45
1:B:402:PRO:O	1:B:405:VAL:HG22	2.17	0.45
1:C:124:GLY:N	1:C:292:PHE:O	2.49	0.45
1:B:77:TYR:HD2	1:B:81:TYR:HD2	1.65	0.45
1:D:296:LYS:HE3	4:D:545:HOH:O	2.16	0.45
1:B:180:LEU:HB2	1:B:183:VAL:CG2	2.47	0.45
1:D:9:GLU:OE1	1:D:77:TYR:OH	2.30	0.45
1:D:35:ASP:OD2	1:D:38:TRP:HZ3	1.99	0.45
1:B:228:HIS:ND1	1:B:257:ASP:O	2.50	0.45
1:C:32:VAL:CG1	1:C:110:LEU:HD22	2.47	0.45
1:C:118:GLN:NE2	4:C:540:HOH:O	2.50	0.45
1:B:152:ASP:OD2	1:B:155:MET:N	2.50	0.45
1:D:387:GLN:NE2	4:D:595:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TYR:HA	1:A:159:PRO:HD3	1.58	0.45
1:C:93:LYS:HE3	1:C:96:THR:HG22	1.99	0.45
1:D:110:LEU:O	1:D:117:TYR:HB3	2.16	0.45
1:D:380:TYR:O	1:D:392:ARG:NH2	2.50	0.45
1:B:22:PRO:HD3	1:B:425:GLY:O	2.16	0.45
1:C:91:THR:HA	1:C:415:VAL:HA	1.98	0.45
1:B:61:THR:N	1:B:64:ASP:OD2	2.50	0.45
1:C:401:VAL:HB	1:C:404:GLU:HB2	1.98	0.45
1:A:413:GLN:NE2	1:A:413:GLN:O	2.50	0.45
1:D:163:ALA:HB1	1:D:167:TYR:CG	2.52	0.44
1:D:71:ILE:HD11	1:D:163:ALA:CB	2.47	0.44
1:C:267:ARG:HA	1:C:391:ALA:O	2.18	0.44
1:C:32:VAL:HG12	1:C:110:LEU:HA	2.00	0.44
1:D:251:ARG:NH2	2:D:431:CBI:O6	2.50	0.44
1:A:300:TYR:CD1	1:A:307:LYS:HD2	2.52	0.44
1:A:197:SER:OG	1:A:198:ASP:N	2.50	0.44
1:C:198:ASP:OD1	1:C:201:ALA:N	2.50	0.44
1:A:274:TYR:HA	1:A:280:LEU:O	2.17	0.44
1:A:280:LEU:CD2	1:A:308:ILE:HG21	2.47	0.44
1:B:349:GLU:HA	1:B:352:ASN:OD1	2.17	0.44
1:D:218:SER:OG	1:D:219:ASN:N	2.49	0.44
1:C:116:LYS:HG2	1:C:116:LYS:H	1.38	0.44
1:B:175:GLN:NE2	3:B:431:CTT:O6C	2.50	0.44
1:B:67:GLU:OE2	1:B:162:GLN:NE2	2.50	0.44
1:D:38:TRP:CZ2	1:D:106:SER:HA	2.52	0.44
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.79	0.44
1:A:12:PRO:O	1:A:32:VAL:N	2.50	0.44
1:B:354:ALA:O	1:B:357:VAL:N	2.50	0.44
1:D:16:TRP:HZ3	1:D:421:PHE:HB3	1.82	0.44
1:A:1:PCA:HG3	1:A:182:PHE:CD1	2.52	0.44
1:A:55:TRP:HE3	1:A:189:ILE:HD12	1.81	0.44
1:A:381:PRO:HA	1:A:382:PRO:HD3	1.83	0.44
1:D:65:CYS:HB3	1:D:182:PHE:HZ	1.82	0.44
1:C:212:GLU:O	1:C:228:HIS:HD2	2.00	0.44
1:A:133:LEU:HA	1:A:136:VAL:HG23	1.99	0.44
1:C:291:ARG:HE	1:C:424:ILE:CG2	2.30	0.44
1:B:82:GLY:O	1:B:93:LYS:N	2.50	0.44
1:B:26:GLN:NE2	1:B:27:THR:O	2.50	0.44
1:B:178:ARG:HD2	1:B:207:GLY:HA3	2.00	0.44
1:B:243:CYS:O	1:B:254:GLY:N	2.50	0.44
1:B:84:SER:O	1:B:90:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ASP:OD1	1:C:267:ARG:NH1	2.50	0.44
1:B:94:PHE:CE2	1:B:95:VAL:HG23	2.52	0.44
1:C:34:ILE:HB	1:C:77:TYR:HE2	1.82	0.44
1:D:303:GLN:O	1:D:306:ARG:N	2.50	0.44
1:A:42:HIS:NE2	1:A:72:GLU:OE2	2.50	0.44
1:C:176:CYS:O	1:C:178:ARG:N	2.50	0.44
1:C:213:ILE:HD12	1:C:213:ILE:N	2.33	0.44
1:C:333:PHE:O	1:C:337:ASN:N	2.50	0.44
1:B:44:ASP:OD1	1:B:45:ASN:N	2.50	0.44
1:A:239:GLU:O	1:A:242:ASN:ND2	2.50	0.44
1:A:337:ASN:ND2	4:A:461:HOH:O	2.50	0.44
1:D:76:ASP:OD2	1:D:79:GLY:N	2.50	0.44
1:C:92:LEU:HB2	1:C:414:VAL:CG1	2.46	0.44
1:D:219:ASN:ND2	1:D:377:ASP:OD2	2.50	0.44
1:B:174:ALA:O	1:B:258:ALA:HA	2.17	0.44
1:B:183:VAL:N	1:B:186:LYS:O	2.50	0.44
1:D:96:THR:N	1:D:103:ASN:O	2.50	0.44
1:A:149:MET:HE2	1:A:360:VAL:CG2	2.44	0.44
1:D:342:PHE:HZ	1:D:348:PHE:HA	1.83	0.44
1:A:376:LEU:O	1:A:392:ARG:HB3	2.18	0.44
1:B:229:ALA:N	4:B:557:HOH:O	2.49	0.44
1:D:50:TYR:OH	1:D:200:ASN:O	2.35	0.44
1:C:18:ARG:NH2	4:C:540:HOH:O	2.50	0.44
1:B:48:ASN:ND2	1:B:50:TYR:O	2.50	0.44
1:B:209:CYS:O	1:B:210:CYS:HB3	2.17	0.44
1:A:45:ASN:O	1:A:46:MET:HB2	2.17	0.44
1:D:4:GLY:HA3	1:D:72:GLU:CD	2.38	0.44
1:B:342:PHE:O	1:B:347:GLY:HA2	2.16	0.44
1:C:339:ARG:NH2	4:C:498:HOH:O	2.50	0.44
1:D:31:GLU:HG3	1:D:111:MET:HE2	1.99	0.44
1:D:2:ARG:CB	1:D:70:MET:HB3	2.48	0.44
1:D:134:SER:O	1:D:134:SER:OG	2.29	0.44
1:D:280:LEU:HD23	1:D:308:ILE:HG21	1.99	0.44
1:D:246:THR:OG1	1:D:251:ARG:NH1	2.50	0.44
1:C:18:ARG:O	1:C:25:CYS:HA	2.17	0.44
1:D:327:GLU:O	1:D:331:THR:OG1	2.30	0.44
1:C:369:HIS:ND1	1:C:402:PRO:HG3	2.32	0.44
1:B:172:CYS:HB2	1:B:209:CYS:C	2.38	0.44
1:C:326:PRO:HG2	1:C:327:GLU:OE2	2.18	0.44
1:A:21:ALA:O	1:A:23:GLY:N	2.49	0.44
1:D:334:ASP:OD2	1:D:334:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ASP:OD1	1:C:88:ASP:N	2.50	0.44
4:A:463:HOH:O	1:B:116:LYS:HE2	2.17	0.44
1:C:319:PRO:HG2	1:C:328:LEU:HD23	1.99	0.44
1:D:295:ASN:N	1:D:295:ASN:OD1	2.50	0.44
1:D:129:PHE:CE2	1:D:131:VAL:HB	2.52	0.44
1:A:50:TYR:O	1:A:51:ASP:HB2	2.18	0.44
1:B:17:GLN:O	1:B:420:ARG:HA	2.17	0.44
1:A:380:TYR:HA	1:A:381:PRO:HA	1.61	0.44
1:B:80:THR:HG22	1:B:81:TYR:CD1	2.52	0.44
1:C:357:VAL:HA	1:C:358:PRO:HD2	1.78	0.44
1:B:197:SER:CB	1:B:369:HIS:HB2	2.47	0.44
1:C:244:GLY:HA2	1:C:253:ALA:HB3	2.00	0.44
1:C:226:THR:CG2	1:C:262:ASP:HB3	2.42	0.44
1:C:268:MET:O	1:C:313:PRO:HB3	2.18	0.44
1:C:128:ALA:HB2	1:C:289:VAL:HG22	2.00	0.44
1:A:90:LEU:HD12	1:A:91:THR:N	2.31	0.44
1:A:267:ARG:NE	1:A:389:GLY:O	2.50	0.44
1:A:302:ILE:O	1:A:302:ILE:HG22	2.17	0.44
1:A:315:TRP:CH2	1:A:388:PRO:HB3	2.53	0.44
1:C:119:MET:HB3	1:C:119:MET:HE2	1.76	0.44
1:B:160:SER:OG	1:B:185:GLY:HA3	2.18	0.44
1:A:262:ASP:N	1:A:262:ASP:OD1	2.50	0.44
1:D:2:ARG:HG2	1:D:69:CYS:O	2.18	0.44
1:B:290:SER:OG	1:B:299:GLN:NE2	2.50	0.44
1:B:274:TYR:O	1:B:278:LYS:HD2	2.17	0.44
1:A:380:TYR:O	1:A:392:ARG:NH2	2.50	0.44
1:D:50:TYR:OH	1:D:192:TRP:NE1	2.50	0.44
1:D:247:TYR:HB2	4:D:608:HOH:O	2.18	0.44
1:A:152:ASP:OD2	1:A:156:ALA:HB2	2.18	0.44
1:A:120:PHE:N	1:A:359:MET:O	2.50	0.43
1:A:146:PHE:HB3	1:A:359:MET:CB	2.38	0.43
1:C:133:LEU:HD11	1:C:286:PHE:CE2	2.52	0.43
1:D:428:TYR:O	1:D:430:PHE:N	2.50	0.43
1:A:51:ASP:N	1:A:54:GLN:O	2.50	0.43
1:C:41:LEU:HD23	1:C:70:MET:C	2.38	0.43
1:D:375:TRP:CZ2	2:D:431:CBI:H5	2.53	0.43
1:B:130:ASP:OD1	1:B:130:ASP:N	2.50	0.43
1:C:208:SER:HG	1:C:235:TYR:HH	1.61	0.43
1:B:152:ASP:CG	1:B:155:MET:H	2.22	0.43
1:C:89:ALA:HA	1:C:416:TRP:O	2.18	0.43
1:B:178:ARG:HH21	1:B:248:SER:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:THR:HG23	1:B:186:LYS:HE3	2.00	0.43
1:B:257:ASP:OD2	1:B:260:GLY:N	2.50	0.43
1:C:14:LEU:O	1:C:30:ALA:O	2.36	0.43
1:D:262:ASP:OD1	1:D:262:ASP:N	2.50	0.43
1:D:280:LEU:HD11	1:D:286:PHE:CD1	2.52	0.43
1:A:59:CYS:HB3	1:A:189:ILE:HD13	1.99	0.43
1:C:125:ASN:HD22	1:C:423:PRO:N	2.17	0.43
1:D:133:LEU:H	1:D:133:LEU:HG	1.62	0.43
1:A:150:GLU:H	1:A:150:GLU:HG3	1.29	0.43
1:D:77:TYR:HB3	1:D:83:ALA:CB	2.33	0.43
1:B:145:TYR:O	1:B:362:VAL:HG23	2.18	0.43
1:B:324:ILE:HG22	1:B:324:ILE:O	2.17	0.43
1:A:43:ASP:OD1	1:A:68:LYS:NZ	2.50	0.43
1:A:3:ALA:C	1:A:70:MET:HB2	2.38	0.43
1:A:142:SER:HB3	1:A:414:VAL:HB	2.00	0.43
1:C:52:GLY:O	1:C:200:ASN:HA	2.17	0.43
1:B:144:LEU:HD23	1:B:145:TYR:H	1.83	0.43
1:A:148:ALA:HB2	1:A:359:MET:CE	2.49	0.43
1:A:357:VAL:CG1	1:A:358:PRO:HD2	2.46	0.43
1:A:342:PHE:CD2	1:A:343:GLU:HG3	2.39	0.43
1:A:182:PHE:O	1:A:183:VAL:HG23	2.18	0.43
1:C:192:TRP:HE1	1:C:202:GLY:HA3	1.84	0.43
1:B:368:ASP:HB3	1:B:373:MET:HE2	1.99	0.43
1:C:228:HIS:ND1	1:C:257:ASP:O	2.50	0.43
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.17	0.43
1:A:171:TYR:O	1:A:180:LEU:HD11	2.18	0.43
1:D:181:LYS:O	1:D:188:ASN:HB2	2.18	0.43
1:C:43:ASP:OD2	1:C:47:GLN:N	2.49	0.43
1:C:409:PHE:N	1:C:410:PRO:HD3	2.33	0.43
1:B:133:LEU:HD13	1:B:219:ASN:O	2.19	0.43
1:A:60:SER:HB3	1:A:64:ASP:OD1	2.19	0.43
1:D:266:TYR:CD2	1:D:271:PRO:HA	2.54	0.43
1:B:384:LYS:O	1:B:385:GLU:HB3	2.18	0.43
1:D:63:THR:HB	1:D:64:ASP:H	1.69	0.43
1:C:144:LEU:HD23	1:C:215:VAL:HB	1.99	0.43
1:D:245:GLY:HA2	1:D:258:ALA:HB2	2.00	0.43
1:D:401:VAL:C	1:D:405:VAL:HG22	2.38	0.43
1:D:180:LEU:N	1:D:180:LEU:HD23	2.33	0.43
1:A:369:HIS:CG	1:A:402:PRO:HG2	2.54	0.43
1:D:137:GLU:O	1:D:219:ASN:ND2	2.52	0.43
1:C:82:GLY:CA	1:C:96:THR:HG21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:PRO:HB3	1:C:321:SER:CA	2.48	0.43
1:A:119:MET:HE1	1:A:149:MET:O	2.19	0.43
1:A:362:VAL:HG12	1:A:363:MET:N	2.34	0.43
1:B:354:ALA:O	1:B:357:VAL:HB	2.19	0.43
1:A:2:ARG:O	1:A:70:MET:HA	2.18	0.43
1:A:259:ASN:N	1:A:259:ASN:OD1	2.51	0.43
1:D:263:TYR:OH	1:D:312:PRO:HA	2.19	0.43
1:C:64:ASP:OD1	1:C:68:LYS:HD2	2.19	0.43
1:A:368:ASP:H	1:A:373:MET:HE2	1.83	0.43
1:D:61:THR:O	1:D:64:ASP:OD2	2.37	0.43
1:C:216:TRP:NE1	1:C:218:SER:OG	2.50	0.43
1:A:17:GLN:HE21	1:A:25:CYS:CB	2.32	0.43
1:A:134:SER:HB2	1:A:283:SER:O	2.19	0.43
1:D:182:PHE:CZ	1:D:187:ALA:HB2	2.53	0.43
1:B:39:ARG:HH11	1:B:39:ARG:HD3	1.68	0.43
1:C:136:VAL:HG12	1:C:140:ILE:HB	2.00	0.43
1:D:272:ASP:C	1:D:278:LYS:HD3	2.38	0.43
1:C:275:GLY:C	1:C:278:LYS:HG3	2.39	0.43
1:A:17:GLN:HB2	1:A:26:GLN:O	2.18	0.43
1:A:333:PHE:O	1:A:337:ASN:N	2.50	0.43
1:D:374:LEU:O	1:D:378:SER:HB3	2.19	0.43
1:B:17:GLN:HG3	4:B:520:HOH:O	2.19	0.43
1:A:378:SER:O	1:A:392:ARG:HD2	2.18	0.43
1:D:146:PHE:CE2	1:D:361:LEU:HB2	2.54	0.43
1:A:13:PRO:HA	1:A:31:GLU:HA	2.00	0.43
1:D:318:MET:HG2	1:D:331:THR:O	2.19	0.43
1:A:302:ILE:HG12	1:A:430:PHE:CE1	2.52	0.43
1:A:63:THR:O	1:A:63:THR:HG22	2.18	0.43
1:B:1:PCA:HB2	1:B:2:ARG:H	1.61	0.43
1:B:110:LEU:HB2	1:B:361:LEU:HD23	2.01	0.43
1:D:123:MET:SD	1:D:294:GLU:HG3	2.58	0.43
1:D:18:ARG:NH1	1:D:118:GLN:HE22	2.16	0.43
1:A:83:ALA:HB2	1:A:108:PHE:HZ	1.83	0.43
1:C:315:TRP:O	1:C:318:MET:HB2	2.19	0.43
1:B:9:GLU:HB2	1:B:167:TYR:CZ	2.54	0.43
1:C:55:TRP:CZ2	1:C:181:LYS:HG2	2.54	0.43
1:B:139:GLY:HA2	1:B:377:ASP:OD2	2.19	0.42
1:A:31:GLU:HG2	1:A:111:MET:HB2	2.01	0.42
1:A:114:PRO:HB2	1:A:166:ARG:NH2	2.34	0.42
1:C:173:ASP:HB2	1:C:174:ALA:H	1.68	0.42
1:A:300:TYR:CG	1:A:307:LYS:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ILE:HG12	1:A:430:PHE:HE1	1.83	0.42
1:D:149:MET:SD	1:D:171:TYR:HD1	2.42	0.42
1:C:198:ASP:HB2	1:C:369:HIS:HE2	1.84	0.42
1:D:40:TRP:HB3	1:D:72:GLU:HB2	2.01	0.42
1:A:398:ASP:OD1	1:A:398:ASP:N	2.50	0.42
1:D:21:ALA:HB1	1:D:22:PRO:HD2	2.00	0.42
1:A:323:GLU:HG2	1:A:323:GLU:H	1.32	0.42
1:D:35:ASP:HB3	1:D:38:TRP:HZ3	1.84	0.42
1:C:263:TYR:HE1	1:C:328:LEU:HG	1.84	0.42
1:C:34:ILE:HD12	1:C:108:PHE:CE1	2.54	0.42
1:C:176:CYS:HB3	1:C:207:GLY:HA3	2.01	0.42
1:C:197:SER:OG	1:C:198:ASP:N	2.50	0.42
1:C:82:GLY:HA3	1:C:96:THR:HG21	2.01	0.42
1:B:188:ASN:O	1:B:192:TRP:HE3	2.01	0.42
1:D:111:MET:HE3	1:D:111:MET:HB3	1.86	0.42
1:B:122:LEU:HB3	1:B:355:LEU:HD13	2.02	0.42
1:C:133:LEU:HD21	1:C:216:TRP:CZ2	2.54	0.42
1:D:123:MET:HE1	1:D:352:ASN:HB3	2.01	0.42
1:D:372:ASN:HB2	1:D:374:LEU:HG	2.01	0.42
1:C:299:GLN:O	1:C:310:ILE:HD12	2.19	0.42
1:A:35:ASP:OD2	1:A:107:ARG:NH2	2.49	0.42
1:B:131:VAL:HG13	1:B:286:PHE:CE2	2.54	0.42
1:D:379:ILE:HG12	1:D:391:ALA:HA	2.02	0.42
1:C:381:PRO:HB3	4:C:491:HOH:O	2.19	0.42
1:C:20:THR:OG1	1:C:21:ALA:N	2.51	0.42
1:B:177:ALA:HB1	1:B:180:LEU:HG	1.99	0.42
1:B:254:GLY:O	1:B:256:CYS:N	2.50	0.42
1:C:145:TYR:CE2	1:C:362:VAL:HB	2.55	0.42
1:D:295:ASN:HA	1:D:348:PHE:CE2	2.54	0.42
1:C:306:ARG:NH2	1:D:302:ILE:HG22	2.34	0.42
1:C:178:ARG:HB3	1:C:207:GLY:HA2	2.00	0.42
1:B:99:GLU:HA	1:C:40:TRP:CE3	2.54	0.42
1:D:180:LEU:HB2	1:D:183:VAL:HG23	2.01	0.42
1:A:336:PHE:HD1	1:A:336:PHE:HA	1.70	0.42
1:C:193:LYS:HD2	1:C:203:VAL:HG12	2.02	0.42
1:A:21:ALA:HB1	1:A:22:PRO:HD2	2.00	0.42
1:C:284:ARG:NH1	1:C:304:ASP:OD2	2.50	0.42
1:C:155:MET:HB2	1:C:164:GLY:HA3	2.00	0.42
1:D:109:TYR:CE1	1:D:362:VAL:HG13	2.54	0.42
1:C:384:LYS:HE3	1:C:387:GLN:NE2	2.31	0.42
1:C:38:TRP:CH2	1:C:107:ARG:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LYS:HZ3	1:A:276:LYS:HG2	1.75	0.42
1:B:155:MET:HG3	1:B:164:GLY:CA	2.47	0.42
1:D:40:TRP:CE3	1:D:72:GLU:HG3	2.54	0.42
1:C:147:VAL:HG12	1:C:212:GLU:HB2	2.01	0.42
1:B:58:ALA:HB1	1:B:68:LYS:CE	2.50	0.42
1:D:133:LEU:HA	1:D:136:VAL:HG23	2.02	0.42
1:C:213:ILE:HA	1:C:227:PRO:HA	2.01	0.42
1:D:84:SER:O	1:D:90:LEU:HD12	2.20	0.42
1:A:339:ARG:HH11	1:A:339:ARG:HD2	1.61	0.42
1:D:12:PRO:HD3	1:D:77:TYR:CE1	2.54	0.42
1:D:117:TYR:OH	1:D:169:THR:O	2.30	0.42
1:D:39:ARG:HB3	1:D:71:ILE:CG2	2.47	0.42
1:D:93:LYS:HD2	1:D:413:GLN:OE1	2.19	0.42
1:B:378:SER:O	1:B:392:ARG:HB2	2.19	0.42
1:A:106:SER:OG	1:A:108:PHE:HE1	2.02	0.42
1:A:77:TYR:O	1:A:82:GLY:N	2.52	0.42
1:B:134:SER:HA	1:B:282:THR:O	2.19	0.42
1:D:232:THR:OG1	1:D:255:LYS:NZ	2.49	0.42
1:D:319:PRO:HG3	1:D:327:GLU:HB2	2.00	0.42
1:B:152:ASP:OD1	1:B:154:GLY:N	2.50	0.42
1:C:430:PHE:HD2	1:D:304:ASP:OD1	2.02	0.42
1:B:58:ALA:HB1	1:B:68:LYS:HE2	2.02	0.42
1:A:325:THR:HG1	1:A:327:GLU:HG2	1.81	0.42
1:B:272:ASP:O	1:B:278:LYS:HB2	2.19	0.42
1:A:380:TYR:CG	1:A:381:PRO:HA	2.55	0.42
1:B:183:VAL:CG1	1:B:206:TYR:HB3	2.50	0.42
1:C:226:THR:HG22	1:C:226:THR:O	2.20	0.42
1:C:123:MET:HA	1:C:292:PHE:O	2.20	0.42
1:C:60:SER:HB3	1:C:64:ASP:OD2	2.19	0.42
1:C:104:VAL:HG21	1:C:406:GLU:OE1	2.20	0.42
1:C:234:GLU:HG2	1:C:234:GLU:H	1.53	0.42
1:B:302:ILE:O	1:B:302:ILE:HG22	2.20	0.42
1:B:18:ARG:O	1:B:26:GLN:N	2.50	0.42
1:B:133:LEU:HD13	1:B:219:ASN:C	2.40	0.42
1:A:76:ASP:O	1:A:80:THR:N	2.50	0.42
1:D:226:THR:HG23	1:D:262:ASP:CB	2.40	0.42
1:A:206:TYR:HA	1:A:206:TYR:HD2	1.71	0.42
1:C:237:VAL:HG12	1:C:238:CYS:N	2.35	0.42
1:A:77:TYR:O	1:A:83:ALA:N	2.50	0.42
1:A:426:SER:OG	1:A:426:SER:O	2.37	0.42
1:D:401:VAL:O	1:D:405:VAL:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:MET:HE2	1:A:46:MET:HA	2.01	0.42
1:C:273:PHE:CE1	1:C:311:PRO:HD3	2.55	0.42
1:D:287:THR:O	1:D:301:PHE:HA	2.20	0.42
1:B:205:PRO:O	1:B:239:GLU:HA	2.20	0.41
1:B:122:LEU:HD23	1:B:213:ILE:HD13	2.02	0.41
1:D:91:THR:HG23	1:D:415:VAL:HB	2.02	0.41
1:A:17:GLN:HB2	1:A:27:THR:CA	2.43	0.41
1:D:286:PHE:CB	1:D:303:GLN:HG2	2.50	0.41
1:A:55:TRP:HH2	1:A:182:PHE:CE1	2.38	0.41
1:B:97:LYS:HD2	1:C:6:GLU:CD	2.40	0.41
1:D:230:CYS:CB	1:D:256:CYS:HA	2.50	0.41
1:B:117:TYR:N	1:B:151:GLU:O	2.50	0.41
1:C:293:GLU:O	1:C:296:LYS:N	2.50	0.41
1:B:39:ARG:HD2	1:B:72:GLU:O	2.20	0.41
1:A:307:LYS:HD3	1:A:430:PHE:CG	2.54	0.41
1:C:148:ALA:HB2	1:C:359:MET:CG	2.48	0.41
1:C:353:ASN:HA	1:C:356:ARG:HD2	2.02	0.41
1:B:348:PHE:O	1:B:352:ASN:OD1	2.38	0.41
1:C:16:TRP:HB2	1:C:419:ILE:HB	2.02	0.41
1:C:179:ASP:HB3	1:C:247:TYR:CZ	2.55	0.41
1:B:318:MET:CE	1:B:332:MET:HA	2.50	0.41
1:B:384:LYS:HD2	1:B:387:GLN:CB	2.47	0.41
1:D:414:VAL:HG13	1:D:414:VAL:O	2.19	0.41
1:A:41:LEU:HD11	1:A:182:PHE:HZ	1.84	0.41
1:C:178:ARG:HB3	1:C:207:GLY:CA	2.51	0.41
1:A:83:ALA:HB2	1:A:108:PHE:CZ	2.55	0.41
1:A:274:TYR:CZ	1:A:282:THR:HG21	2.55	0.41
1:D:197:SER:HB2	1:D:369:HIS:HD2	1.83	0.41
1:A:295:ASN:N	1:A:352:ASN:OD1	2.51	0.41
1:D:107:ARG:NH2	2:D:432:CBI:O6	2.49	0.41
1:A:340:ASN:ND2	1:A:342:PHE:H	2.17	0.41
1:A:104:VAL:O	2:A:432:CBI:H62	2.20	0.41
1:B:374:LEU:CD2	1:B:397:THR:HA	2.51	0.41
1:C:341:ARG:NH1	1:C:344:GLU:OE1	2.50	0.41
1:D:85:THR:HA	1:D:89:ALA:O	2.20	0.41
1:C:230:CYS:HB3	1:C:255:LYS:C	2.40	0.41
1:B:82:GLY:HA3	1:B:93:LYS:CB	2.50	0.41
1:A:22:PRO:HB2	1:A:429:ASP:CG	2.41	0.41
1:C:275:GLY:O	1:C:281:ASP:HA	2.20	0.41
1:C:7:THR:HA	1:C:8:PRO:HD2	1.94	0.41
1:B:313:PRO:HD3	1:B:321:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LYS:O	1:B:187:ALA:HA	2.21	0.41
1:B:257:ASP:CG	1:B:260:GLY:H	2.23	0.41
1:A:189:ILE:HG23	1:A:190:GLU:N	2.35	0.41
1:A:2:ARG:HH22	1:A:70:MET:HE1	1.85	0.41
1:C:205:PRO:HB2	1:C:206:TYR:H	1.47	0.41
1:C:127:LEU:HG	1:C:128:ALA:N	2.32	0.41
1:C:78:LEU:HB3	1:C:79:GLY:H	1.58	0.41
1:C:80:THR:HB	1:C:81:TYR:CE2	2.56	0.41
1:D:11:HIS:HD2	1:D:33:VAL:HB	1.84	0.41
1:C:193:LYS:CA	1:C:193:LYS:HZ3	2.32	0.41
1:C:45:ASN:O	1:C:46:MET:HB2	2.19	0.41
1:B:189:ILE:HG23	1:B:190:GLU:N	2.36	0.41
1:B:267:ARG:HH12	3:B:431:CTT:H6B	1.85	0.41
1:A:362:VAL:HG12	1:A:363:MET:H	1.85	0.41
1:A:343:GLU:CG	1:A:347:GLY:HA2	2.47	0.41
1:A:33:VAL:HG22	1:A:34:ILE:N	2.35	0.41
1:B:325:THR:H	1:B:328:LEU:HB2	1.85	0.41
1:C:122:LEU:HD23	1:C:292:PHE:CE2	2.56	0.41
1:A:196:THR:OG1	1:A:197:SER:N	2.53	0.41
1:C:154:GLY:C	1:C:161:ASN:HD22	2.23	0.41
1:A:144:LEU:O	1:A:145:TYR:HB3	2.21	0.41
1:D:280:LEU:HD11	1:D:286:PHE:CG	2.56	0.41
1:A:143:ALA:N	1:A:364:SER:O	2.49	0.41
1:A:93:LYS:H	1:A:93:LYS:HG3	1.52	0.41
1:A:130:ASP:N	1:A:417:SER:O	2.50	0.41
1:C:158:TYR:HA	1:C:159:PRO:HD2	1.70	0.41
1:B:387:GLN:HA	1:B:388:PRO:HD3	1.91	0.41
1:D:36:ALA:HA	1:D:39:ARG:CD	2.43	0.41
1:B:95:VAL:CG2	1:B:104:VAL:HG13	2.51	0.41
1:C:144:LEU:HG	1:C:145:TYR:N	2.36	0.41
1:D:307:LYS:O	1:D:308:ILE:HG13	2.21	0.41
1:A:41:LEU:CD1	1:A:49:CYS:HB2	2.51	0.41
1:B:325:THR:H	1:B:328:LEU:CB	2.34	0.41
1:D:230:CYS:HB3	1:D:256:CYS:HA	2.03	0.41
1:D:242:ASN:HA	4:D:524:HOH:O	2.20	0.41
1:C:383:GLU:H	1:C:383:GLU:HG2	1.51	0.41
1:B:137:GLU:HG3	1:B:409:PHE:CG	2.56	0.41
1:A:403:ALA:O	1:A:406:GLU:N	2.53	0.41
1:B:310:ILE:HA	1:B:311:PRO:HD2	1.85	0.41
1:A:296:LYS:NZ	1:A:323:GLU:OE2	2.49	0.41
1:D:2:ARG:HH21	1:D:68:LYS:CA	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:CYS:HB3	1:C:256:CYS:CA	2.51	0.41
1:C:297:LEU:HD12	1:C:297:LEU:HA	1.79	0.41
1:B:394:ASP:N	1:B:394:ASP:OD2	2.53	0.41
1:B:178:ARG:HD2	1:B:243:CYS:SG	2.60	0.41
1:B:255:LYS:HD2	4:B:499:HOH:O	2.20	0.41
1:B:86:SER:O	1:B:89:ALA:HB3	2.20	0.41
1:B:145:TYR:HE2	1:B:212:GLU:OE1	2.04	0.41
1:A:145:TYR:CB	1:A:214:ASP:HA	2.51	0.41
1:A:125:ASN:HD22	1:A:423:PRO:HA	1.85	0.41
1:A:145:TYR:O	1:A:362:VAL:N	2.50	0.41
1:C:145:TYR:HB3	1:C:214:ASP:HA	2.02	0.41
1:B:99:GLU:HG3	1:C:40:TRP:HB2	2.02	0.41
1:B:328:LEU:HD13	1:B:328:LEU:HA	1.79	0.41
1:B:163:ALA:O	1:B:166:ARG:HG3	2.20	0.41
1:D:325:THR:HB	1:D:327:GLU:OE1	2.20	0.41
1:D:350:GLN:OE1	1:D:353:ASN:OD1	2.38	0.41
1:C:174:ALA:HB2	1:C:212:GLU:HG2	2.02	0.41
1:A:250:ASP:OD2	1:A:253:ALA:HB2	2.20	0.41
1:C:351:LEU:O	1:C:354:ALA:N	2.52	0.41
1:B:141:ASN:HB3	1:B:366:TRP:CE2	2.56	0.41
1:A:225:PHE:CZ	1:A:297:LEU:HG	2.56	0.41
1:C:144:LEU:HB3	1:C:216:TRP:HB3	2.03	0.41
1:B:11:HIS:CD2	1:B:33:VAL:HG23	2.56	0.41
1:B:273:PHE:HE2	1:B:301:PHE:HE1	1.69	0.41
1:D:45:ASN:ND2	4:D:488:HOH:O	2.50	0.41
1:C:374:LEU:O	1:C:378:SER:N	2.50	0.41
1:A:371:ALA:O	1:A:374:LEU:HG	2.21	0.41
1:C:280:LEU:HA	1:C:280:LEU:HD22	1.88	0.41
1:A:85:THR:HG22	1:A:87:GLY:H	1.86	0.41
1:D:94:PHE:O	1:D:105:GLY:N	2.50	0.40
1:C:380:TYR:HE2	2:C:431:CBI:O2'	2.01	0.40
1:C:2:ARG:O	1:C:70:MET:HB3	2.20	0.40
1:A:38:TRP:NE1	2:A:432:CBI:H62	2.35	0.40
1:C:228:HIS:HA	1:C:342:PHE:HE1	1.85	0.40
1:B:6:GLU:HB3	1:B:7:THR:H	1.57	0.40
1:C:346:GLY:CA	1:C:350:GLN:HB2	2.50	0.40
1:D:195:SER:CB	1:D:198:ASP:HB3	2.51	0.40
1:B:232:THR:HG22	1:B:234:GLU:HG2	2.03	0.40
1:D:78:LEU:HD22	1:D:78:LEU:O	2.21	0.40
1:C:115:ASP:O	1:C:165:ALA:HB3	2.21	0.40
1:C:225:PHE:HE1	1:C:298:SER:O	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:PHE:O	1:C:362:VAL:HG13	2.21	0.40
1:B:123:MET:CE	1:B:356:ARG:HE	2.24	0.40
1:A:97:LYS:HA	1:A:102:THR:HA	2.03	0.40
1:D:35:ASP:HA	1:D:168:GLY:O	2.22	0.40
1:D:145:TYR:HH	2:D:432:CBI:HO1'	1.62	0.40
1:A:251:ARG:NH2	2:A:431:CBI:O3'	2.55	0.40
1:A:336:PHE:CE1	1:A:388:PRO:HB2	2.56	0.40
1:A:212:GLU:OE2	1:A:214:ASP:OD1	2.40	0.40
1:A:228:HIS:ND1	1:A:257:ASP:O	2.54	0.40
1:A:75:GLY:O	1:A:77:TYR:N	2.55	0.40
1:D:380:TYR:HE2	2:D:431:CBI:O2'	2.04	0.40
1:A:245:GLY:O	1:A:251:ARG:HG3	2.22	0.40
1:B:325:THR:HB	1:B:327:GLU:OE2	2.22	0.40
1:C:307:LYS:HD2	1:C:430:PHE:HB3	2.04	0.40
1:A:315:TRP:CZ3	1:A:388:PRO:HB3	2.57	0.40
1:A:155:MET:HE3	1:A:155:MET:HB3	1.76	0.40
1:D:198:ASP:OD1	1:D:201:ALA:N	2.50	0.40
1:D:274:TYR:C	1:D:278:LYS:HD2	2.42	0.40
1:B:143:ALA:O	1:B:364:SER:OG	2.36	0.40
1:A:232:THR:HG22	1:A:234:GLU:HG2	2.03	0.40
1:A:124:GLY:O	1:A:125:ASN:ND2	2.54	0.40
1:A:41:LEU:HD22	1:A:41:LEU:HA	1.88	0.40
1:C:193:LYS:NZ	1:C:193:LYS:N	2.70	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	428/430 (100%)	354 (83%)	57 (13%)	17 (4%)	4 1
1	B	428/430 (100%)	336 (78%)	64 (15%)	28 (6%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	428/430 (100%)	332 (78%)	69 (16%)	27 (6%)	2 0
1	D	428/430 (100%)	331 (77%)	71 (17%)	26 (6%)	2 0
All	All	1712/1720 (100%)	1353 (79%)	261 (15%)	98 (6%)	2 0

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	CYS
1	A	122	LEU
1	A	278	LYS
1	A	347	GLY
1	B	6	GLU
1	B	30	ALA
1	B	78	LEU
1	B	86	SER
1	B	187	ALA
1	B	188	ASN
1	B	240	THR
1	B	273	PHE
1	B	304	ASP
1	B	385	GLU
1	B	399	SER
1	C	46	MET
1	C	94	PHE
1	C	205	PRO
1	C	385	GLU
1	C	399	SER
1	C	402	PRO
1	D	43	ASP
1	D	51	ASP
1	D	94	PHE
1	D	114	PRO
1	D	135	THR
1	D	190	GLU
1	D	199	PRO
1	D	235	TYR
1	D	260	GLY
1	D	372	ASN
1	A	30	ALA
1	A	129	PHE
1	A	176	CYS

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Mol	Chain	Res	Type
1	B	210	CYS
1	B	335	VAL
1	C	43	ASP
1	C	73	GLY
1	C	79	GLY
1	C	87	GLY
1	C	165	ALA
1	C	180	LEU
1	C	200	ASN
1	C	240	THR
1	C	429	ASP
1	D	87	GLY
1	D	98	HIS
1	D	113	GLY
1	D	385	GLU
1	A	52	GLY
1	A	315	TRP
1	A	337	ASN
1	A	384	LYS
1	A	403	ALA
1	B	94	PHE
1	B	123	MET
1	B	184	GLY
1	B	212	GLU
1	B	338	ASP
1	C	78	LEU
1	C	173	ASP
1	C	206	TYR
1	C	383	GLU
1	C	388	PRO
1	C	404	GLU
1	D	63	THR
1	D	106	SER
1	D	191	GLY
1	D	205	PRO
1	D	319	PRO
1	A	385	GLU
1	B	62	ALA
1	B	211	ALA
1	B	412	ALA
1	B	424	ILE
1	C	177	ALA

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Mol	Chain	Res	Type
1	C	219	ASN
1	C	414	VAL
1	D	22	PRO
1	D	71	ILE
1	D	176	CYS
1	D	285	LYS
1	D	328	LEU
1	A	76	ASP
1	A	390	ALA
1	B	176	CYS
1	A	260	GLY
1	A	391	ALA
1	B	8	PRO
1	B	138	CYS
1	C	159	PRO
1	B	402	PRO
1	C	164	GLY
1	B	345	VAL
1	B	52	GLY
1	D	313	PRO
1	D	402	PRO
1	C	424	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	354/354 (100%)	240 (68%)	114 (32%)	0 0
1	B	354/354 (100%)	251 (71%)	103 (29%)	0 0
1	C	354/354 (100%)	255 (72%)	99 (28%)	0 0
1	D	354/354 (100%)	259 (73%)	95 (27%)	0 0
All	All	1416/1416 (100%)	1005 (71%)	411 (29%)	0 0

All (411) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	GLU
1	A	7	THR
1	A	17	GLN
1	A	20	THR
1	A	26	GLN
1	A	27	THR
1	A	29	ASN
1	A	32	VAL
1	A	34	ILE
1	A	37	ASN
1	A	41	LEU
1	A	45	ASN
1	A	46	MET
1	A	54	GLN
1	A	57	ASN
1	A	59	CYS
1	A	64	ASP
1	A	71	ILE
1	A	76	ASP
1	A	78	LEU
1	A	84	SER
1	A	86	SER
1	A	92	LEU
1	A	93	LYS
1	A	97	LYS
1	A	104	VAL
1	A	110	LEU
1	A	116	LYS
1	A	121	ASN
1	A	122	LEU
1	A	130	ASP
1	A	133	LEU
1	A	135	THR
1	A	137	GLU
1	A	140	ILE
1	A	142	SER
1	A	144	LEU
1	A	147	VAL
1	A	149	MET
1	A	150	GLU
1	A	155	MET
1	A	157	SER

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	181	LYS
1	A	193	LYS
1	A	194	SER
1	A	196	THR
1	A	198	ASP
1	A	206	TYR
1	A	209	CYS
1	A	212	GLU
1	A	215	VAL
1	A	219	ASN
1	A	225	PHE
1	A	231	THR
1	A	233	ASN
1	A	239	GLU
1	A	241	THR
1	A	247	TYR
1	A	249	GLU
1	A	251	ARG
1	A	252	PHE
1	A	255	LYS
1	A	259	ASN
1	A	261	CYS
1	A	266	TYR
1	A	267	ARG
1	A	272	ASP
1	A	276	LYS
1	A	280	LEU
1	A	284	ARG
1	A	285	LYS
1	A	290	SER
1	A	291	ARG
1	A	293	GLU
1	A	294	GLU
1	A	297	LEU
1	A	298	SER
1	A	300	TYR
1	A	304	ASP
1	A	307	LYS
1	A	308	ILE
1	A	309	GLU
1	A	314	THR

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Mol	Chain	Res	Type
1	A	323	GLU
1	A	328	LEU
1	A	332	MET
1	A	334	ASP
1	A	336	PHE
1	A	337	ASN
1	A	338	ASP
1	A	339	ARG
1	A	340	ASN
1	A	341	ARG
1	A	348	PHE
1	A	352	ASN
1	A	353	ASN
1	A	356	ARG
1	A	357	VAL
1	A	361	LEU
1	A	364	SER
1	A	366	TRP
1	A	385	GLU
1	A	392	ARG
1	A	397	THR
1	A	398	ASP
1	A	401	VAL
1	A	404	GLU
1	A	409	PHE
1	A	413	GLN
1	A	417	SER
1	A	426	SER
1	A	429	ASP
1	B	2	ARG
1	B	6	GLU
1	B	7	THR
1	B	9	GLU
1	B	20	THR
1	B	24	ASN
1	B	31	GLU
1	B	34	ILE
1	B	41	LEU
1	B	44	ASP
1	B	45	ASN
1	B	46	MET
1	B	47	GLN

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Mol	Chain	Res	Type
1	B	48	ASN
1	B	49	CYS
1	B	59	CYS
1	B	63	THR
1	B	64	ASP
1	B	67	GLU
1	B	68	LYS
1	B	71	ILE
1	B	76	ASP
1	B	78	LEU
1	B	86	SER
1	B	88	ASP
1	B	93	LYS
1	B	96	THR
1	B	98	HIS
1	B	106	SER
1	B	111	MET
1	B	115	ASP
1	B	123	MET
1	B	127	LEU
1	B	130	ASP
1	B	135	THR
1	B	144	LEU
1	B	145	TYR
1	B	149	MET
1	B	155	MET
1	B	166	ARG
1	B	169	THR
1	B	178	ARG
1	B	179	ASP
1	B	181	LYS
1	B	190	GLU
1	B	193	LYS
1	B	196	THR
1	B	197	SER
1	B	200	ASN
1	B	209	CYS
1	B	212	GLU
1	B	214	ASP
1	B	217	GLU
1	B	240	THR
1	B	243	CYS

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Mol	Chain	Res	Type
1	B	249	GLU
1	B	255	LYS
1	B	262	ASP
1	B	264	ASN
1	B	267	ARG
1	B	268	MET
1	B	278	LYS
1	B	281	ASP
1	B	284	ARG
1	B	285	LYS
1	B	287	THR
1	B	293	GLU
1	B	298	SER
1	B	299	GLN
1	B	306	ARG
1	B	310	ILE
1	B	316	GLU
1	B	320	ASN
1	B	323	GLU
1	B	327	GLU
1	B	328	LEU
1	B	330	SER
1	B	332	MET
1	B	334	ASP
1	B	337	ASN
1	B	338	ASP
1	B	340	ASN
1	B	348	PHE
1	B	349	GLU
1	B	352	ASN
1	B	353	ASN
1	B	355	LEU
1	B	356	ARG
1	B	365	ILE
1	B	367	ASP
1	B	369	HIS
1	B	374	LEU
1	B	376	LEU
1	B	383	GLU
1	B	384	LYS
1	B	385	GLU
1	B	394	ASP

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Mol	Chain	Res	Type
1	B	395	CYS
1	B	397	THR
1	B	398	ASP
1	B	404	GLU
1	B	415	VAL
1	B	416	TRP
1	C	2	ARG
1	C	5	ASN
1	C	11	HIS
1	C	20	THR
1	C	28	VAL
1	C	32	VAL
1	C	33	VAL
1	C	39	ARG
1	C	44	ASP
1	C	46	MET
1	C	47	GLN
1	C	53	ASN
1	C	57	ASN
1	C	59	CYS
1	C	61	THR
1	C	64	ASP
1	C	70	MET
1	C	77	TYR
1	C	78	LEU
1	C	86	SER
1	C	88	ASP
1	C	96	THR
1	C	97	LYS
1	C	98	HIS
1	C	99	GLU
1	C	111	MET
1	C	115	ASP
1	C	116	LYS
1	C	118	GLN
1	C	119	MET
1	C	121	ASN
1	C	123	MET
1	C	133	LEU
1	C	144	LEU
1	C	149	MET
1	C	166	ARG

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Mol	Chain	Res	Type
1	C	167	TYR
1	C	173	ASP
1	C	175	GLN
1	C	180	LEU
1	C	193	LYS
1	C	200	ASN
1	C	208	SER
1	C	209	CYS
1	C	223	PHE
1	C	225	PHE
1	C	228	HIS
1	C	230	CYS
1	C	232	THR
1	C	234	GLU
1	C	238	CYS
1	C	240	THR
1	C	241	THR
1	C	242	ASN
1	C	243	CYS
1	C	246	THR
1	C	249	GLU
1	C	252	PHE
1	C	255	LYS
1	C	263	TYR
1	C	265	PRO
1	C	267	ARG
1	C	270	ASN
1	C	272	ASP
1	C	284	ARG
1	C	290	SER
1	C	291	ARG
1	C	294	GLU
1	C	297	LEU
1	C	298	SER
1	C	299	GLN
1	C	303	GLN
1	C	306	ARG
1	C	316	GLU
1	C	318	MET
1	C	335	VAL
1	C	337	ASN
1	C	341	ARG

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Mol	Chain	Res	Type
1	C	342	PHE
1	C	348	PHE
1	C	349	GLU
1	C	351	LEU
1	C	352	ASN
1	C	361	LEU
1	C	366	TRP
1	C	373	MET
1	C	379	ILE
1	C	383	GLU
1	C	384	LYS
1	C	392	ARG
1	C	394	ASP
1	C	397	THR
1	C	398	ASP
1	C	404	GLU
1	C	413	GLN
1	C	415	VAL
1	C	419	ILE
1	C	420	ARG
1	C	424	ILE
1	D	2	ARG
1	D	10	ASN
1	D	27	THR
1	D	29	ASN
1	D	38	TRP
1	D	39	ARG
1	D	41	LEU
1	D	57	ASN
1	D	59	CYS
1	D	60	SER
1	D	61	THR
1	D	64	ASP
1	D	68	LYS
1	D	70	MET
1	D	71	ILE
1	D	78	LEU
1	D	84	SER
1	D	93	LYS
1	D	96	THR
1	D	97	LYS
1	D	98	HIS

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Mol	Chain	Res	Type
1	D	99	GLU
1	D	104	VAL
1	D	110	LEU
1	D	111	MET
1	D	114	PRO
1	D	117	TYR
1	D	119	MET
1	D	123	MET
1	D	126	GLU
1	D	133	LEU
1	D	134	SER
1	D	135	THR
1	D	138	CYS
1	D	145	TYR
1	D	146	PHE
1	D	150	GLU
1	D	155	MET
1	D	166	ARG
1	D	171	TYR
1	D	175	GLN
1	D	178	ARG
1	D	181	LYS
1	D	186	LYS
1	D	189	ILE
1	D	193	LYS
1	D	194	SER
1	D	196	THR
1	D	197	SER
1	D	200	ASN
1	D	208	SER
1	D	225	PHE
1	D	226	THR
1	D	228	HIS
1	D	230	CYS
1	D	234	GLU
1	D	236	HIS
1	D	242	ASN
1	D	249	GLU
1	D	251	ARG
1	D	270	ASN
1	D	280	LEU
1	D	281	ASP

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Mol	Chain	Res	Type
1	D	290	SER
1	D	291	ARG
1	D	294	GLU
1	D	295	ASN
1	D	296	LYS
1	D	297	LEU
1	D	306	ARG
1	D	309	GLU
1	D	315	TRP
1	D	320	ASN
1	D	324	ILE
1	D	325	THR
1	D	327	GLU
1	D	330	SER
1	D	334	ASP
1	D	340	ASN
1	D	344	GLU
1	D	352	ASN
1	D	355	LEU
1	D	361	LEU
1	D	365	ILE
1	D	373	MET
1	D	381	PRO
1	D	384	LYS
1	D	387	GLN
1	D	392	ARG
1	D	394	ASP
1	D	397	THR
1	D	405	VAL
1	D	426	SER
1	D	429	ASP
1	D	430	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	24	ASN
1	A	26	GLN
1	A	29	ASN
1	A	48	ASN
1	A	103	ASN

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Mol	Chain	Res	Type
1	A	236	HIS
1	A	270	ASN
1	A	303	GLN
1	A	320	ASN
1	A	337	ASN
1	A	340	ASN
1	A	353	ASN
1	A	369	HIS
1	A	372	ASN
1	A	408	GLN
1	A	413	GLN
1	B	5	ASN
1	B	26	GLN
1	B	45	ASN
1	B	103	ASN
1	B	125	ASN
1	B	175	GLN
1	B	270	ASN
1	B	299	GLN
1	B	320	ASN
1	B	340	ASN
1	B	372	ASN
1	B	387	GLN
1	C	5	ASN
1	C	17	GLN
1	C	29	ASN
1	C	37	ASN
1	C	45	ASN
1	C	118	GLN
1	C	121	ASN
1	C	125	ASN
1	C	161	ASN
1	C	270	ASN
1	C	320	ASN
1	C	337	ASN
1	C	352	ASN
1	C	353	ASN
1	C	387	GLN
1	D	10	ASN
1	D	24	ASN
1	D	29	ASN
1	D	103	ASN

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Mol	Chain	Res	Type
1	D	125	ASN
1	D	242	ASN
1	D	264	ASN
1	D	340	ASN
1	D	352	ASN
1	D	353	ASN
1	D	369	HIS
1	D	372	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PCA	A	1	1	7,8,9	1.88	1 (14%)	9,10,12	1.56	2 (22%)
1	PCA	B	1	1	7,8,9	1.74	1 (14%)	9,10,12	1.43	3 (33%)
1	PCA	C	1	1	7,8,9	1.77	1 (14%)	9,10,12	1.35	2 (22%)
1	PCA	D	1	1	7,8,9	1.81	1 (14%)	9,10,12	1.30	1 (11%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	CD-N	4.28	1.47	1.33
1	B	1	PCA	CD-N	4.31	1.48	1.33
1	D	1	PCA	CD-N	4.34	1.48	1.33
1	A	1	PCA	CD-N	4.45	1.48	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	PCA	OE-CD-CG	-2.66	120.87	126.81
1	B	1	PCA	CB-CA-C	-2.48	109.37	112.76
1	C	1	PCA	CB-CA-C	-2.16	109.81	112.76
1	A	1	PCA	CB-CA-C	-2.09	109.91	112.76
1	B	1	PCA	O-C-CA	-2.07	119.98	125.44
1	D	1	PCA	CB-CA-C	-2.05	109.96	112.76
1	B	1	PCA	OE-CD-CG	-2.03	122.28	126.81
1	C	1	PCA	CB-CG-CD	2.08	108.44	104.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	4	0
1	B	1	PCA	4	0
1	C	1	PCA	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CBI	A	431	-	24,24,24	0.49	0	35,35,35	1.19	3 (8%)
2	CBI	A	432	-	24,24,24	0.44	0	35,35,35	1.17	4 (11%)
3	CTT	B	431	-	48,48,48	0.47	0	71,71,71	1.21	8 (11%)
2	CBI	C	431	-	24,24,24	0.46	0	35,35,35	1.13	3 (8%)
2	CBI	D	431	-	24,24,24	0.48	0	35,35,35	1.03	2 (5%)
2	CBI	D	432	-	24,24,24	0.46	0	35,35,35	1.27	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CBI	A	431	-	-	0/8/48/48	0/2/2/2
2	CBI	A	432	-	-	0/8/48/48	0/2/2/2
3	CTT	B	431	-	-	0/20/100/100	0/4/4/4
2	CBI	C	431	-	-	0/8/48/48	0/2/2/2
2	CBI	D	431	-	-	0/8/48/48	0/2/2/2
2	CBI	D	432	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	432	CBI	C1-O4'-C4'	-4.33	106.70	118.01
2	A	431	CBI	C1-O4'-C4'	-3.95	107.68	118.01
3	B	431	CTT	C1D-O4C-C4C	-3.35	109.25	118.01
3	B	431	CTT	C1E-O4D-C4D	-3.27	109.47	118.01
2	C	431	CBI	C1-O4'-C4'	-3.16	109.76	118.01
2	A	432	CBI	C1-O5-C5	-3.15	107.63	113.75
2	A	432	CBI	C1-O4'-C4'	-2.98	110.23	118.01
2	D	431	CBI	C1-O4'-C4'	-2.88	110.47	118.01
2	C	431	CBI	C6-C5-C4	-2.49	106.88	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	432	CBI	C1'-O5'-C5'	-2.42	108.99	113.47
3	B	431	CTT	C1C-O5C-C5C	-2.27	109.34	113.75
2	D	431	CBI	C1'-O5'-C5'	-2.12	109.55	113.47
2	A	432	CBI	C3'-C4'-C5'	-2.05	106.20	110.84
3	B	431	CTT	C3D-C4D-C5D	-2.04	106.22	110.84
3	B	431	CTT	O5B-C5B-C4B	2.05	114.07	109.75
2	C	431	CBI	C2'-C3'-C4'	2.06	114.13	109.60
2	A	432	CBI	O5-C5-C6	2.07	111.59	106.36
2	A	431	CBI	O5-C5-C6	2.12	111.72	106.36
3	B	431	CTT	O4D-C4D-C3D	2.29	113.09	107.17
3	B	431	CTT	O5D-C5D-C6D	2.50	112.67	106.36
2	A	431	CBI	O4'-C4'-C3'	2.59	113.86	107.17
3	B	431	CTT	O4D-C4D-C5D	3.21	117.75	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	431	CBI	3	0
2	A	432	CBI	8	0
3	B	431	CTT	9	0
2	C	431	CBI	3	0
2	D	431	CBI	5	0
2	D	432	CBI	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	429/430 (99%)	-0.55	1 (0%)	95	96	12, 32, 53, 70	0
1	B	429/430 (99%)	-0.55	1 (0%)	95	96	11, 33, 55, 80	0
1	C	429/430 (99%)	-0.59	2 (0%)	91	93	10, 31, 53, 83	0
1	D	429/430 (99%)	-0.62	2 (0%)	91	93	10, 31, 49, 68	0
All	All	1716/1720 (99%)	-0.57	6 (0%)	94	95	10, 32, 53, 83	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	VAL	5.2
1	C	100	TYR	4.7
1	B	19	CYS	2.4
1	D	100	TYR	2.3
1	C	191	GLY	2.2
1	D	40	TRP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	PCA	A	1	8/9	0.96	0.08	-	15,28,31,49	0
1	PCA	D	1	8/9	0.97	0.06	-	19,25,30,40	0
1	PCA	B	1	8/9	0.96	0.09	-	28,41,48,52	0
1	PCA	C	1	8/9	0.93	0.11	-	21,32,43,57	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CTT	B	431	45/45	0.94	0.10	0.25	15,35,48,60	0
2	CBI	D	431	23/23	0.96	0.09	0.20	6,25,36,59	0
2	CBI	C	431	23/23	0.97	0.07	-0.42	17,22,37,50	0
2	CBI	A	431	23/23	0.95	0.08	-0.46	18,38,49,57	0
2	CBI	D	432	23/23	0.96	0.08	-0.47	7,30,42,51	0
2	CBI	A	432	23/23	0.97	0.08	-0.48	12,24,44,50	0

6.5 Other polymers (i)

There are no such residues in this entry.