Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 12:44 AM EDT

PDB ID	:	2D5H
Title	:	Crystal Structure of Recombinant Soybean Proglycinin A3B4 subunit, its Comparison with Mature Glycinin A3B4 subunit, Responsible for Hexamer Assembly
Authors	:	Itoh, T.; Adachi, M.; Masuda, T.; Mikami, B.; Utsumi, S.
Deposited on	:	2005-11-01
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

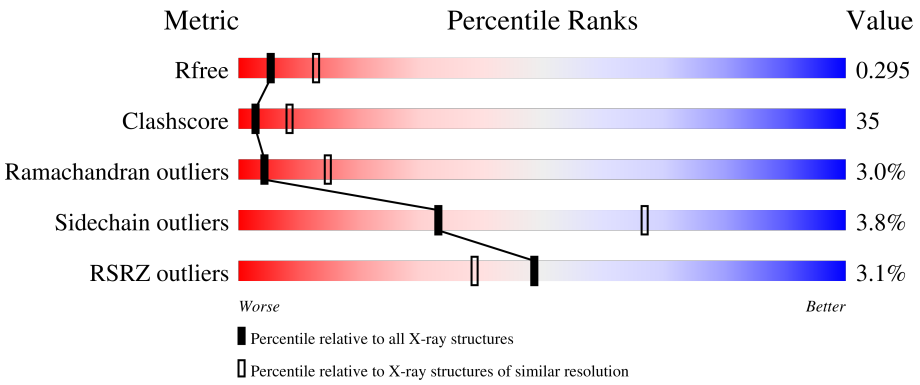
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	493	4% 32% 40% • 24%
1	B	493	2% 33% 39% • 25%
1	C	493	5% 26% 44% 5% 25%
1	D	493	% 36% 38% • 24%
1	E	493	% 40% 34% • 23%

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Mol	Chain	Length	Quality of chain
1	F	493	% 36% 36% • 24%

2 Entry composition (i)

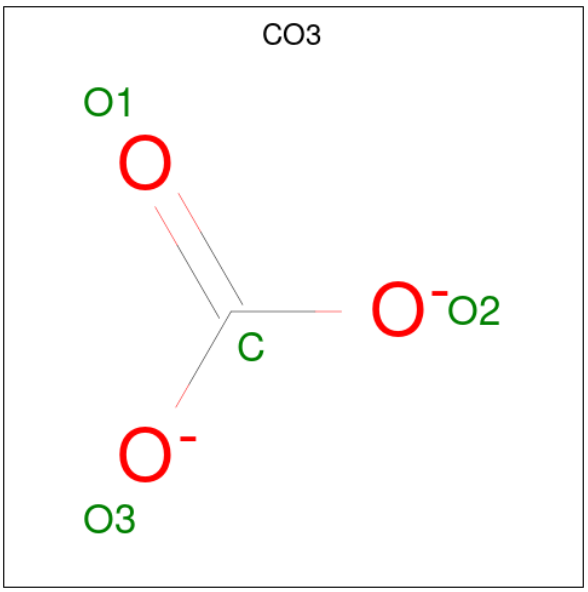
There are 3 unique types of molecules in this entry. The entry contains 17703 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycinin A3B4 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2937	1844	523	562	8	0	0	0
1	B	372	2920	1835	520	557	8	0	0	0
1	C	370	2905	1827	517	553	8	0	0	0
1	D	377	2967	1861	529	569	8	0	0	0
1	E	380	2981	1872	530	571	8	0	0	0
1	F	377	2963	1860	528	567	8	0	0	0

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

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

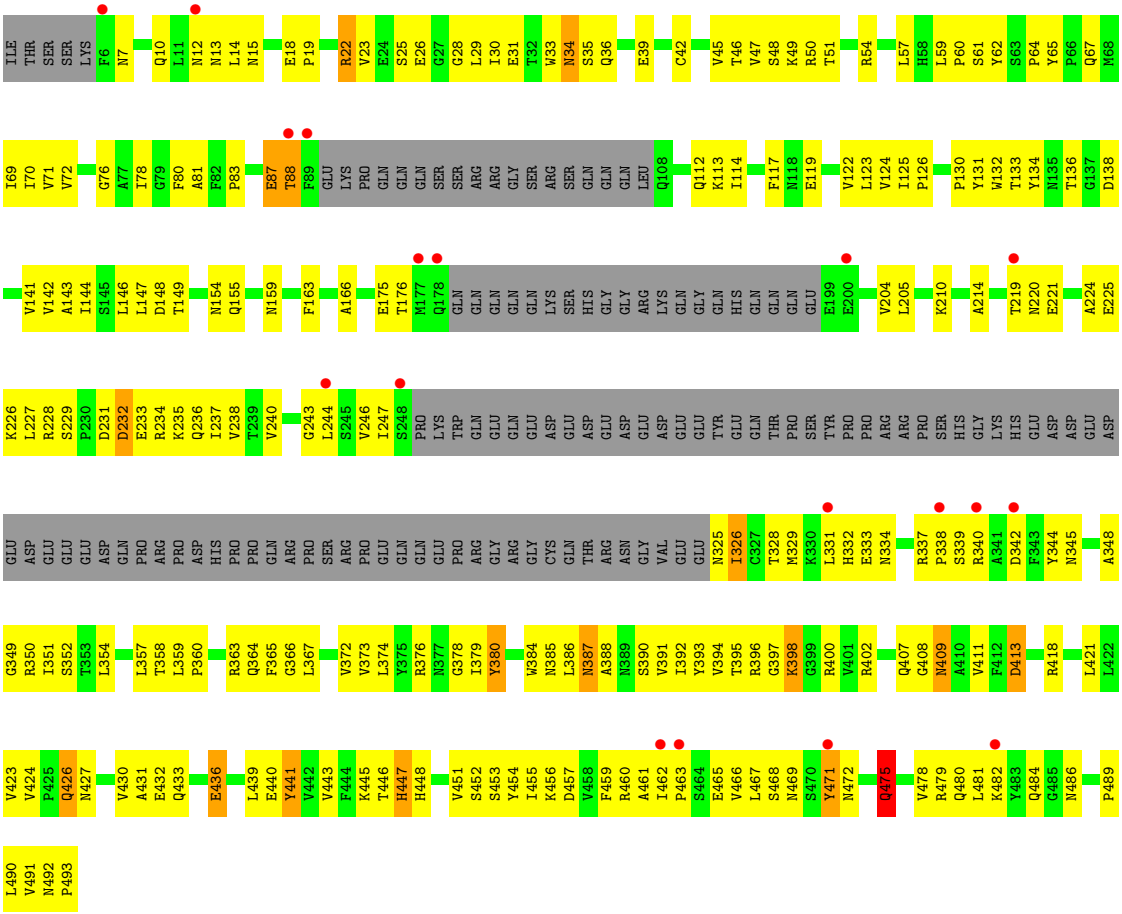
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0
3	F	1	1	1	0	0

3 Residue-property plots (i)

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

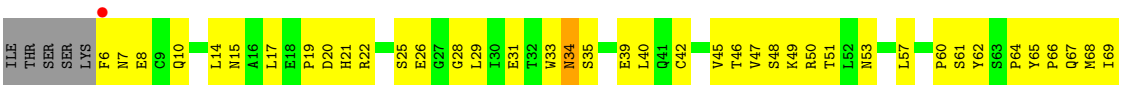
• Molecule 1: glycinin A3B4 subunit

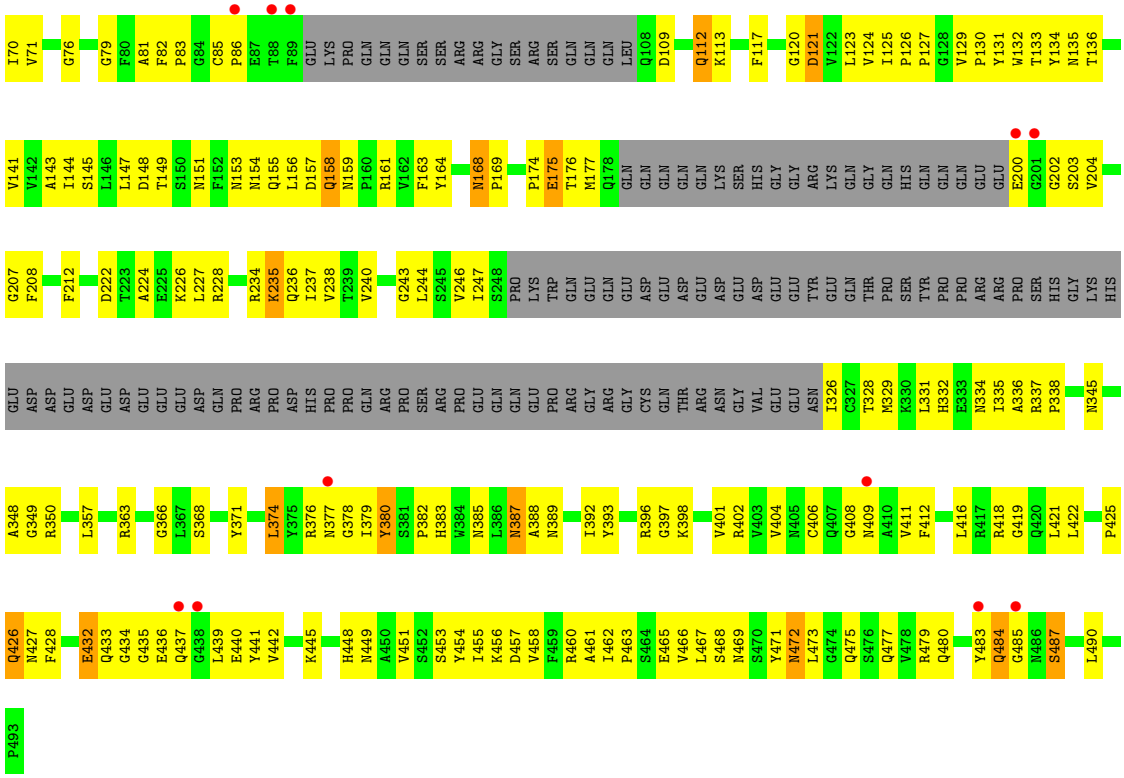
Chain A: 4% 32% 40% • 24%



• Molecule 1: glycinin A3B4 subunit

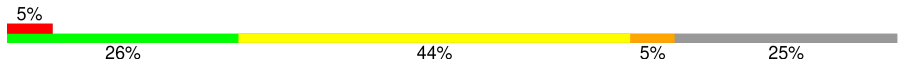
Chain B: 2% 33% 39% • 25%

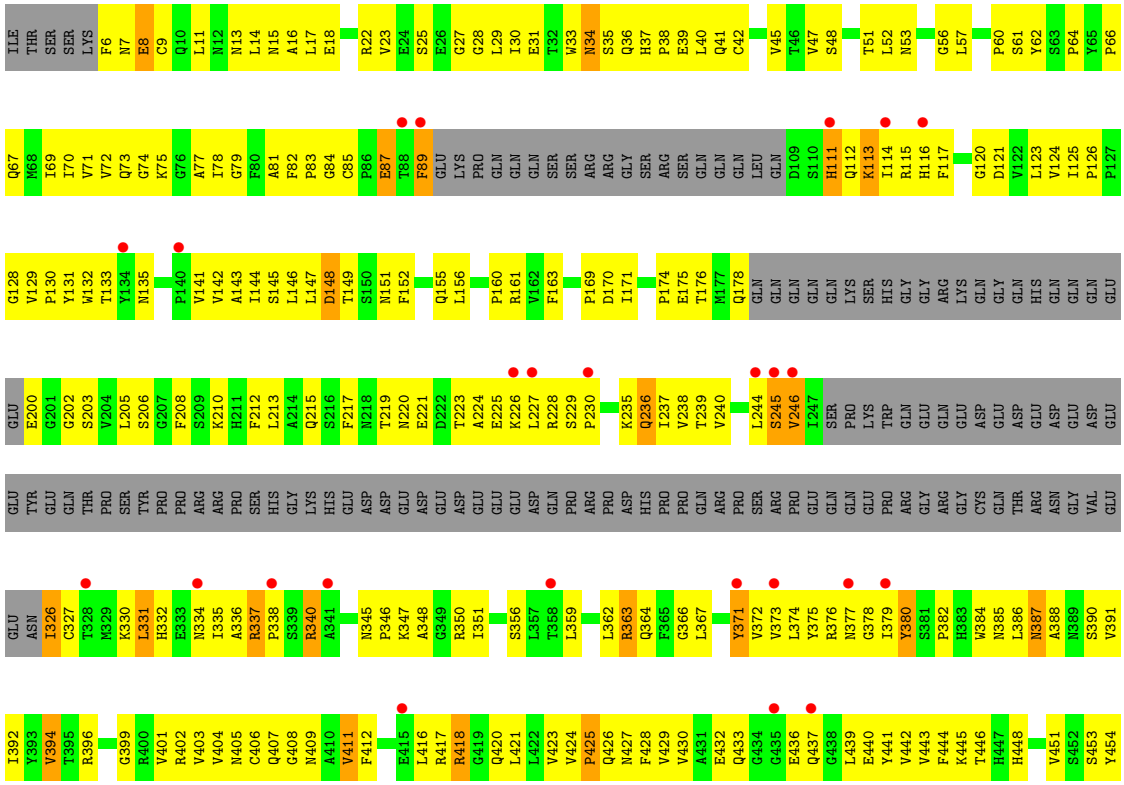


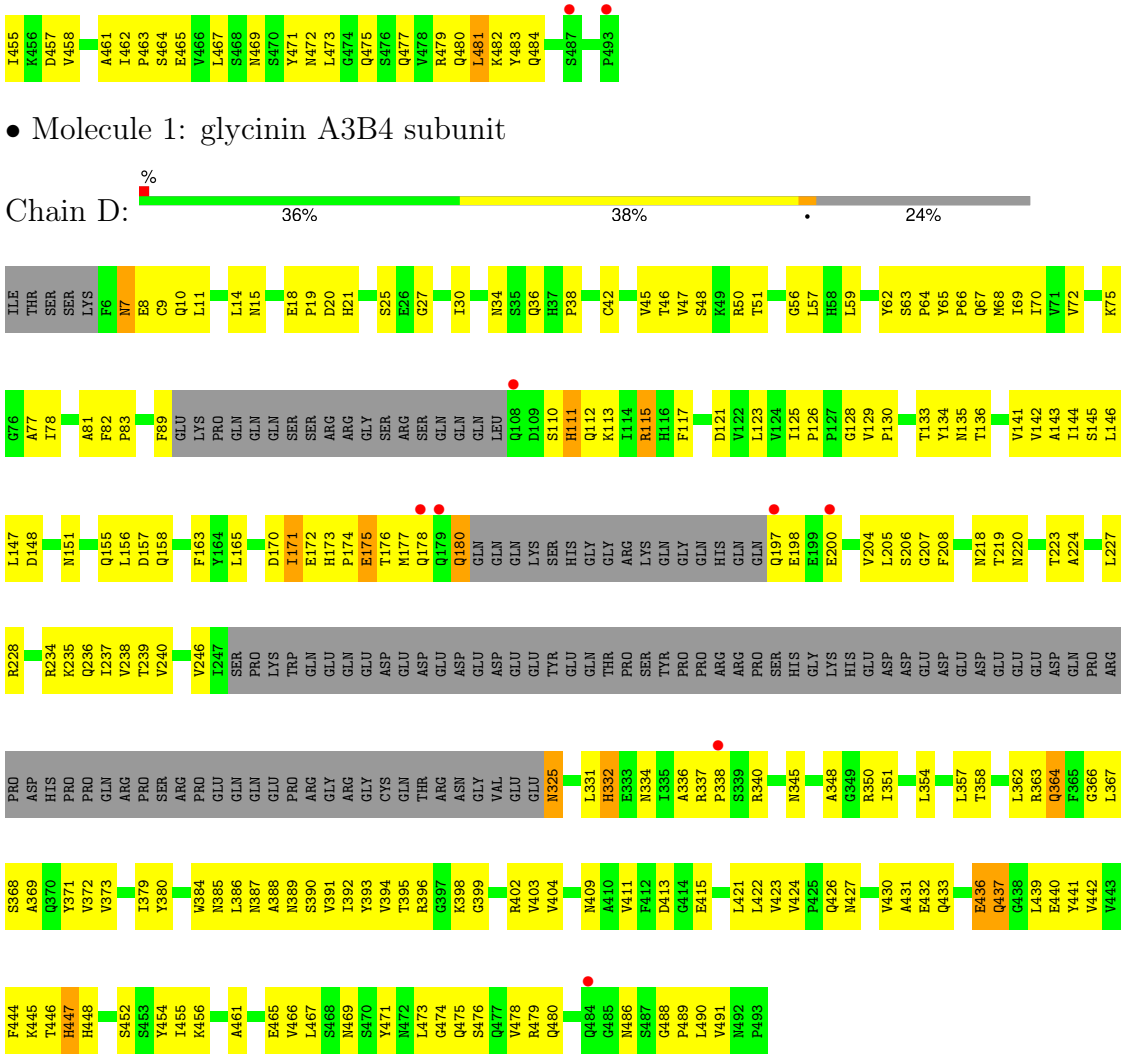


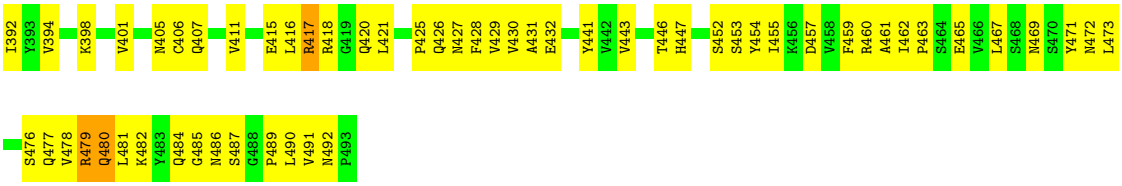
- Molecule 1: glycinin A3B4 subunit

Chain C:



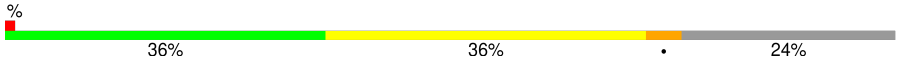


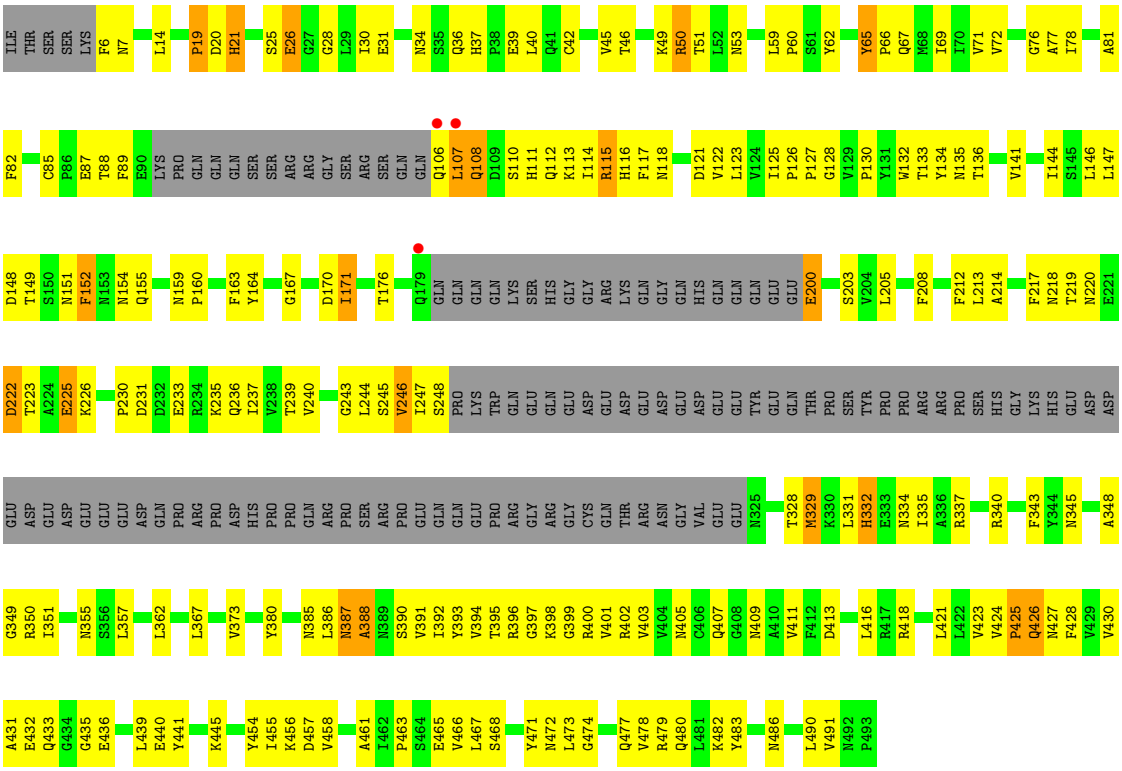

I455 K456 D457 V458 A461 I462 P463 S464 E465 V466 L467 S468 N469 S470 Y471 N472 L473 G474 Q475 S476 Q477 V478 R479 Q480 L481 K482 Y483 Q484 S487 P493
• Molecule 1: glycinin A3B4 subunit
Chain D:
%
36%
38%
24%
ILE THR SER SER LYS F6 N7 E8 C9 Q10 L11 L14 N15 E18 P19 D20 H21 S25 E26 G27 I30 N34 S35 Q36 H37 P38 C42 V45 T46 V47 S48 K49 R50 T51 G56 L57 H58 L59 Y62 S63 P64 Y65 P66 Q67 M68 I69 I70 V71 V72 K75
G76 A77 I78 A81 F82 P83 F89 GLU LYS PRO GLN GLN GLN SER SER ARG ARG GLY SER ARG SER GLN GLN GLN LEU Q108 D109 S110 H111 Q112 K113 I114 R115 H116 F117 D121 V122 L123 V124 I125 P126 P127 G128 V129 P130 T133 Y134 N135 T136 V141 V142 A143 I144 S145 L146
L147 D148 N151 Q155 L156 D157 Q158 F163 Y164 L165 D170 I171 E172 H173 P174 E175 T176 M177 Q178 Q179 Q180 GLN GLN GLN LYS SER HIS GLY GLY ARG LYS GLN GLY GLN HIS GLN GLN Q197 E198 E199 E200 V204 L205 S206 G207 F208 N218 T219 N220 T223 A224 L227
R228 R234 K235 Q236 I237 V238 T239 V240 V246 I247 SER PRO LYS TRP GLN GLU GLN GLU ASP GLU ASP GLU ASP GLU GLU GLU TYR GLU GLN THR PRO SER TYR PRO PRO ARG ARG PRO SER HIS GLY LYS HIS GLU ASP ASP GLU ASP GLU GLU ASP GLN PRO ARG
PRO ASP HIS PRO PRO GLN ARG PRO PRO SER ARG PRO GLU GLN GLN GLU PRO ARG GLY ARG GLY CYS GLN THR ARG ASN GLY VAL GLU GLU N325 L331 H332 E333 N334 T335 A336 R337 P338 S339 R340 N345 A348 G349 R350 I351 L354 I357 T358 L362 R363 Q364 F365 G366 L367
S368 A369 Q370 Y371 V372 V373 I379 Y380 W384 N385 L386 N387 A388 N389 S390 V391 I392 Y393 V394 T395 R396 G397 K398 G399 R402 V403 V404 N409 A410 V411 F412 D413 G414 E415 L421 L422 V423 V424 P425 Q426 N427 V430 A431 E432 Q433 E436 Q437 G438 L439 E440 Y441 V442 V443
F444 K445 T446 H447 H448 S452 S453 Y454 I455 K456 A461 E465 V466 L467 S468 N469 S470 Y471 N472 L473 G474 Q475 S476 Q477 V478 R479 Q480 Q484 G485 N486 S487 G488 P489 L490 V491 N492 P493
• Molecule 1: glycinin A3B4 subunit
Chain E:
%
40%
34%
23%
I1 T2 S3 S4 K5 F6 C9 L14 N15 A16 L17 E18 P19 D20 H21 R22 V23 L29 I30 E31 T32 W33 N34 S35 Q36 H37 P38 E39 L40 V45 T46 V47 S48 K49 L57 H58 L59 P60 S61 Y62 P66 I69 I70 V71 V72 Q73 G74 K75 F82 C85
T88 F89 GLU LYS PRO GLN GLN GLN SER SER ARG ARG GLY SER ARG SER GLN GLN GLN L107 Q108 D109 S110 H111 I114 R115 N118 V122 L123 P127 G128 V129 W132 N135 V141 V142 A143 I144 S145 L146 L147 D148 N151 L156 D157 Q158 N159 P160 Y164 L165
P169 D170 I171 E172 H173 P174 E175 Q178 GLN GLN GLN GLN GLN LYS SER HIS GLY GLY ARG LYS GLN GLY GLN HIS GLN GLN GLU E199 E200 G201 L205 S206 G207 F208 S209 K210 H211 F212 L213 A214 T219 N220 E221 D222 T223 A224 E225 K226 L227 R228 S229 R234 K235 Q236
L244 S245 V246 I247 S248 PRO LYS TRP GLN GLU GLN GLU ASP GLU ASP GLU ASP GLU GLU TYR GLU GLN THR PRO ARG ARG PRO SER HIS GLY LYS HIS GLU ASP ASP GLU ASP GLU ASP GLU GLU GLU ASP GLN PRO ARG PRO ASP HIS PRO PRO GLN ARG
PRO SER ARG PRO GLU GLN GLN GLU PRO ARG GLY ARG GLY CYS GLN THR ARG ASN GLY VAL GLU GLU N325 I326 C327 T328 M329 K330 L331 H332 E333 N334 I335 R340 N345 A348 G349 L354 N355 S356 L357 A369 V372 R376 N377 Y380 N385 L386 N387 A388



- Molecule 1: glycinin A3B4 subunit

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.38Å 223.74Å 88.66Å 90.00° 119.85° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 45.36 – 2.78	Depositor EDS
% Data completeness (in resolution range)	85.1 (15.00-2.80) 83.1 (45.36-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.325 0.222 , 0.295	Depositor DCC
R_{free} test set	5961 reflections (9.43%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.047 for -h-l,k,h 0.047 for l,k,-h-l 0.034 for -h-l,-k,l 0.035 for l,-k,h 0.034 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	17703	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CSD, CO3

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	0.27	0/2995	0.49	0/4068
1	B	0.27	0/2978	0.49	0/4045
1	C	0.27	0/2963	0.50	0/4025
1	D	0.26	0/3025	0.51	0/4108
1	E	0.28	0/3039	0.52	0/4127
1	F	0.27	0/3021	0.51	0/4103
All	All	0.27	0/18021	0.50	0/24476

There are no bond length outliers.

There are no bond angle outliers.

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	2937	0	2841	248	0
1	B	2920	0	2830	251	0
1	C	2905	0	2817	265	0
1	D	2967	0	2867	193	0
1	E	2981	0	2897	183	0
1	F	2963	0	2868	211	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	1	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	17703	0	17120	1233	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 35.

All (1233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ASN:HD22	1:C:337:ARG:HG2	1.17	1.08
1:F:159:ASN:HD22	1:F:176:THR:HG22	1.20	1.06
1:F:115:ARG:HH22	1:F:331:LEU:HD12	1.20	1.04
1:E:247:ILE:HG12	1:E:248:SER:H	1.19	1.04
1:B:159:ASN:HD22	1:B:176:THR:HG22	1.29	0.98
1:C:81:ALA:HB3	1:C:130:PRO:HG2	1.46	0.98
1:B:156:LEU:HB3	1:B:161:ARG:HH21	1.27	0.98
1:D:36:GLN:HE21	1:D:175:GLU:HB2	1.30	0.95
1:B:123:LEU:HD23	1:B:332:HIS:HB3	1.48	0.94
1:A:340:ARG:HB3	1:A:340:ARG:NH1	1.83	0.93
1:A:426:GLN:HE22	1:C:155:GLN:H	1.17	0.92
1:F:34:ASN:HD21	1:F:36:GLN:HB2	1.34	0.92
1:E:247:ILE:HD13	1:E:247:ILE:H	1.35	0.91
1:F:334:ASN:ND2	1:F:337:ARG:HG2	1.86	0.91
1:A:60:PRO:HG3	1:A:132:TRP:HB3	1.51	0.90
1:A:340:ARG:HB3	1:A:340:ARG:HH11	1.34	0.87
1:D:364:GLN:H	1:D:364:GLN:HE21	1.19	0.86
1:E:376:ARG:HH11	1:E:376:ARG:HB3	1.41	0.85
1:E:486:ASN:HD21	1:E:491:VAL:HG22	1.40	0.85
1:A:334:ASN:ND2	1:A:337:ARG:HG2	1.92	0.85
1:D:115:ARG:H	1:D:115:ARG:HD2	1.41	0.85
1:C:124:VAL:H	1:C:331:LEU:HD12	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLN:HE21	1:A:175:GLU:HB2	1.40	0.84
1:A:340:ARG:NH1	1:A:350:ARG:HD2	1.92	0.83
1:F:334:ASN:HD22	1:F:337:ARG:HG2	1.43	0.83
1:D:384:TRP:HE1	1:D:386:LEU:HD12	1.44	0.83
1:B:14:LEU:HD13	1:B:411:VAL:HB	1.60	0.82
1:D:456:LYS:HE2	1:F:217:PHE:HA	1.60	0.82
1:A:373:VAL:HG22	1:A:440:GLU:HG3	1.60	0.82
1:C:124:VAL:HB	1:C:331:LEU:HD11	1.62	0.82
1:C:338:PRO:HG3	1:C:350:ARG:HH11	1.43	0.82
1:D:68:MET:HE1	1:D:369:ALA:HB2	1.62	0.81
1:F:171:ILE:HD12	1:F:171:ILE:H	1.45	0.81
1:D:72:VAL:HG22	1:D:142:VAL:O	1.78	0.81
1:F:486:ASN:HD21	1:F:491:VAL:HG22	1.44	0.81
1:C:373:VAL:HG22	1:C:440:GLU:HG3	1.60	0.81
1:B:480:GLN:NE2	1:B:484:GLN:HE21	1.78	0.80
1:F:328:THR:HG23	1:F:329:MET:H	1.45	0.80
1:A:372:VAL:HB	1:A:441:TYR:HE2	1.48	0.79
1:D:486:ASN:HD21	1:D:491:VAL:HG22	1.45	0.79
1:C:477:GLN:O	1:C:480:GLN:HB3	1.82	0.79
1:D:83:PRO:HB3	1:E:453:SER:HB2	1.63	0.79
1:E:405:ASN:HD22	1:E:411:VAL:HG13	1.47	0.79
1:D:334:ASN:HD22	1:D:337:ARG:HB2	1.46	0.79
1:C:462:ILE:HB	1:C:467:LEU:HD11	1.63	0.78
1:F:50:ARG:HH22	1:F:67:GLN:HE22	1.30	0.78
1:A:224:ALA:HA	1:A:227:LEU:HD12	1.66	0.78
1:C:52:LEU:HD23	1:C:237:ILE:HD13	1.66	0.77
1:E:73:GLN:HB3	1:E:142:VAL:HG12	1.65	0.77
1:B:396:ARG:HH11	1:B:440:GLU:HG3	1.49	0.77
1:E:460:ARG:NH2	1:E:487:SER:HB2	2.00	0.77
1:A:334:ASN:HD21	1:A:337:ARG:H	1.31	0.77
1:D:45:VAL:HG12	1:D:148:ASP:HA	1.67	0.77
1:C:210:LYS:HD3	1:C:225:GLU:HG2	1.64	0.77
1:D:46:THR:HG23	1:D:147:LEU:HD12	1.67	0.77
1:E:465:GLU:CD	1:E:465:GLU:H	1.85	0.77
1:E:247:ILE:HG12	1:E:248:SER:N	1.98	0.76
1:C:392:ILE:HG12	1:C:443:VAL:HG22	1.65	0.76
1:C:367:LEU:HD23	1:C:446:THR:HA	1.67	0.76
1:D:34:ASN:ND2	1:D:36:GLN:HB2	2.01	0.76
1:B:112:GLN:HE21	1:C:461:ALA:HB1	1.51	0.76
1:A:388:ALA:HA	1:C:155:GLN:OE1	1.86	0.75
1:E:376:ARG:HB3	1:E:376:ARG:NH1	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:ARG:NH2	1:F:67:GLN:HE22	1.83	0.75
1:F:107:LEU:H	1:F:107:LEU:HD22	1.51	0.75
1:A:159:ASN:HD22	1:A:176:THR:HA	1.52	0.75
1:A:372:VAL:HB	1:A:441:TYR:CE2	2.22	0.75
1:F:486:ASN:ND2	1:F:491:VAL:HG22	2.01	0.75
1:B:387:ASN:HD22	1:B:387:ASN:H	1.35	0.75
1:B:135:ASN:ND2	1:B:141:VAL:HG23	2.01	0.74
1:C:89:PHE:HB2	1:C:113:LYS:HA	1.70	0.74
1:B:477:GLN:O	1:B:480:GLN:HB3	1.88	0.74
1:E:235:LYS:HA	1:E:235:LYS:HE3	1.69	0.74
1:E:486:ASN:ND2	1:E:491:VAL:HG22	2.02	0.73
1:F:85:CYS:HB2	1:F:112:GLN:HE22	1.52	0.73
1:F:399:GLY:HA3	1:F:439:LEU:HD22	1.70	0.73
1:B:156:LEU:HD13	1:B:161:ARG:HE	1.54	0.73
1:D:246:VAL:HG11	1:E:463:PRO:HB3	1.69	0.73
1:C:391:VAL:HG23	1:C:444:PHE:HB2	1.70	0.72
1:F:135:ASN:ND2	1:F:141:VAL:HG23	2.04	0.72
1:F:240:VAL:HG11	1:F:244:LEU:HD12	1.72	0.72
1:C:363:ARG:HE	1:C:448:HIS:CD2	2.07	0.72
1:F:334:ASN:ND2	1:F:337:ARG:H	1.88	0.72
1:B:64:PRO:HG3	1:B:156:LEU:HD12	1.71	0.72
1:C:390:SER:HB2	1:C:424:VAL:HB	1.71	0.71
1:D:403:VAL:HG22	1:D:430:VAL:HG23	1.70	0.71
1:B:480:GLN:HA	1:B:484:GLN:NE2	2.05	0.71
1:F:400:ARG:HB3	1:F:433:GLN:HB3	1.73	0.71
1:A:463:PRO:HB2	1:A:466:VAL:HG23	1.70	0.71
1:A:366:GLY:HA2	1:A:448:HIS:HB3	1.73	0.71
1:D:364:GLN:H	1:D:364:GLN:NE2	1.88	0.71
1:F:85:CYS:HB2	1:F:112:GLN:NE2	2.06	0.71
1:A:455:ILE:HD13	1:C:205:LEU:HD21	1.72	0.71
1:D:465:GLU:OE1	1:F:246:VAL:HG23	1.91	0.71
1:A:459:PHE:HE2	1:A:471:TYR:HH	1.37	0.70
1:B:156:LEU:HB3	1:B:161:ARG:NH2	2.05	0.70
1:C:124:VAL:H	1:C:331:LEU:CD1	2.03	0.70
1:D:240:VAL:HG13	1:E:469:ASN:HD21	1.57	0.70
1:D:390:SER:HB2	1:D:424:VAL:HB	1.74	0.70
1:C:60:PRO:HG3	1:C:132:TRP:HB3	1.73	0.70
1:D:338:PRO:HG3	1:D:350:ARG:HH11	1.56	0.70
1:D:384:TRP:NE1	1:D:386:LEU:HD12	2.07	0.70
1:A:46:THR:HG23	1:A:147:LEU:HD12	1.74	0.69
1:B:401:VAL:HG21	1:B:416:LEU:HD22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:H	1:B:113:LYS:HD2	1.55	0.69
1:C:391:VAL:CG2	1:C:444:PHE:HB2	2.23	0.69
1:E:326:ILE:HD13	1:E:326:ILE:O	1.91	0.69
1:A:480:GLN:O	1:A:484:GLN:HB2	1.93	0.69
1:E:37:HIS:HB2	1:E:40:LEU:HD23	1.74	0.69
1:B:83:PRO:HB3	1:C:453:SER:HB2	1.75	0.69
1:B:123:LEU:HD23	1:B:332:HIS:CB	2.22	0.69
1:D:50:ARG:HH12	1:D:67:GLN:HE22	1.39	0.69
1:D:391:VAL:HG22	1:D:421:LEU:HD11	1.74	0.69
1:E:16:ALA:HB1	1:E:420:GLN:HE21	1.56	0.69
1:A:221:GLU:O	1:A:225:GLU:HB2	1.92	0.69
1:B:126:PRO:HB2	1:B:129:VAL:HG21	1.75	0.69
1:C:67:GLN:HB2	1:C:125:ILE:HB	1.74	0.69
1:C:480:GLN:NE2	1:C:484:GLN:HG3	2.08	0.69
1:A:453:SER:OG	1:C:83:PRO:HB3	1.93	0.69
1:B:244:LEU:HB2	1:B:247:ILE:HD13	1.75	0.68
1:B:385:ASN:HD21	1:B:445:LYS:NZ	1.90	0.68
1:A:159:ASN:HB3	1:A:176:THR:HG22	1.75	0.68
1:B:155:GLN:OE1	1:C:388:ALA:HA	1.92	0.68
1:E:460:ARG:HH22	1:E:487:SER:HB2	1.56	0.68
1:F:46:THR:HG23	1:F:147:LEU:HD12	1.76	0.68
1:F:123:LEU:HD23	1:F:332:HIS:HB3	1.73	0.68
1:C:70:ILE:HD12	1:C:442:VAL:HG21	1.74	0.68
1:A:357:LEU:H	1:A:357:LEU:HD12	1.57	0.68
1:D:394:VAL:HA	1:D:441:TYR:HB3	1.76	0.68
1:A:367:LEU:O	1:A:448:HIS:HA	1.93	0.68
1:A:409:ASN:N	1:A:409:ASN:HD22	1.92	0.68
1:E:385:ASN:HD22	1:E:452:SER:HB3	1.59	0.68
1:B:368:SER:OG	1:B:445:LYS:HB2	1.94	0.68
1:D:67:GLN:HB2	1:D:125:ILE:HB	1.75	0.68
1:A:14:LEU:HD13	1:A:411:VAL:HB	1.75	0.67
1:A:112:GLN:HE21	1:B:461:ALA:HB1	1.59	0.67
1:B:467:LEU:HD22	1:B:467:LEU:H	1.59	0.67
1:B:240:VAL:HG21	1:B:244:LEU:HD11	1.75	0.67
1:E:345:ASN:HB3	1:E:348:ALA:HB3	1.77	0.67
1:F:66:PRO:HG3	1:F:151:ASN:ND2	2.10	0.67
1:D:364:GLN:HE21	1:D:364:GLN:N	1.90	0.66
1:A:155:GLN:OE1	1:B:388:ALA:HA	1.94	0.66
1:A:374:LEU:HD12	1:A:439:LEU:HD23	1.76	0.66
1:C:403:VAL:O	1:C:411:VAL:HG22	1.95	0.66
1:B:14:LEU:C	1:B:15:ASN:HD22	1.99	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLY:O	1:B:335:ILE:HG22	1.96	0.66
1:B:159:ASN:ND2	1:B:176:THR:HG22	2.07	0.66
1:C:169:PRO:HA	1:C:236:GLN:OE1	1.95	0.66
1:C:463:PRO:O	1:C:467:LEU:HD13	1.95	0.66
1:B:387:ASN:HD21	1:B:451:VAL:H	1.43	0.66
1:C:69:ILE:HG12	1:C:145:SER:OG	1.95	0.66
1:B:40:LEU:HD21	1:B:46:THR:HA	1.77	0.66
1:D:334:ASN:ND2	1:D:337:ARG:HB2	2.09	0.66
1:B:26:GLU:OE1	1:B:234:ARG:HG2	1.94	0.66
1:C:121:ASP:HA	1:C:334:ASN:HA	1.78	0.66
1:E:75:LYS:HB3	1:E:118:ASN:HA	1.77	0.66
1:F:159:ASN:ND2	1:F:176:THR:HG22	2.03	0.66
1:E:425:PRO:HB2	1:E:428:PHE:CD2	2.31	0.66
1:C:56:GLY:H	1:C:135:ASN:HB3	1.61	0.65
1:D:396:ARG:HB3	1:D:440:GLU:HB2	1.77	0.65
1:A:481:LEU:HD22	1:C:217:PHE:HB3	1.77	0.65
1:C:229:SER:N	1:C:230:PRO:HD3	2.10	0.65
1:A:31:GLU:OE1	1:A:49:LYS:HD2	1.95	0.65
1:F:30:ILE:HG12	1:F:50:ARG:HG3	1.78	0.65
1:F:115:ARG:NH2	1:F:331:LEU:HD12	2.02	0.65
1:F:401:VAL:HG22	1:F:432:GLU:HG3	1.77	0.65
1:A:426:GLN:NE2	1:C:155:GLN:H	1.92	0.65
1:E:169:PRO:HB3	1:E:236:GLN:HB3	1.77	0.65
1:A:454:TYR:CE1	1:A:457:ASP:HB2	2.30	0.65
1:A:10:GLN:HA	1:C:161:ARG:HH22	1.61	0.65
1:A:400:ARG:HG2	1:A:402:ARG:NH2	2.11	0.65
1:E:148:ASP:OD2	1:E:151:ASN:HB2	1.97	0.65
1:A:205:LEU:HD21	1:B:455:ILE:HD13	1.79	0.65
1:B:393:TYR:HB3	1:B:442:VAL:CG1	2.28	0.65
1:F:14:LEU:HD13	1:F:411:VAL:HB	1.77	0.65
1:C:382:PRO:HB2	1:C:455:ILE:HD12	1.78	0.64
1:D:240:VAL:HG13	1:E:469:ASN:ND2	2.12	0.64
1:E:208:PHE:HB2	1:E:213:LEU:HD21	1.79	0.64
1:C:394:VAL:HG11	1:C:416:LEU:HG	1.79	0.64
1:A:463:PRO:HG3	1:C:111:HIS:ND1	2.13	0.64
1:E:244:LEU:HB3	1:E:247:ILE:HD11	1.77	0.64
1:C:51:THR:HG23	1:C:142:VAL:HG22	1.78	0.64
1:F:19:PRO:HB3	1:F:31:GLU:HB3	1.78	0.64
1:B:22:ARG:HB3	1:B:22:ARG:HH11	1.62	0.64
1:B:463:PRO:HB2	1:B:466:VAL:HG23	1.78	0.64
1:A:334:ASN:ND2	1:A:337:ARG:H	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:PRO:N	1:B:127:PRO:HG3	2.12	0.64
1:B:374:LEU:HD11	1:B:378:GLY:C	2.18	0.64
1:A:342:ASP:HB2	1:A:351:ILE:O	1.97	0.64
1:B:22:ARG:NH2	1:B:29:LEU:HD21	2.13	0.64
1:C:208:PHE:HB2	1:C:213:LEU:HD21	1.80	0.64
1:A:326:ILE:HD13	1:A:326:ILE:O	1.98	0.63
1:B:475:GLN:NE2	1:B:479:ARG:HB2	2.13	0.63
1:F:25:SER:HB3	1:F:235:LYS:HB2	1.81	0.63
1:C:124:VAL:HG21	1:C:362:LEU:HD23	1.81	0.63
1:A:235:LYS:HB3	1:A:236:GLN:OE1	1.99	0.63
1:A:480:GLN:HE21	1:A:480:GLN:HA	1.63	0.63
1:F:81:ALA:HB3	1:F:130:PRO:HB2	1.79	0.63
1:A:112:GLN:NE2	1:B:461:ALA:HB1	2.14	0.63
1:B:456:LYS:HG2	1:B:460:ARG:NH2	2.13	0.63
1:C:205:LEU:HD13	1:C:227:LEU:HB3	1.79	0.63
1:D:224:ALA:HA	1:D:227:LEU:HD12	1.81	0.63
1:D:455:ILE:HD13	1:F:205:LEU:HD21	1.81	0.63
1:F:67:GLN:HE21	1:F:69:ILE:HD11	1.63	0.63
1:B:388:ALA:O	1:B:426:GLN:HA	1.98	0.63
1:A:363:ARG:HE	1:A:448:HIS:CD2	2.16	0.63
1:D:176:THR:O	1:D:177:MET:HE2	1.99	0.63
1:D:391:VAL:CG1	1:D:444:PHE:HB2	2.28	0.63
1:E:73:GLN:HE21	1:E:142:VAL:CG1	2.12	0.63
1:A:392:ILE:HG12	1:A:443:VAL:HG22	1.79	0.63
1:C:62:TYR:CE2	1:C:163:PHE:HB2	2.34	0.63
1:D:398:LYS:HE3	1:D:415:GLU:HB3	1.80	0.63
1:F:50:ARG:HH22	1:F:67:GLN:NE2	1.97	0.62
1:C:326:ILE:HG23	1:C:327:CYS:N	2.14	0.62
1:E:60:PRO:HG3	1:E:132:TRP:HB3	1.80	0.62
1:F:14:LEU:HD23	1:F:423:VAL:O	2.00	0.62
1:E:459:PHE:O	1:E:482:LYS:HE2	2.00	0.62
1:A:340:ARG:HB2	1:A:352:SER:OG	1.99	0.62
1:A:349:GLY:HA3	1:A:373:VAL:O	2.00	0.62
1:A:471:TYR:HB3	1:C:226:LYS:O	1.99	0.62
1:B:388:ALA:N	1:B:426:GLN:HE21	1.98	0.62
1:D:14:LEU:HD13	1:D:411:VAL:HB	1.81	0.62
1:E:330:LYS:HE3	1:E:332:HIS:O	2.00	0.62
1:C:351:ILE:HG12	1:C:372:VAL:HG13	1.82	0.62
1:D:70:ILE:HD12	1:D:442:VAL:HG21	1.81	0.62
1:D:364:GLN:NE2	1:D:364:GLN:N	2.47	0.62
1:A:57:LEU:HD12	1:A:133:THR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:THR:O	1:C:226:LYS:HB2	1.99	0.61
1:D:379:ILE:HD11	1:F:212:PHE:CZ	2.35	0.61
1:F:454:TYR:CE1	1:F:457:ASP:HB2	2.35	0.61
1:B:113:LYS:HD2	1:B:113:LYS:N	2.14	0.61
1:B:224:ALA:HA	1:B:227:LEU:HD12	1.82	0.61
1:F:345:ASN:HB3	1:F:348:ALA:HB3	1.82	0.61
1:C:27:GLY:HA2	1:C:239:THR:HG23	1.82	0.61
1:D:366:GLY:HA2	1:D:448:HIS:H	1.65	0.61
1:E:109:ASP:HA	1:F:483:TYR:OH	2.01	0.61
1:B:46:THR:CG2	1:B:147:LEU:HB2	2.30	0.61
1:B:136:THR:HG22	1:B:247:ILE:HG21	1.82	0.61
1:E:144:ILE:N	1:E:144:ILE:HD12	2.16	0.61
1:E:135:ASN:ND2	1:E:141:VAL:HG23	2.14	0.61
1:C:64:PRO:HG3	1:C:156:LEU:HD12	1.83	0.61
1:D:446:THR:O	1:D:447:HIS:HB2	1.99	0.61
1:E:156:LEU:HD21	1:F:426:GLN:H	1.65	0.61
1:F:170:ASP:HB2	1:F:235:LYS:HD2	1.82	0.61
1:D:437:GLN:H	1:D:437:GLN:NE2	1.99	0.60
1:A:468:SER:OG	1:A:478:VAL:HG21	2.01	0.60
1:B:31:GLU:HB2	1:B:49:LYS:HB3	1.83	0.60
1:C:52:LEU:CD2	1:C:237:ILE:HD13	2.31	0.60
1:A:234:ARG:CB	1:A:238:VAL:HG12	2.31	0.60
1:A:471:TYR:CD2	1:C:227:LEU:HA	2.36	0.60
1:B:454:TYR:CZ	1:B:457:ASP:HB2	2.36	0.60
1:D:351:ILE:HG23	1:D:372:VAL:HG22	1.82	0.60
1:F:28:GLY:HA3	1:F:237:ILE:HG21	1.84	0.60
1:B:148:ASP:OD2	1:B:151:ASN:HB2	2.01	0.60
1:D:126:PRO:HB2	1:D:129:VAL:HG21	1.82	0.60
1:D:338:PRO:HG3	1:D:350:ARG:NH1	2.16	0.60
1:C:114:ILE:HD12	1:C:132:TRP:HZ2	1.66	0.60
1:C:326:ILE:HG23	1:C:327:CYS:H	1.65	0.60
1:D:325:ASN:N	1:D:325:ASN:HD22	1.97	0.60
1:A:409:ASN:N	1:A:409:ASN:ND2	2.49	0.60
1:B:240:VAL:HG13	1:C:469:ASN:HD21	1.67	0.60
1:B:387:ASN:C	1:B:426:GLN:HE21	2.04	0.60
1:D:489:PRO:O	1:D:491:VAL:HG23	2.02	0.60
1:B:246:VAL:HG23	1:C:465:GLU:OE2	2.01	0.60
1:E:17:LEU:HD22	1:E:37:HIS:ND1	2.17	0.60
1:A:33:TRP:CE3	1:A:47:VAL:HB	2.37	0.59
1:B:69:ILE:HG12	1:B:145:SER:HA	1.84	0.59
1:A:407:GLN:HB2	1:A:409:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ARG:HD3	1:B:436:GLU:O	2.02	0.59
1:D:34:ASN:HD21	1:D:36:GLN:HB2	1.66	0.59
1:A:374:LEU:HB2	1:A:439:LEU:HB3	1.83	0.59
1:B:240:VAL:HG13	1:C:469:ASN:ND2	2.17	0.59
1:B:475:GLN:HE21	1:B:479:ARG:HB2	1.67	0.59
1:A:34:ASN:HD22	1:A:35:SER:N	2.00	0.59
1:C:213:LEU:HD12	1:C:217:PHE:HE1	1.66	0.59
1:C:350:ARG:HH21	1:C:350:ARG:HG3	1.68	0.59
1:C:363:ARG:HE	1:C:448:HIS:CG	2.21	0.59
1:E:234:ARG:O	1:E:235:LYS:HB2	2.02	0.59
1:D:392:ILE:O	1:D:421:LEU:HD12	2.02	0.59
1:A:60:PRO:HA	1:A:131:TYR:O	2.03	0.59
1:A:123:LEU:HD23	1:A:332:HIS:HB3	1.83	0.59
1:A:471:TYR:CE2	1:C:205:LEU:HD12	2.38	0.59
1:B:326:ILE:HG13	1:B:329:MET:SD	2.43	0.59
1:C:14:LEU:C	1:C:15:ASN:HD22	2.05	0.59
1:B:65:TYR:C	1:B:127:PRO:HG3	2.23	0.58
1:D:123:LEU:HD23	1:D:332:HIS:HB3	1.84	0.58
1:F:395:THR:O	1:F:418:ARG:HG3	2.02	0.58
1:C:399:GLY:HA3	1:C:439:LEU:HD22	1.86	0.58
1:B:348:ALA:O	1:B:374:LEU:HD22	2.03	0.58
1:F:107:LEU:H	1:F:107:LEU:CD2	2.16	0.58
1:A:159:ASN:ND2	1:A:176:THR:HA	2.19	0.58
1:B:338:PRO:HG3	1:B:350:ARG:HH21	1.68	0.58
1:C:23:VAL:HG11	1:C:170:ASP:HB3	1.85	0.58
1:E:47:VAL:HG21	1:E:421:LEU:HD11	1.84	0.58
1:F:387:ASN:O	1:F:388:ALA:HB2	2.04	0.58
1:B:121:ASP:HA	1:B:334:ASN:HA	1.84	0.58
1:C:8:GLU:O	1:C:42:CYS:HB2	2.03	0.58
1:D:386:LEU:HG	1:F:128:GLY:HA3	1.84	0.58
1:A:45:VAL:HG12	1:A:148:ASP:HA	1.86	0.58
1:C:174:PRO:O	1:C:178:GLN:HG3	2.02	0.58
1:E:62:TYR:HE2	1:F:427:ASN:HB3	1.67	0.58
1:F:164:TYR:O	1:F:203:SER:HB2	2.04	0.58
1:D:368:SER:HB3	1:D:445:LYS:HB2	1.85	0.58
1:A:22:ARG:HH12	1:A:29:LEU:HD21	1.69	0.57
1:A:378:GLY:O	1:A:433:GLN:HA	2.04	0.57
1:B:393:TYR:HB3	1:B:442:VAL:HG12	1.85	0.57
1:D:480:GLN:OE1	1:F:219:THR:HA	2.04	0.57
1:B:387:ASN:HA	1:B:426:GLN:NE2	2.20	0.57
1:D:135:ASN:ND2	1:D:141:VAL:HG23	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HD12	1:A:144:ILE:N	2.20	0.57
1:A:326:ILE:HA	1:A:329:MET:CE	2.34	0.57
1:A:354:LEU:HD12	1:A:358:THR:OG1	2.04	0.57
1:B:387:ASN:HD22	1:B:387:ASN:N	1.98	0.57
1:C:338:PRO:CG	1:C:350:ARG:HH11	2.17	0.57
1:B:34:ASN:HD22	1:B:35:SER:N	2.03	0.57
1:B:124:VAL:HG12	1:B:331:LEU:O	2.05	0.57
1:F:71:VAL:HG21	1:F:117:PHE:CD2	2.39	0.57
1:F:456:LYS:NZ	1:F:486:ASN:HD21	2.02	0.57
1:A:71:VAL:HG21	1:A:117:PHE:CD2	2.40	0.57
1:A:463:PRO:HB2	1:A:466:VAL:CG2	2.35	0.57
1:B:134:TYR:OH	1:B:243:GLY:HA2	2.05	0.57
1:C:345:ASN:HD22	1:C:348:ALA:HB3	1.68	0.57
1:E:73:GLN:HE21	1:E:142:VAL:HG12	1.69	0.57
1:F:219:THR:OG1	1:F:223:THR:HB	2.04	0.57
1:D:391:VAL:HG13	1:D:391:VAL:O	2.05	0.57
1:A:22:ARG:NH1	1:A:22:ARG:HB2	2.19	0.57
1:D:175:GLU:O	1:D:178:GLN:HG3	2.05	0.57
1:C:386:LEU:HD12	1:C:386:LEU:H	1.70	0.57
1:D:83:PRO:HB3	1:E:453:SER:CB	2.34	0.57
1:F:245:SER:C	1:F:247:ILE:H	2.08	0.57
1:A:234:ARG:HB2	1:A:238:VAL:HG12	1.86	0.57
1:A:357:LEU:H	1:A:357:LEU:CD1	2.17	0.57
1:D:379:ILE:HG13	1:D:433:GLN:HB2	1.87	0.57
1:B:168:ASN:ND2	1:B:202:GLY:HA2	2.20	0.57
1:E:20:ASP:OD2	1:E:34:ASN:HB2	2.05	0.57
1:B:22:ARG:HB3	1:B:22:ARG:NH1	2.20	0.56
1:C:337:ARG:HA	1:C:337:ARG:HH21	1.69	0.56
1:E:17:LEU:HD13	1:E:37:HIS:ND1	2.20	0.56
1:D:14:LEU:HD23	1:D:423:VAL:O	2.05	0.56
1:D:34:ASN:OD1	1:D:175:GLU:HB3	2.06	0.56
1:D:144:ILE:HG13	1:D:393:TYR:CE2	2.40	0.56
1:D:427:ASN:HB3	1:F:62:TYR:HE2	1.70	0.56
1:E:430:VAL:HG22	1:E:431:ALA:N	2.21	0.56
1:D:170:ASP:O	1:D:172:GLU:N	2.38	0.56
1:A:396:ARG:HG2	1:A:396:ARG:HH11	1.71	0.56
1:B:28:GLY:HA3	1:B:237:ILE:HG21	1.87	0.56
1:D:47:VAL:HG13	1:D:145:SER:O	2.05	0.56
1:C:124:VAL:CB	1:C:331:LEU:HD11	2.34	0.56
1:C:123:LEU:HD23	1:C:331:LEU:O	2.06	0.56
1:E:333:GLU:HG3	1:E:340:ARG:HH12	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:THR:HA	1:F:141:VAL:O	2.05	0.56
1:F:477:GLN:O	1:F:480:GLN:HB3	2.06	0.56
1:C:66:PRO:HG3	1:C:151:ASN:ND2	2.21	0.56
1:C:69:ILE:HG12	1:C:145:SER:CB	2.36	0.56
1:D:36:GLN:HE22	1:D:178:GLN:NE2	2.04	0.56
1:E:417:ARG:HG3	1:E:420:GLN:OE1	2.05	0.56
1:A:204:VAL:O	1:B:404:VAL:HG11	2.06	0.56
1:D:234:ARG:O	1:D:235:LYS:HB2	2.06	0.56
1:D:345:ASN:HB3	1:D:348:ALA:HB3	1.88	0.56
1:C:6:PHE:C	1:C:7:ASN:HD22	2.08	0.55
1:C:371:TYR:HE1	1:C:440:GLU:HG2	1.69	0.55
1:C:394:VAL:HG21	1:C:417:ARG:O	2.05	0.55
1:F:67:GLN:HG2	1:F:125:ILE:HB	1.88	0.55
1:A:385:ASN:HD21	1:A:445:LYS:CE	2.20	0.55
1:B:61:SER:O	1:B:130:PRO:HA	2.06	0.55
1:B:144:ILE:N	1:B:144:ILE:HD12	2.22	0.55
1:C:394:VAL:O	1:C:418:ARG:HA	2.05	0.55
1:E:226:LYS:HB2	1:F:473:LEU:HD21	1.88	0.55
1:F:214:ALA:HB1	1:F:219:THR:O	2.06	0.55
1:C:47:VAL:HG12	1:C:48:SER:N	2.22	0.55
1:D:173:HIS:HB3	1:D:175:GLU:OE1	2.06	0.55
1:B:471:TYR:O	1:B:472:ASN:HB2	2.06	0.55
1:C:126:PRO:HB2	1:C:129:VAL:HG21	1.89	0.55
1:C:417:ARG:HG2	1:C:417:ARG:HH11	1.71	0.55
1:A:373:VAL:HG22	1:A:440:GLU:CG	2.35	0.55
1:B:349:GLY:O	1:B:490:LEU:HD13	2.06	0.55
1:D:466:VAL:HG22	1:F:244:LEU:HD21	1.89	0.55
1:A:26:GLU:OE1	1:A:234:ARG:HG2	2.06	0.55
1:C:71:VAL:HG21	1:C:117:PHE:CD2	2.42	0.55
1:E:73:GLN:HB3	1:E:142:VAL:CG1	2.36	0.55
1:A:214:ALA:HB1	1:A:219:THR:O	2.07	0.55
1:B:82:PHE:HZ	1:B:331:LEU:HD11	1.71	0.55
1:C:61:SER:O	1:C:130:PRO:HA	2.06	0.55
1:C:144:ILE:HD12	1:C:144:ILE:N	2.21	0.55
1:F:246:VAL:HG12	1:F:246:VAL:O	2.06	0.55
1:A:390:SER:HB2	1:A:424:VAL:HB	1.88	0.55
1:A:409:ASN:ND2	1:A:409:ASN:H	2.03	0.55
1:F:214:ALA:HA	1:F:219:THR:HG22	1.88	0.55
1:E:70:ILE:HG23	1:E:70:ILE:O	2.05	0.55
1:E:333:GLU:CG	1:E:340:ARG:HH12	2.19	0.55
1:F:349:GLY:O	1:F:490:LEU:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:HB	1:A:30:ILE:HB	1.89	0.55
1:A:357:LEU:HD12	1:A:357:LEU:N	2.22	0.55
1:A:395:THR:C	1:A:418:ARG:HG3	2.27	0.55
1:A:22:ARG:HA	1:A:30:ILE:O	2.07	0.54
1:B:34:ASN:HD22	1:B:35:SER:H	1.55	0.54
1:B:385:ASN:HD21	1:B:445:LYS:HZ2	1.53	0.54
1:E:2:THR:HA	1:E:5:LYS:NZ	2.22	0.54
1:B:479:ARG:HE	1:B:483:TYR:HD2	1.53	0.54
1:E:244:LEU:HD21	1:F:466:VAL:CG2	2.37	0.54
1:E:405:ASN:HD22	1:E:411:VAL:CG1	2.18	0.54
1:F:208:PHE:HB2	1:F:213:LEU:HD21	1.88	0.54
1:A:350:ARG:NH1	1:A:373:VAL:HG21	2.22	0.54
1:D:156:LEU:HA	1:E:9:CYS:SG	2.46	0.54
1:E:208:PHE:CD1	1:F:402:ARG:HD3	2.43	0.54
1:F:235:LYS:HB3	1:F:236:GLN:OE1	2.08	0.54
1:C:30:ILE:HD12	1:C:236:GLN:HG3	1.90	0.54
1:F:25:SER:OG	1:F:237:ILE:HB	2.07	0.54
1:A:358:THR:O	1:A:360:PRO:HD3	2.07	0.54
1:B:65:TYR:CE2	1:B:147:LEU:HB3	2.43	0.54
1:B:387:ASN:HA	1:B:426:GLN:HE21	1.72	0.54
1:C:206:SER:HA	1:C:228:ARG:HG2	1.90	0.54
1:C:403:VAL:HG22	1:C:430:VAL:HG23	1.89	0.54
1:F:218:ASN:HD22	1:F:218:ASN:N	2.04	0.54
1:A:340:ARG:CZ	1:A:350:ARG:HD2	2.37	0.54
1:A:407:GLN:HB2	1:A:409:ASN:ND2	2.22	0.54
1:C:11:LEU:HD21	1:C:38:PRO:HB3	1.89	0.54
1:C:135:ASN:ND2	1:C:141:VAL:HG23	2.22	0.54
1:E:36:GLN:HE21	1:E:175:GLU:HB2	1.73	0.54
1:E:478:VAL:O	1:E:482:LYS:HB2	2.08	0.54
1:A:46:THR:HG23	1:A:147:LEU:HB2	1.90	0.54
1:A:400:ARG:HG2	1:A:402:ARG:HH22	1.72	0.54
1:B:67:GLN:HE21	1:B:147:LEU:CD2	2.20	0.54
1:D:69:ILE:CG2	1:D:143:ALA:HB1	2.38	0.54
1:A:325:ASN:HA	1:A:328:THR:HG22	1.89	0.54
1:C:60:PRO:HA	1:C:131:TYR:O	2.08	0.54
1:C:210:LYS:HD3	1:C:225:GLU:CG	2.35	0.54
1:D:466:VAL:HG22	1:F:244:LEU:CD2	2.38	0.54
1:F:25:SER:CB	1:F:235:LYS:HB2	2.38	0.54
1:F:334:ASN:HB3	1:F:340:ARG:NH1	2.22	0.54
1:A:25:SER:OG	1:A:237:ILE:HB	2.08	0.54
1:B:35:SER:OG	1:B:175:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:HD12	1:C:386:LEU:N	2.23	0.54
1:D:246:VAL:HG13	1:E:465:GLU:CD	2.28	0.54
1:A:124:VAL:O	1:A:126:PRO:HD3	2.08	0.54
1:A:351:ILE:HG12	1:A:372:VAL:HG22	1.89	0.54
1:B:46:THR:HG23	1:B:147:LEU:HB2	1.90	0.54
1:A:350:ARG:HH12	1:A:373:VAL:HG21	1.73	0.53
1:E:376:ARG:HH11	1:E:376:ARG:CB	2.18	0.53
1:F:402:ARG:NH2	1:F:413:ASP:OD1	2.41	0.53
1:A:163:PHE:CZ	1:B:406:CSD:HB2	2.43	0.53
1:A:491:VAL:HG12	1:A:492:ASN:N	2.23	0.53
1:D:50:ARG:HH12	1:D:67:GLN:NE2	2.05	0.53
1:F:34:ASN:ND2	1:F:36:GLN:HB2	2.14	0.53
1:A:122:VAL:O	1:A:332:HIS:HA	2.08	0.53
1:D:394:VAL:HA	1:D:441:TYR:CB	2.38	0.53
1:F:343:PHE:HB2	1:F:351:ILE:HB	1.89	0.53
1:C:326:ILE:HD13	1:C:326:ILE:C	2.28	0.53
1:D:180:GLN:NE2	1:D:180:GLN:N	2.56	0.53
1:D:218:ASN:OD1	1:E:485:GLY:HA3	2.08	0.53
1:E:16:ALA:HB1	1:E:420:GLN:NE2	2.22	0.53
1:A:15:ASN:HB2	1:A:39:GLU:OE2	2.09	0.53
1:A:391:VAL:CG1	1:A:421:LEU:HD11	2.37	0.53
1:D:115:ARG:HD2	1:D:115:ARG:N	2.20	0.53
1:D:171:ILE:HG12	1:D:198:GLU:O	2.08	0.53
1:A:465:GLU:OE2	1:C:245:SER:HB2	2.09	0.53
1:A:493:PRO:HB3	1:C:215:GLN:OE1	2.08	0.53
1:B:425:PRO:HB2	1:B:428:PHE:CD2	2.44	0.53
1:D:36:GLN:NE2	1:D:175:GLU:HB2	2.12	0.53
1:F:170:ASP:HA	1:F:200:GLU:HA	1.89	0.53
1:B:462:ILE:HG22	1:B:466:VAL:HB	1.91	0.53
1:E:325:ASN:HA	1:E:328:THR:HG22	1.90	0.53
1:E:335:ILE:HG12	1:E:335:ILE:O	2.09	0.53
1:F:171:ILE:HD13	1:F:200:GLU:N	2.24	0.53
1:A:391:VAL:HG12	1:A:421:LEU:HD11	1.90	0.53
1:D:27:GLY:HA3	1:D:239:THR:HG23	1.90	0.53
1:E:39:GLU:N	1:E:39:GLU:OE1	2.39	0.53
1:E:170:ASP:OD2	1:E:235:LYS:HE2	2.09	0.53
1:F:20:ASP:O	1:F:21:HIS:HB2	2.08	0.53
1:B:396:ARG:HA	1:B:418:ARG:HG3	1.91	0.53
1:C:454:TYR:CE1	1:C:457:ASP:HB2	2.44	0.53
1:D:430:VAL:HG22	1:D:431:ALA:N	2.24	0.53
1:B:69:ILE:CG2	1:B:143:ALA:HB1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLU:HG3	1:C:112:GLN:N	2.24	0.53
1:F:405:ASN:OD1	1:F:407:GLN:HG3	2.08	0.53
1:B:31:GLU:OE1	1:B:49:LYS:HD3	2.08	0.52
1:E:247:ILE:H	1:E:247:ILE:CD1	2.16	0.52
1:E:376:ARG:O	1:E:377:ASN:HB2	2.10	0.52
1:A:70:ILE:O	1:A:70:ILE:HG23	2.09	0.52
1:A:461:ALA:HA	1:C:87:GLU:CG	2.39	0.52
1:C:372:VAL:HB	1:C:441:TYR:CZ	2.44	0.52
1:F:107:LEU:HD22	1:F:107:LEU:N	2.20	0.52
1:A:386:LEU:HD13	1:A:452:SER:HA	1.90	0.52
1:B:15:ASN:HD22	1:B:15:ASN:N	2.05	0.52
1:B:379:ILE:HG12	1:B:433:GLN:HG3	1.91	0.52
1:C:34:ASN:HD22	1:C:35:SER:N	2.07	0.52
1:C:146:LEU:HB2	1:C:444:PHE:CD1	2.43	0.52
1:E:40:LEU:HD12	1:E:45:VAL:O	2.10	0.52
1:F:244:LEU:O	1:F:247:ILE:HD13	2.09	0.52
1:A:387:ASN:HD21	1:A:451:VAL:H	1.57	0.52
1:B:69:ILE:HA	1:B:144:ILE:O	2.09	0.52
1:B:81:ALA:HA	1:B:112:GLN:NE2	2.24	0.52
1:B:240:VAL:HG11	1:B:244:LEU:CD1	2.39	0.52
1:C:213:LEU:HD22	1:C:213:LEU:H	1.75	0.52
1:C:240:VAL:HG11	1:C:244:LEU:HD13	1.91	0.52
1:C:345:ASN:HD22	1:C:348:ALA:CB	2.23	0.52
1:B:335:ILE:HG23	1:B:336:ALA:N	2.25	0.52
1:C:394:VAL:CG1	1:C:416:LEU:HG	2.39	0.52
1:D:62:TYR:HE2	1:E:427:ASN:HB3	1.74	0.52
1:E:57:LEU:HD12	1:E:59:LEU:HD23	1.91	0.52
1:F:6:PHE:C	1:F:7:ASN:HD22	2.13	0.52
1:A:61:SER:O	1:A:130:PRO:HA	2.10	0.52
1:A:351:ILE:HG13	1:A:490:LEU:HD11	1.91	0.52
1:E:235:LYS:HE3	1:E:235:LYS:CA	2.40	0.52
1:E:244:LEU:HD11	1:F:465:GLU:HB3	1.91	0.52
1:F:152:PHE:H	1:F:152:PHE:HD1	1.56	0.52
1:B:76:GLY:HA2	1:B:136:THR:H	1.75	0.52
1:B:85:CYS:HB3	1:B:113:LYS:NZ	2.24	0.52
1:D:59:LEU:HG	1:D:236:GLN:O	2.10	0.52
1:A:334:ASN:HD21	1:A:337:ARG:HG2	1.71	0.52
1:A:395:THR:O	1:A:418:ARG:HG3	2.09	0.52
1:B:480:GLN:O	1:B:484:GLN:HB2	2.10	0.52
1:C:174:PRO:C	1:C:178:GLN:HE21	2.13	0.52
1:A:34:ASN:HD22	1:A:35:SER:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASP:H	1:C:236:GLN:CD	2.13	0.52
1:C:406:CSD:C	1:C:408:GLY:H	2.23	0.52
1:C:425:PRO:HB2	1:C:428:PHE:CG	2.45	0.52
1:F:357:LEU:N	1:F:357:LEU:HD12	2.25	0.51
1:F:391:VAL:CG1	1:F:421:LEU:HD11	2.40	0.51
1:B:204:VAL:HB	1:C:429:VAL:HG21	1.93	0.51
1:B:335:ILE:HD11	1:B:371:TYR:N	2.25	0.51
1:D:21:HIS:HE1	1:D:197:GLN:HG3	1.75	0.51
1:F:46:THR:CG2	1:F:147:LEU:HB2	2.41	0.51
1:C:392:ILE:O	1:C:421:LEU:HD12	2.11	0.51
1:E:128:GLY:O	1:F:386:LEU:HG	2.09	0.51
1:E:462:ILE:HB	1:E:467:LEU:HD21	1.92	0.51
1:F:170:ASP:H	1:F:236:GLN:HE22	1.58	0.51
1:B:234:ARG:O	1:B:235:LYS:HB2	2.10	0.51
1:C:25:SER:HB3	1:C:28:GLY:O	2.11	0.51
1:A:22:ARG:CB	1:A:22:ARG:HH11	2.24	0.51
1:A:23:VAL:O	1:A:29:LEU:HD12	2.11	0.51
1:C:225:GLU:OE1	1:C:225:GLU:HA	2.11	0.51
1:C:378:GLY:O	1:C:433:GLN:HA	2.11	0.51
1:E:62:TYR:CE2	1:F:427:ASN:HB3	2.44	0.51
1:E:210:LYS:HG3	1:E:221:GLU:OE2	2.10	0.51
1:F:106:GLN:HE21	1:F:106:GLN:HA	1.76	0.51
1:A:14:LEU:HD23	1:A:423:VAL:O	2.10	0.51
1:A:18:GLU:CA	1:A:33:TRP:HE1	2.24	0.51
1:B:240:VAL:HG11	1:B:244:LEU:HD12	1.92	0.51
1:B:357:LEU:HD23	1:B:449:ASN:ND2	2.25	0.51
1:D:57:LEU:HD12	1:D:133:THR:O	2.11	0.51
1:D:126:PRO:HB2	1:D:129:VAL:CG2	2.40	0.51
1:D:469:ASN:ND2	1:F:240:VAL:HG13	2.26	0.51
1:A:69:ILE:HG22	1:A:143:ALA:HB1	1.93	0.51
1:A:462:ILE:HG22	1:A:466:VAL:HB	1.91	0.51
1:A:480:GLN:HA	1:A:480:GLN:NE2	2.24	0.51
1:E:227:LEU:HA	1:F:471:TYR:HD2	1.75	0.51
1:B:164:TYR:CD1	1:B:169:PRO:HG3	2.45	0.51
1:C:223:THR:O	1:C:227:LEU:HD22	2.11	0.51
1:A:166:ALA:HB2	1:B:471:TYR:CZ	2.45	0.51
1:A:344:TYR:CE1	1:F:233:GLU:HB2	2.46	0.51
1:C:27:GLY:HA3	1:C:237:ILE:HG22	1.92	0.51
1:F:430:VAL:HG22	1:F:431:ALA:N	2.25	0.51
1:C:72:VAL:HG23	1:C:73:GLN:N	2.26	0.51
1:A:475:GLN:CG	1:A:479:ARG:HH12	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:PRO:HG3	1:C:350:ARG:NH1	2.21	0.50
1:D:475:GLN:O	1:D:479:ARG:HG2	2.11	0.50
1:F:403:VAL:HG22	1:F:430:VAL:HG23	1.92	0.50
1:A:76:GLY:HA2	1:A:136:THR:H	1.76	0.50
1:B:200:GLU:N	1:B:200:GLU:OE1	2.44	0.50
1:B:408:GLY:C	1:B:409:ASN:HD22	2.14	0.50
1:F:40:LEU:N	1:F:40:LEU:HD12	2.26	0.50
1:F:144:ILE:HD12	1:F:144:ILE:N	2.26	0.50
1:A:134:TYR:OH	1:A:243:GLY:HA2	2.12	0.50
1:A:460:ARG:O	1:C:87:GLU:HG2	2.11	0.50
1:B:136:THR:CG2	1:B:247:ILE:HG21	2.41	0.50
1:C:143:ALA:C	1:C:144:ILE:HD12	2.32	0.50
1:C:221:GLU:O	1:C:224:ALA:HB3	2.12	0.50
1:D:115:ARG:H	1:D:115:ARG:CD	2.17	0.50
1:F:114:ILE:HD12	1:F:132:TRP:HZ2	1.74	0.50
1:F:220:ASN:OD1	1:F:222:ASP:HB2	2.11	0.50
1:D:8:GLU:O	1:D:42:CYS:HB2	2.11	0.50
1:D:14:LEU:C	1:D:15:ASN:HD22	2.15	0.50
1:D:427:ASN:HB2	1:F:163:PHE:CZ	2.47	0.50
1:E:369:ALA:HA	1:E:443:VAL:O	2.12	0.50
1:B:134:TYR:CZ	1:B:244:LEU:HD13	2.46	0.50
1:B:404:VAL:HA	1:B:409:ASN:O	2.12	0.50
1:C:79:GLY:HA3	1:C:132:TRP:CE2	2.47	0.50
1:C:213:LEU:HD12	1:C:217:PHE:CE1	2.46	0.50
1:C:418:ARG:HH21	1:C:418:ARG:HG3	1.76	0.50
1:D:219:THR:OG1	1:D:220:ASN:N	2.44	0.50
1:D:473:LEU:HD21	1:F:226:LYS:HB2	1.94	0.50
1:E:157:ASP:OD2	1:E:159:ASN:HB2	2.11	0.50
1:A:23:VAL:HG11	1:A:236:GLN:NE2	2.27	0.50
1:B:326:ILE:O	1:B:329:MET:HG2	2.11	0.50
1:B:345:ASN:CG	1:B:348:ALA:HB3	2.31	0.50
1:F:236:GLN:OE1	1:F:236:GLN:N	2.39	0.50
1:F:474:GLY:O	1:F:478:VAL:HG23	2.11	0.50
1:B:34:ASN:HD21	1:B:175:GLU:HB3	1.76	0.50
1:C:36:GLN:HE21	1:C:175:GLU:HB2	1.76	0.50
1:C:57:LEU:HD22	1:C:240:VAL:HG22	1.94	0.50
1:C:114:ILE:HD12	1:C:132:TRP:CZ2	2.47	0.50
1:C:479:ARG:HH11	1:C:479:ARG:HG2	1.77	0.50
1:E:326:ILE:O	1:E:329:MET:HG2	2.12	0.50
1:F:385:ASN:HD21	1:F:445:LYS:CE	2.25	0.50
1:A:379:ILE:HB	1:A:491:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:GLN:HE21	1:E:461:ALA:HB1	1.76	0.50
1:D:389:ASN:ND2	1:F:155:GLN:HB3	2.27	0.50
1:E:476:SER:O	1:E:479:ARG:HB2	2.11	0.50
1:F:65:TYR:CE1	1:F:149:THR:HG22	2.47	0.50
1:A:226:LYS:HE3	1:A:231:ASP:OD1	2.11	0.50
1:B:61:SER:HB3	1:B:164:TYR:CD2	2.47	0.50
1:B:244:LEU:HD12	1:B:244:LEU:N	2.27	0.50
1:C:9:CYS:C	1:C:11:LEU:H	2.16	0.50
1:D:66:PRO:HG3	1:D:151:ASN:ND2	2.26	0.50
1:E:372:VAL:HB	1:E:441:TYR:CE1	2.47	0.50
1:B:67:GLN:O	1:B:124:VAL:HA	2.12	0.49
1:B:396:ARG:HA	1:B:418:ARG:CG	2.42	0.49
1:C:228:ARG:HB3	1:C:230:PRO:HG3	1.94	0.49
1:D:402:ARG:HG3	1:D:402:ARG:HH11	1.76	0.49
1:A:331:LEU:O	1:A:359:LEU:HD21	2.12	0.49
1:F:50:ARG:NH2	1:F:67:GLN:NE2	2.57	0.49
1:B:17:LEU:HB2	1:B:421:LEU:HB3	1.94	0.49
1:B:70:ILE:CG2	1:B:144:ILE:HB	2.42	0.49
1:B:392:ILE:HG23	1:B:441:TYR:HD2	1.78	0.49
1:D:204:VAL:HB	1:E:429:VAL:HG21	1.94	0.49
1:D:404:VAL:HG13	1:D:409:ASN:O	2.13	0.49
1:E:205:LEU:HD21	1:F:455:ILE:HD13	1.93	0.49
1:A:124:VAL:HG11	1:A:365:PHE:CD2	2.47	0.49
1:B:374:LEU:HD11	1:B:378:GLY:O	2.12	0.49
1:F:59:LEU:HD13	1:F:167:GLY:HA3	1.94	0.49
1:F:386:LEU:N	1:F:386:LEU:HD12	2.27	0.49
1:B:25:SER:OG	1:B:237:ILE:HB	2.13	0.49
1:C:377:ASN:O	1:C:433:GLN:HG3	2.13	0.49
1:C:386:LEU:HD13	1:C:451:VAL:HG23	1.93	0.49
1:C:396:ARG:HD2	1:C:396:ARG:C	2.33	0.49
1:E:247:ILE:HD13	1:E:247:ILE:N	2.17	0.49
1:A:247:ILE:HD12	1:A:247:ILE:N	2.27	0.49
1:A:480:GLN:CD	1:A:484:GLN:HG3	2.32	0.49
1:B:33:TRP:CE3	1:B:47:VAL:HB	2.46	0.49
1:B:34:ASN:HA	1:B:175:GLU:OE2	2.13	0.49
1:B:109:ASP:HA	1:C:483:TYR:OH	2.12	0.49
1:D:146:LEU:HB2	1:D:444:PHE:CD2	2.48	0.49
1:E:349:GLY:O	1:E:490:LEU:HD13	2.11	0.49
1:A:462:ILE:HB	1:A:467:LEU:HD21	1.95	0.49
1:B:144:ILE:HG12	1:B:393:TYR:CD2	2.48	0.49
1:B:363:ARG:HA	1:B:448:HIS:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ALA:HB2	1:C:116:HIS:ND1	2.28	0.49
1:D:68:MET:HB2	1:D:367:LEU:HD13	1.94	0.49
1:E:88:THR:O	1:E:110:SER:HA	2.13	0.49
1:A:155:GLN:HB3	1:B:389:ASN:ND2	2.28	0.49
1:A:329:MET:O	1:A:329:MET:HG3	2.11	0.49
1:B:396:ARG:HA	1:B:418:ARG:CD	2.43	0.49
1:B:402:ARG:HG3	1:B:402:ARG:HH11	1.78	0.49
1:C:34:ASN:HD22	1:C:35:SER:H	1.59	0.49
1:C:376:ARG:NH1	1:C:376:ARG:HB2	2.28	0.49
1:F:46:THR:CG2	1:F:147:LEU:HD12	2.42	0.49
1:A:72:VAL:HG22	1:A:142:VAL:O	2.13	0.49
1:C:236:GLN:OE1	1:C:236:GLN:N	2.46	0.49
1:C:385:ASN:HD21	1:C:445:LYS:CE	2.26	0.49
1:C:404:VAL:HA	1:C:409:ASN:O	2.13	0.49
1:E:46:THR:HG23	1:E:147:LEU:HD12	1.94	0.49
1:E:57:LEU:HD13	1:E:57:LEU:C	2.33	0.49
1:A:59:LEU:HG	1:A:236:GLN:O	2.13	0.49
1:A:71:VAL:HG21	1:A:117:PHE:HD2	1.78	0.49
1:A:166:ALA:HB2	1:B:471:TYR:CE2	2.48	0.49
1:D:357:LEU:HD12	1:D:357:LEU:N	2.27	0.49
1:F:45:VAL:HG21	1:F:146:LEU:HD21	1.94	0.49
1:F:401:VAL:HG21	1:F:416:LEU:HD23	1.95	0.49
1:A:471:TYR:HE2	1:C:205:LEU:HD12	1.79	0.48
1:F:394:VAL:HG21	1:F:416:LEU:HG	1.94	0.48
1:F:409:ASN:N	1:F:409:ASN:HD22	2.11	0.48
1:A:46:THR:CG2	1:A:147:LEU:HB2	2.43	0.48
1:A:159:ASN:HB3	1:A:176:THR:CG2	2.41	0.48
1:B:227:LEU:HD21	1:C:481:LEU:HD11	1.96	0.48
1:C:376:ARG:HB2	1:C:376:ARG:HH11	1.77	0.48
1:F:31:GLU:OE1	1:F:49:LYS:HD2	2.12	0.48
1:F:400:ARG:O	1:F:432:GLU:HA	2.13	0.48
1:A:234:ARG:HB3	1:A:238:VAL:HG12	1.95	0.48
1:A:240:VAL:HG13	1:B:469:ASN:ND2	2.29	0.48
1:A:475:GLN:HG2	1:A:479:ARG:HH22	1.78	0.48
1:A:481:LEU:CD2	1:C:217:PHE:HB3	2.42	0.48
1:B:67:GLN:HB2	1:B:125:ILE:HB	1.95	0.48
1:B:383:HIS:HB3	1:B:454:TYR:HB3	1.96	0.48
1:E:22:ARG:HH11	1:E:22:ARG:HB3	1.77	0.48
1:E:398:LYS:HE2	1:E:415:GLU:OE1	2.12	0.48
1:F:218:ASN:N	1:F:218:ASN:ND2	2.61	0.48
1:F:328:THR:HG23	1:F:329:MET:N	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:PHE:O	1:A:482:LYS:HE2	2.13	0.48
1:D:82:PHE:HZ	1:D:331:LEU:HD11	1.78	0.48
1:D:469:ASN:HD21	1:F:240:VAL:HG13	1.78	0.48
1:E:244:LEU:CD1	1:F:465:GLU:HB3	2.42	0.48
1:F:134:TYR:CE1	1:F:244:LEU:HD13	2.49	0.48
1:A:337:ARG:HG3	1:A:337:ARG:HH11	1.78	0.48
1:A:475:GLN:HG2	1:A:479:ARG:HH12	1.78	0.48
1:D:9:CYS:C	1:D:11:LEU:H	2.16	0.48
1:D:47:VAL:HG12	1:D:48:SER:N	2.28	0.48
1:E:1:ILE:HD11	1:F:155:GLN:HA	1.95	0.48
1:F:65:TYR:HE1	1:F:160:PRO:HA	1.79	0.48
1:F:123:LEU:HD23	1:F:332:HIS:CB	2.40	0.48
1:C:350:ARG:HG3	1:C:350:ARG:NH2	2.27	0.48
1:E:486:ASN:HD21	1:E:491:VAL:CG2	2.20	0.48
1:A:12:ASN:O	1:A:411:VAL:HG12	2.14	0.48
1:A:454:TYR:HD1	1:A:456:LYS:HB2	1.77	0.48
1:B:65:TYR:OH	1:B:147:LEU:HD13	2.13	0.48
1:B:70:ILE:HG22	1:B:144:ILE:HB	1.96	0.48
1:A:469:ASN:ND2	1:C:240:VAL:HG13	2.29	0.48
1:C:40:LEU:HD12	1:C:45:VAL:HG23	1.94	0.48
1:C:57:LEU:HD22	1:C:240:VAL:CG2	2.43	0.48
1:D:7:ASN:ND2	1:D:10:GLN:HB2	2.29	0.48
1:E:480:GLN:HG3	1:E:481:LEU:N	2.29	0.48
1:B:374:LEU:HD12	1:B:434:GLY:HA3	1.95	0.48
1:B:387:ASN:CA	1:B:426:GLN:HE21	2.27	0.48
1:D:205:LEU:HD21	1:E:455:ILE:HD13	1.96	0.48
1:D:325:ASN:N	1:D:325:ASN:ND2	2.62	0.48
1:F:337:ARG:HH21	1:F:337:ARG:HG3	1.78	0.48
1:A:87:GLU:O	1:A:88:THR:C	2.53	0.48
1:A:348:ALA:O	1:A:374:LEU:HA	2.14	0.48
1:D:21:HIS:CE1	1:D:197:GLN:HG3	2.49	0.48
1:D:51:THR:HA	1:D:141:VAL:O	2.14	0.48
1:A:326:ILE:HA	1:A:329:MET:HE3	1.96	0.47
1:B:335:ILE:CD1	1:B:371:TYR:HB2	2.44	0.47
1:A:175:GLU:HG2	1:A:176:THR:N	2.29	0.47
1:B:460:ARG:NH1	1:B:487:SER:HA	2.29	0.47
1:C:62:TYR:HD1	1:C:130:PRO:HB3	1.78	0.47
1:C:425:PRO:HB2	1:C:428:PHE:CD2	2.48	0.47
1:C:464:SER:HB3	1:C:475:GLN:HE22	1.79	0.47
1:E:23:VAL:O	1:E:29:LEU:HD12	2.14	0.47
1:A:392:ILE:O	1:A:421:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ARG:NH1	1:C:212:PHE:HE2	2.12	0.47
1:B:396:ARG:HD3	1:B:396:ARG:C	2.34	0.47
1:C:111:HIS:CD2	1:C:111:HIS:H	2.32	0.47
1:C:392:ILE:HG23	1:C:441:TYR:CD2	2.50	0.47
1:C:396:ARG:HG3	1:C:396:ARG:HH11	1.79	0.47
1:E:5:LYS:HB3	1:E:6:PHE:H	1.51	0.47
1:E:75:LYS:CB	1:E:118:ASN:HA	2.42	0.47
1:F:170:ASP:H	1:F:236:GLN:NE2	2.12	0.47
1:A:467:LEU:HD12	1:A:471:TYR:HE1	1.79	0.47
1:C:170:ASP:HB2	1:C:235:LYS:HD2	1.95	0.47
1:C:362:LEU:HD22	1:C:367:LEU:O	2.14	0.47
1:E:61:SER:HB3	1:E:164:TYR:CD2	2.49	0.47
1:E:392:ILE:HG23	1:E:441:TYR:CD2	2.49	0.47
1:E:405:ASN:OD1	1:E:407:GLN:HB2	2.14	0.47
1:E:421:LEU:C	1:E:421:LEU:HD23	2.35	0.47
1:B:385:ASN:HD21	1:B:445:LYS:HZ3	1.62	0.47
1:D:476:SER:O	1:D:479:ARG:HB2	2.15	0.47
1:F:480:GLN:HA	1:F:480:GLN:HE21	1.78	0.47
1:A:351:ILE:HG23	1:A:372:VAL:HG22	1.96	0.47
1:B:425:PRO:O	1:B:428:PHE:HB2	2.15	0.47
1:C:385:ASN:HD21	1:C:445:LYS:HE2	1.79	0.47
1:E:394:VAL:HA	1:E:441:TYR:HB3	1.97	0.47
1:A:394:VAL:HB	1:A:418:ARG:HA	1.96	0.47
1:B:387:ASN:H	1:B:387:ASN:ND2	2.07	0.47
1:C:112:GLN:O	1:C:114:ILE:N	2.47	0.47
1:D:78:ILE:O	1:D:78:ILE:HG23	2.14	0.47
1:D:110:SER:O	1:D:111:HIS:HB3	2.15	0.47
1:D:128:GLY:O	1:E:386:LEU:HG	2.15	0.47
1:E:123:LEU:HD23	1:E:332:HIS:HB3	1.97	0.47
1:E:340:ARG:NH2	1:E:354:LEU:HD13	2.29	0.47
1:A:47:VAL:HG12	1:A:48:SER:N	2.30	0.47
1:A:83:PRO:HB3	1:B:453:SER:OG	2.13	0.47
1:A:380:TYR:HB3	1:A:432:GLU:H	1.80	0.47
1:B:426:GLN:HG2	1:B:427:ASN:N	2.29	0.47
1:D:56:GLY:O	1:D:134:TYR:HA	2.15	0.47
1:E:394:VAL:HG21	1:E:416:LEU:HG	1.96	0.47
1:F:148:ASP:OD2	1:F:151:ASN:HB2	2.14	0.47
1:F:170:ASP:O	1:F:171:ILE:C	2.52	0.47
1:F:334:ASN:HD22	1:F:337:ARG:H	1.59	0.47
1:A:144:ILE:HG12	1:A:393:TYR:CE2	2.50	0.47
1:A:210:LYS:HD3	1:A:225:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASN:HD22	1:B:176:THR:CG2	2.12	0.47
1:B:387:ASN:N	1:B:387:ASN:ND2	2.63	0.47
1:B:388:ALA:H	1:B:426:GLN:HG3	1.80	0.47
1:B:473:LEU:HB3	1:B:477:GLN:HB2	1.96	0.47
1:C:6:PHE:CD2	1:C:6:PHE:N	2.81	0.47
1:C:401:VAL:HG13	1:C:432:GLU:HG3	1.97	0.47
1:F:40:LEU:HD12	1:F:40:LEU:H	1.80	0.47
1:F:454:TYR:HD1	1:F:456:LYS:HB3	1.80	0.47
1:B:60:PRO:HG3	1:B:132:TRP:HB3	1.97	0.47
1:B:437:GLN:HA	1:B:437:GLN:NE2	2.30	0.47
1:C:22:ARG:NH1	1:C:31:GLU:HG2	2.29	0.47
1:C:340:ARG:H	1:C:340:ARG:HD2	1.80	0.47
1:E:107:LEU:HA	1:F:479:ARG:HH21	1.79	0.47
1:E:228:ARG:HB3	1:E:228:ARG:NH1	2.30	0.47
1:E:489:PRO:O	1:E:491:VAL:HG23	2.15	0.47
1:A:22:ARG:NH2	1:A:29:LEU:HD11	2.31	0.46
1:A:363:ARG:O	1:A:363:ARG:CZ	2.64	0.46
1:B:134:TYR:CE2	1:B:244:LEU:HD13	2.51	0.46
1:F:392:ILE:HG23	1:F:441:TYR:CD2	2.51	0.46
1:A:396:ARG:HG2	1:A:396:ARG:NH1	2.29	0.46
1:B:398:LYS:N	1:B:439:LEU:HD13	2.30	0.46
1:D:223:THR:OG1	1:E:477:GLN:NE2	2.48	0.46
1:E:223:THR:O	1:E:227:LEU:HG	2.15	0.46
1:B:33:TRP:CD2	1:B:421:LEU:HD22	2.51	0.46
1:B:371:TYR:OH	1:B:440:GLU:HB3	2.15	0.46
1:B:382:PRO:HB2	1:B:455:ILE:HD12	1.98	0.46
1:D:336:ALA:HA	1:D:371:TYR:HD1	1.80	0.46
1:D:392:ILE:N	1:D:422:LEU:O	2.42	0.46
1:E:19:PRO:HG3	1:E:33:TRP:CZ2	2.50	0.46
1:E:211:HIS:O	1:E:214:ALA:HB3	2.15	0.46
1:C:114:ILE:HG22	1:C:115:ARG:N	2.29	0.46
1:C:394:VAL:HG22	1:C:420:GLN:O	2.16	0.46
1:D:336:ALA:HA	1:D:371:TYR:CD1	2.50	0.46
1:E:244:LEU:HD21	1:F:466:VAL:HG22	1.98	0.46
1:D:206:SER:C	1:D:208:PHE:H	2.19	0.46
1:D:388:ALA:HA	1:F:155:GLN:OE1	2.16	0.46
1:E:418:ARG:HG2	1:E:418:ARG:HH21	1.81	0.46
1:A:50:ARG:HH22	1:A:67:GLN:HE22	1.64	0.46
1:B:15:ASN:N	1:B:15:ASN:ND2	2.63	0.46
1:B:57:LEU:C	1:B:57:LEU:HD23	2.36	0.46
1:B:338:PRO:HG3	1:B:350:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:GLU:OE1	1:C:228:ARG:HD3	2.15	0.46
1:B:20:ASP:O	1:B:21:HIS:HB2	2.16	0.46
1:B:46:THR:HG23	1:B:147:LEU:HD12	1.96	0.46
1:B:174:PRO:C	1:B:176:THR:H	2.18	0.46
1:D:8:GLU:OE2	1:D:8:GLU:N	2.48	0.46
1:D:171:ILE:HG21	1:D:174:PRO:HA	1.97	0.46
1:D:235:LYS:HD2	1:D:235:LYS:N	2.31	0.46
1:F:171:ILE:HD12	1:F:171:ILE:N	2.23	0.46
1:A:463:PRO:HA	1:C:111:HIS:HB3	1.98	0.46
1:D:336:ALA:O	1:D:338:PRO:HD3	2.16	0.46
1:C:376:ARG:HG3	1:C:376:ARG:O	2.15	0.46
1:D:36:GLN:NE2	1:D:178:GLN:NE2	2.64	0.46
1:D:70:ILE:HG22	1:D:144:ILE:O	2.16	0.46
1:D:391:VAL:CG2	1:D:421:LEU:HD11	2.43	0.46
1:D:398:LYS:HE3	1:D:415:GLU:CB	2.46	0.46
1:F:108:GLN:N	1:F:108:GLN:OE1	2.49	0.46
1:F:108:GLN:O	1:F:108:GLN:HG2	2.16	0.46
1:A:71:VAL:O	1:A:119:GLU:HA	2.15	0.45
1:B:376:ARG:C	1:B:378:GLY:H	2.18	0.45
1:B:387:ASN:O	1:B:388:ALA:HB2	2.16	0.45
1:B:425:PRO:HB2	1:B:428:PHE:CG	2.51	0.45
1:B:460:ARG:CZ	1:B:487:SER:HA	2.46	0.45
1:C:57:LEU:HD12	1:C:133:THR:O	2.16	0.45
1:C:74:GLY:HA3	1:C:141:VAL:HG22	1.97	0.45
1:C:75:LYS:N	1:C:141:VAL:HG22	2.32	0.45
1:C:169:PRO:HD2	1:C:202:GLY:HA2	1.98	0.45
1:C:213:LEU:HD22	1:C:213:LEU:N	2.30	0.45
1:C:351:ILE:CG2	1:C:372:VAL:HG22	2.46	0.45
1:D:455:ILE:CD1	1:F:205:LEU:HD21	2.45	0.45
1:E:201:GLY:HA2	1:F:407:GLN:O	2.16	0.45
1:E:388:ALA:HB2	1:E:447:HIS:HB2	1.97	0.45
1:E:471:TYR:HB2	1:E:473:LEU:HG	1.97	0.45
1:F:240:VAL:HG21	1:F:244:LEU:HD11	1.98	0.45
1:A:163:PHE:CE1	1:B:406:CSD:HB2	2.52	0.45
1:A:340:ARG:NE	1:A:350:ARG:HB2	2.31	0.45
1:D:157:ASP:HB2	1:E:5:LYS:O	2.16	0.45
1:E:326:ILE:HD13	1:E:326:ILE:C	2.36	0.45
1:F:159:ASN:HB3	1:F:176:THR:CG2	2.45	0.45
1:F:479:ARG:HG2	1:F:479:ARG:HH11	1.81	0.45
1:B:228:ARG:HB3	1:B:228:ARG:NH1	2.31	0.45
1:C:417:ARG:HG2	1:C:417:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:435:GLY:O	1:F:436:GLU:C	2.54	0.45
1:A:54:ARG:HG3	1:A:54:ARG:HH11	1.82	0.45
1:A:340:ARG:HH11	1:A:340:ARG:CB	2.17	0.45
1:A:384:TRP:O	1:A:452:SER:HB2	2.17	0.45
1:C:148:ASP:OD2	1:C:367:LEU:HD21	2.17	0.45
1:C:418:ARG:HG3	1:C:418:ARG:NH2	2.32	0.45
1:F:76:GLY:HA2	1:F:136:THR:HG23	1.98	0.45
1:F:222:ASP:O	1:F:226:LYS:HG2	2.16	0.45
1:A:7:ASN:N	1:A:7:ASN:HD22	2.14	0.45
1:A:155:GLN:HB3	1:B:389:ASN:HD21	1.81	0.45
1:A:402:ARG:O	1:A:430:VAL:HG23	2.15	0.45
1:C:146:LEU:HD13	1:C:146:LEU:C	2.37	0.45
1:C:471:TYR:CB	1:C:473:LEU:HD13	2.47	0.45
1:E:246:VAL:HG11	1:F:463:PRO:HB3	1.98	0.45
1:F:343:PHE:O	1:F:350:ARG:HA	2.17	0.45
1:A:446:THR:O	1:A:447:HIS:HB2	2.17	0.45
1:B:454:TYR:CE1	1:B:457:ASP:HB2	2.52	0.45
1:B:480:GLN:O	1:B:484:GLN:N	2.49	0.45
1:C:67:GLN:HE21	1:C:147:LEU:HD22	1.80	0.45
1:C:391:VAL:HG23	1:C:391:VAL:O	2.17	0.45
1:D:34:ASN:C	1:D:36:GLN:H	2.20	0.45
1:D:81:ALA:HB3	1:D:130:PRO:HB2	1.98	0.45
1:E:471:TYR:O	1:E:472:ASN:C	2.55	0.45
1:E:480:GLN:O	1:E:484:GLN:HB2	2.17	0.45
1:C:22:ARG:NH1	1:C:22:ARG:HB3	2.32	0.45
1:C:336:ALA:O	1:C:337:ARG:C	2.55	0.45
1:C:338:PRO:HB3	1:C:350:ARG:HE	1.81	0.45
1:D:363:ARG:HD2	1:D:448:HIS:CD2	2.52	0.45
1:E:146:LEU:HD13	1:E:146:LEU:C	2.37	0.45
1:E:355:ASN:OD1	1:E:357:LEU:HB2	2.16	0.45
1:B:8:GLU:O	1:B:42:CYS:HB2	2.16	0.45
1:B:70:ILE:HG23	1:B:70:ILE:O	2.17	0.45
1:B:247:ILE:N	1:B:247:ILE:HD12	2.32	0.45
1:F:34:ASN:HB3	1:F:37:HIS:CD2	2.52	0.45
1:F:72:VAL:HG11	1:F:144:ILE:HD13	1.99	0.45
1:F:349:GLY:HA3	1:F:373:VAL:O	2.17	0.45
1:F:424:VAL:O	1:F:425:PRO:O	2.35	0.45
1:A:229:SER:C	1:A:231:ASP:H	2.20	0.45
1:B:401:VAL:HB	1:B:412:PHE:HE1	1.81	0.45
1:C:387:ASN:O	1:C:388:ALA:HB2	2.17	0.45
1:D:46:THR:HG23	1:D:147:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:TYR:HB2	1:D:473:LEU:HG	1.99	0.45
1:F:144:ILE:HG12	1:F:393:TYR:CE2	2.52	0.45
1:A:246:VAL:HG23	1:B:465:GLU:OE2	2.17	0.45
1:B:71:VAL:HG21	1:B:117:PHE:HD2	1.81	0.45
1:D:30:ILE:HD12	1:D:236:GLN:HG3	1.97	0.45
1:E:114:ILE:HD12	1:E:132:TRP:CZ2	2.52	0.45
1:A:325:ASN:HA	1:A:328:THR:CG2	2.47	0.44
1:B:126:PRO:HB2	1:B:129:VAL:CG2	2.44	0.44
1:D:373:VAL:HG13	1:D:440:GLU:HG2	1.99	0.44
1:D:461:ALA:O	1:F:111:HIS:HB2	2.17	0.44
1:E:165:LEU:HD13	1:F:458:VAL:HG11	1.99	0.44
1:F:77:ALA:HB2	1:F:116:HIS:CE1	2.52	0.44
1:B:6:PHE:CD1	1:B:6:PHE:N	2.84	0.44
1:B:46:THR:HG22	1:B:147:LEU:HB2	1.98	0.44
1:B:124:VAL:HG13	1:B:331:LEU:HD22	1.99	0.44
1:B:379:ILE:HD11	1:B:433:GLN:NE2	2.32	0.44
1:C:39:GLU:HB3	1:C:423:VAL:HG21	2.00	0.44
1:C:337:ARG:HH21	1:C:337:ARG:CA	2.29	0.44
1:C:404:VAL:CG1	1:C:408:GLY:HA2	2.46	0.44
1:F:334:ASN:ND2	1:F:337:ARG:N	2.61	0.44
1:A:240:VAL:HG11	1:A:244:LEU:HD12	1.99	0.44
1:A:385:ASN:HD21	1:A:445:LYS:HE2	1.82	0.44
1:D:171:ILE:HG21	1:D:177:MET:HG3	1.99	0.44
1:D:402:ARG:HG2	1:D:413:ASP:OD1	2.17	0.44
1:B:401:VAL:HG11	1:B:422:LEU:CD2	2.48	0.44
1:C:67:GLN:O	1:C:124:VAL:HA	2.16	0.44
1:C:120:GLY:O	1:C:335:ILE:HG22	2.18	0.44
1:C:147:LEU:O	1:C:149:THR:N	2.49	0.44
1:D:240:VAL:HG22	1:E:469:ASN:ND2	2.33	0.44
1:D:403:VAL:O	1:D:411:VAL:HG22	2.18	0.44
1:E:47:VAL:HG12	1:E:48:SER:N	2.33	0.44
1:A:65:TYR:HD1	1:A:154:ASN:HD22	1.66	0.44
1:A:363:ARG:NE	1:A:448:HIS:CD2	2.86	0.44
1:D:354:LEU:HD12	1:D:358:THR:OG1	2.18	0.44
1:E:235:LYS:HB3	1:E:236:GLN:OE1	2.18	0.44
1:A:224:ALA:HA	1:A:227:LEU:CD1	2.43	0.44
1:A:491:VAL:HG12	1:A:492:ASN:H	1.82	0.44
1:B:158:GLN:OE1	1:B:158:GLN:N	2.50	0.44
1:C:23:VAL:O	1:C:29:LEU:HD12	2.16	0.44
1:C:356:SER:HA	1:C:359:LEU:O	2.18	0.44
1:D:15:ASN:HD22	1:D:15:ASN:N	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ARG:O	1:D:340:ARG:HG2	2.18	0.44
1:D:474:GLY:O	1:D:478:VAL:HG22	2.17	0.44
1:F:89:PHE:CE1	1:F:110:SER:HB3	2.52	0.44
1:D:200:GLU:O	1:D:200:GLU:HG3	2.18	0.44
1:D:218:ASN:N	1:D:218:ASN:HD22	2.15	0.44
1:D:436:GLU:OE1	1:D:436:GLU:HA	2.18	0.44
1:F:247:ILE:HG22	1:F:248:SER:N	2.32	0.44
1:F:425:PRO:HG2	1:F:428:PHE:CE1	2.52	0.44
1:A:28:GLY:HA3	1:A:237:ILE:HG21	2.00	0.44
1:B:65:TYR:CE1	1:B:149:THR:HG22	2.53	0.44
1:C:82:PHE:CE1	1:C:129:VAL:HG11	2.52	0.44
1:C:200:GLU:N	1:C:200:GLU:OE1	2.50	0.44
1:D:11:LEU:HD22	1:D:38:PRO:HB3	1.99	0.44
1:D:228:ARG:HB3	1:D:228:ARG:CZ	2.48	0.44
1:D:461:ALA:HA	1:F:87:GLU:OE1	2.17	0.44
1:F:113:LYS:HD3	1:F:115:ARG:HE	1.82	0.44
1:A:13:ASN:C	1:A:14:LEU:HD12	2.38	0.44
1:A:69:ILE:CG2	1:A:143:ALA:HB1	2.47	0.44
1:B:22:ARG:HH22	1:B:29:LEU:HD21	1.83	0.44
1:B:436:GLU:OE1	1:B:436:GLU:HA	2.18	0.44
1:C:405:ASN:HD22	1:C:411:VAL:CG1	2.31	0.44
1:D:148:ASP:OD2	1:D:151:ASN:HB2	2.18	0.44
1:D:163:PHE:CD2	1:E:406:CSD:HB2	2.52	0.44
1:F:456:LYS:NZ	1:F:486:ASN:ND2	2.65	0.44
1:A:22:ARG:CZ	1:A:29:LEU:HD11	2.48	0.43
1:B:7:ASN:ND2	1:B:10:GLN:NE2	2.66	0.43
1:B:234:ARG:HB3	1:B:238:VAL:HG12	1.99	0.43
1:B:326:ILE:C	1:B:328:THR:H	2.21	0.43
1:C:160:PRO:O	1:C:176:THR:HG21	2.18	0.43
1:C:384:TRP:HH2	1:C:458:VAL:HG21	1.83	0.43
1:D:146:LEU:HD21	1:D:391:VAL:HG11	2.00	0.43
1:F:398:LYS:CB	1:F:398:LYS:NZ	2.82	0.43
1:D:456:LYS:HE2	1:F:217:PHE:CA	2.42	0.43
1:E:210:LYS:CB	1:E:225:GLU:HG2	2.47	0.43
1:F:78:ILE:HG13	1:F:133:THR:HG22	2.00	0.43
1:A:18:GLU:HA	1:A:33:TRP:HE1	1.83	0.43
1:A:22:ARG:NH1	1:A:22:ARG:CB	2.81	0.43
1:A:65:TYR:CE1	1:A:149:THR:HG22	2.53	0.43
1:B:124:VAL:HG13	1:B:124:VAL:O	2.18	0.43
1:B:357:LEU:N	1:B:357:LEU:HD22	2.33	0.43
1:B:379:ILE:HG22	1:B:380:TYR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ALA:HA	1:C:421:LEU:O	2.18	0.43
1:C:38:PRO:HA	1:C:41:GLN:HB2	2.00	0.43
1:C:340:ARG:HH11	1:C:340:ARG:HG2	1.83	0.43
1:D:399:GLY:HA3	1:D:439:LEU:HD22	1.99	0.43
1:E:114:ILE:HD12	1:E:132:TRP:HZ2	1.82	0.43
1:E:478:VAL:O	1:E:478:VAL:HG12	2.18	0.43
1:F:334:ASN:HB3	1:F:340:ARG:HH11	1.84	0.43
1:B:228:ARG:HB3	1:B:228:ARG:CZ	2.49	0.43
1:B:401:VAL:HA	1:B:432:GLU:HB3	2.01	0.43
1:F:244:LEU:HD12	1:F:244:LEU:N	2.34	0.43
1:F:348:ALA:CB	1:F:490:LEU:HB3	2.49	0.43
1:F:373:VAL:HG13	1:F:440:GLU:HG2	1.98	0.43
1:A:240:VAL:HG11	1:A:244:LEU:CD1	2.48	0.43
1:A:326:ILE:HA	1:A:329:MET:HE2	2.00	0.43
1:B:47:VAL:HG12	1:B:48:SER:N	2.34	0.43
1:B:335:ILE:HD11	1:B:371:TYR:H	1.84	0.43
1:C:121:ASP:OD2	1:C:332:HIS:HE1	2.01	0.43
1:C:471:TYR:HB2	1:C:473:LEU:HD13	1.99	0.43
1:E:227:LEU:HA	1:F:471:TYR:CD2	2.53	0.43
1:E:340:ARG:HH22	1:E:354:LEU:HD13	1.84	0.43
1:F:53:ASN:N	1:F:53:ASN:HD22	2.16	0.43
1:F:230:PRO:HG2	1:F:231:ASP:H	1.82	0.43
1:A:345:ASN:HD22	1:A:486:ASN:ND2	2.16	0.43
1:B:156:LEU:CD1	1:B:161:ARG:HE	2.29	0.43
1:C:210:LYS:CD	1:C:225:GLU:HG2	2.42	0.43
1:C:387:ASN:ND2	1:C:387:ASN:H	2.17	0.43
1:D:385:ASN:ND2	1:D:452:SER:HB3	2.33	0.43
1:F:39:GLU:CD	1:F:39:GLU:H	2.22	0.43
1:F:46:THR:HG23	1:F:147:LEU:HB2	2.00	0.43
1:A:64:PRO:O	1:A:154:ASN:HA	2.18	0.43
1:A:386:LEU:HD13	1:A:452:SER:CA	2.48	0.43
1:B:71:VAL:HG21	1:B:117:PHE:CD2	2.52	0.43
1:C:70:ILE:HG23	1:C:70:ILE:O	2.19	0.43
1:C:79:GLY:HA3	1:C:132:TRP:NE1	2.34	0.43
1:C:210:LYS:HE2	1:C:221:GLU:OE2	2.18	0.43
1:C:219:THR:OG1	1:C:220:ASN:N	2.51	0.43
1:D:340:ARG:HG3	1:D:340:ARG:HH11	1.83	0.43
1:D:391:VAL:HG12	1:D:444:PHE:HB2	1.98	0.43
1:C:373:VAL:HG22	1:C:440:GLU:CG	2.41	0.43
1:C:386:LEU:H	1:C:386:LEU:CD1	2.31	0.43
1:D:489:PRO:HG2	1:D:490:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:LEU:HB3	1:F:367:LEU:O	2.19	0.43
1:F:395:THR:C	1:F:418:ARG:HG3	2.39	0.43
1:A:64:PRO:HG2	1:A:65:TYR:CD1	2.54	0.43
1:B:437:GLN:HA	1:B:437:GLN:HE21	1.83	0.43
1:B:472:ASN:N	1:B:472:ASN:HD22	2.15	0.43
1:C:78:ILE:HG12	1:C:79:GLY:N	2.34	0.43
1:C:367:LEU:CD2	1:C:446:THR:HA	2.44	0.43
1:F:122:VAL:O	1:F:332:HIS:HA	2.19	0.43
1:A:78:ILE:HG13	1:A:133:THR:HG22	2.00	0.43
1:A:340:ARG:CD	1:A:350:ARG:HB2	2.49	0.43
1:B:61:SER:HA	1:B:163:PHE:O	2.18	0.43
1:C:34:ASN:HB3	1:C:37:HIS:CD2	2.53	0.43
1:D:113:LYS:O	1:D:115:ARG:HD2	2.18	0.43
1:D:454:TYR:HD1	1:D:456:LYS:HB2	1.83	0.43
1:E:22:ARG:HH11	1:E:22:ARG:CB	2.32	0.43
1:F:213:LEU:H	1:F:213:LEU:HD22	1.83	0.43
1:A:337:ARG:C	1:A:339:SER:H	2.23	0.42
1:B:47:VAL:HA	1:B:145:SER:O	2.19	0.42
1:B:207:GLY:HA2	1:C:408:GLY:O	2.18	0.42
1:C:404:VAL:HG13	1:C:409:ASN:O	2.19	0.42
1:D:228:ARG:HB3	1:D:228:ARG:NH1	2.34	0.42
1:E:82:PHE:HB2	1:E:85:CYS:SG	2.59	0.42
1:E:175:GLU:OE1	1:E:175:GLU:N	2.50	0.42
1:E:236:GLN:H	1:E:236:GLN:CD	2.20	0.42
1:A:112:GLN:O	1:A:114:ILE:N	2.52	0.42
1:A:233:GLU:O	1:A:235:LYS:HE3	2.19	0.42
1:A:387:ASN:O	1:A:388:ALA:HB2	2.18	0.42
1:A:408:GLY:HA2	1:C:203:SER:O	2.19	0.42
1:B:79:GLY:O	1:B:131:TYR:HA	2.19	0.42
1:B:86:PRO:O	1:B:113:LYS:HE3	2.19	0.42
1:C:87:GLU:HA	1:C:112:GLN:HA	2.01	0.42
1:C:471:TYR:O	1:C:472:ASN:HB2	2.19	0.42
1:A:244:LEU:HD12	1:A:244:LEU:N	2.34	0.42
1:A:441:TYR:HD2	1:A:441:TYR:O	2.01	0.42
1:B:398:LYS:HA	1:B:416:LEU:O	2.19	0.42
1:D:70:ILE:HG23	1:D:70:ILE:O	2.18	0.42
1:E:171:ILE:HG21	1:E:174:PRO:HA	2.01	0.42
1:E:376:ARG:O	1:E:377:ASN:CB	2.67	0.42
1:B:169:PRO:HA	1:B:236:GLN:OE1	2.19	0.42
1:B:366:GLY:HA2	1:B:448:HIS:H	1.84	0.42
1:C:17:LEU:HD12	1:C:40:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ALA:O	1:C:374:LEU:HA	2.18	0.42
1:E:22:ARG:CB	1:E:22:ARG:NH1	2.83	0.42
1:E:73:GLN:HE21	1:E:142:VAL:HG11	1.84	0.42
1:F:225:GLU:O	1:F:230:PRO:HD3	2.19	0.42
1:A:7:ASN:N	1:A:7:ASN:ND2	2.66	0.42
1:A:46:THR:CG2	1:A:147:LEU:HD12	2.43	0.42
1:A:454:TYR:CD2	1:A:489:PRO:HB3	2.55	0.42
1:B:133:THR:HG21	2:B:502:CO3:O1	2.20	0.42
1:B:396:ARG:HA	1:B:418:ARG:HD2	2.02	0.42
1:C:151:ASN:OD1	1:C:152:PHE:N	2.52	0.42
1:C:245:SER:OG	1:C:246:VAL:N	2.51	0.42
1:D:155:GLN:OE1	1:E:388:ALA:HA	2.20	0.42
1:E:14:LEU:HD13	1:E:411:VAL:HB	2.01	0.42
1:E:69:ILE:HB	1:E:123:LEU:HB2	2.00	0.42
1:E:246:VAL:HG23	1:F:465:GLU:CD	2.40	0.42
1:E:417:ARG:HG2	1:E:417:ARG:HH11	1.85	0.42
1:C:70:ILE:HG22	1:C:144:ILE:O	2.19	0.42
1:C:72:VAL:HG23	1:C:73:GLN:H	1.84	0.42
1:C:148:ASP:CG	1:C:151:ASN:HB2	2.40	0.42
1:D:363:ARG:HG3	1:D:363:ARG:HH21	1.84	0.42
1:E:72:VAL:HG23	1:E:142:VAL:HG13	2.01	0.42
1:E:228:ARG:O	1:E:229:SER:C	2.57	0.42
1:F:152:PHE:CD1	1:F:152:PHE:N	2.81	0.42
1:A:146:LEU:HD13	1:A:146:LEU:C	2.40	0.42
1:C:326:ILE:CG2	1:C:327:CYS:N	2.82	0.42
1:C:405:ASN:OD1	1:C:406:CSD:N	2.53	0.42
1:E:1:ILE:HD11	1:F:154:ASN:O	2.20	0.42
1:E:160:PRO:HB2	1:E:173:HIS:ND1	2.35	0.42
1:A:148:ASP:OD1	1:A:367:LEU:HD21	2.19	0.42
1:D:350:ARG:HH21	1:D:350:ARG:HG3	1.85	0.42
1:D:387:ASN:HA	1:D:426:GLN:NE2	2.35	0.42
1:E:219:THR:OG1	1:E:220:ASN:N	2.51	0.42
1:F:26:GLU:HG2	1:F:239:THR:OG1	2.20	0.42
1:A:430:VAL:HG22	1:A:431:ALA:N	2.34	0.42
1:B:60:PRO:HA	1:B:131:TYR:O	2.20	0.42
1:B:222:ASP:O	1:B:226:LYS:HG2	2.20	0.42
1:B:392:ILE:HG23	1:B:441:TYR:CD2	2.55	0.42
1:C:7:ASN:O	1:C:9:CYS:N	2.53	0.42
1:C:363:ARG:HH21	1:C:448:HIS:CD2	2.38	0.42
1:D:7:ASN:CG	1:D:10:GLN:HB2	2.40	0.42
1:D:234:ARG:HB3	1:D:238:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:VAL:HG22	1:E:142:VAL:O	2.20	0.42
1:E:122:VAL:O	1:E:332:HIS:HA	2.20	0.42
1:E:392:ILE:O	1:E:421:LEU:HA	2.20	0.42
1:A:402:ARG:O	1:A:430:VAL:HA	2.20	0.42
1:C:148:ASP:HB2	1:C:367:LEU:HD11	2.01	0.42
1:C:345:ASN:O	1:C:347:LYS:N	2.53	0.42
1:F:134:TYR:CZ	1:F:244:LEU:HD13	2.55	0.42
1:F:355:ASN:OD1	1:F:357:LEU:HB2	2.20	0.42
1:A:80:PHE:CD1	1:A:80:PHE:N	2.87	0.41
1:A:376:ARG:HH12	1:A:436:GLU:HG2	1.85	0.41
1:C:47:VAL:HG12	1:C:48:SER:H	1.85	0.41
1:D:25:SER:OG	1:D:237:ILE:HB	2.20	0.41
1:D:402:ARG:HB2	1:F:208:PHE:HE1	1.84	0.41
1:E:31:GLU:OE1	1:E:49:LYS:HD3	2.19	0.41
1:E:111:HIS:HB2	1:F:461:ALA:O	2.19	0.41
1:E:164:TYR:CD1	1:E:169:PRO:HG3	2.54	0.41
1:F:72:VAL:CG1	1:F:144:ILE:HD13	2.50	0.41
1:A:51:THR:HA	1:A:141:VAL:O	2.20	0.41
1:A:387:ASN:C	1:A:387:ASN:HD22	2.24	0.41
1:A:426:GLN:HG2	1:A:427:ASN:N	2.36	0.41
1:B:151:ASN:OD1	1:B:153:ASN:N	2.53	0.41
1:B:397:GLY:HA3	1:B:439:LEU:HA	2.02	0.41
1:C:67:GLN:O	1:C:125:ILE:N	2.53	0.41
1:E:205:LEU:C	1:E:207:GLY:H	2.22	0.41
1:F:467:LEU:HD12	1:F:467:LEU:HA	1.89	0.41
1:A:12:ASN:O	1:A:411:VAL:HA	2.20	0.41
1:B:337:ARG:HA	1:B:338:PRO:HD3	1.90	0.41
1:B:479:ARG:NE	1:B:483:TYR:HD2	2.17	0.41
1:D:11:LEU:HD11	1:D:38:PRO:O	2.21	0.41
1:A:386:LEU:CD1	1:A:452:SER:HA	2.50	0.41
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.85	0.41
1:B:228:ARG:NH1	1:B:228:ARG:CB	2.84	0.41
1:C:337:ARG:HB2	1:C:340:ARG:HE	1.86	0.41
1:C:437:GLN:HE21	1:C:437:GLN:HA	1.85	0.41
1:D:432:GLU:N	1:D:432:GLU:OE2	2.54	0.41
1:E:46:THR:CG2	1:E:147:LEU:HD12	2.50	0.41
1:F:398:LYS:NZ	1:F:398:LYS:HB2	2.36	0.41
1:B:68:MET:HA	1:B:123:LEU:O	2.20	0.41
1:B:79:GLY:HA3	1:B:132:TRP:CE2	2.56	0.41
1:B:129:VAL:HA	1:B:130:PRO:HD3	1.91	0.41
1:B:156:LEU:CB	1:B:161:ARG:HH21	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:THR:C	1:B:177:MET:HE2	2.41	0.41
1:B:234:ARG:CB	1:B:238:VAL:HG12	2.51	0.41
1:D:175:GLU:C	1:D:177:MET:H	2.23	0.41
1:E:71:VAL:HA	1:E:143:ALA:HB2	2.03	0.41
1:F:396:ARG:HG2	1:F:397:GLY:N	2.36	0.41
1:A:397:GLY:O	1:A:398:LYS:HB2	2.19	0.41
1:A:455:ILE:CD1	1:C:205:LEU:HD21	2.48	0.41
1:B:363:ARG:HA	1:B:448:HIS:HB2	2.02	0.41
1:B:437:GLN:HE21	1:B:437:GLN:CA	2.33	0.41
1:C:17:LEU:HD13	1:C:37:HIS:CD2	2.56	0.41
1:C:56:GLY:N	1:C:135:ASN:HB3	2.32	0.41
1:C:84:GLY:O	1:C:85:CYS:C	2.58	0.41
1:D:75:LYS:HG3	1:D:136:THR:OG1	2.21	0.41
1:D:112:GLN:HE21	1:E:461:ALA:CB	2.32	0.41
1:E:2:THR:HG22	1:E:5:LYS:HZ3	1.85	0.41
1:E:70:ILE:HD13	1:E:70:ILE:C	2.41	0.41
1:E:244:LEU:HD21	1:F:466:VAL:HG23	2.02	0.41
1:F:88:THR:HG22	1:F:89:PHE:N	2.35	0.41
1:F:89:PHE:CD1	1:F:110:SER:HB3	2.55	0.41
1:F:335:ILE:O	1:F:335:ILE:HG12	2.21	0.41
1:B:379:ILE:CG2	1:B:380:TYR:N	2.84	0.41
1:C:78:ILE:HB	1:C:133:THR:HG22	2.03	0.41
1:C:89:PHE:HD1	1:C:114:ILE:H	1.67	0.41
1:E:19:PRO:HB3	1:E:31:GLU:HB3	2.03	0.41
1:E:454:TYR:CZ	1:E:457:ASP:HB2	2.55	0.41
1:F:59:LEU:HA	1:F:60:PRO:HD3	1.95	0.41
1:A:461:ALA:HA	1:C:87:GLU:CD	2.41	0.41
1:C:237:ILE:HG22	1:C:238:VAL:N	2.36	0.41
1:D:362:LEU:HD13	1:D:367:LEU:O	2.20	0.41
1:D:366:GLY:HA2	1:D:448:HIS:N	2.34	0.41
1:D:437:GLN:NE2	1:D:437:GLN:N	2.67	0.41
1:F:34:ASN:ND2	1:F:36:GLN:H	2.19	0.41
1:F:82:PHE:HB3	1:F:85:CYS:SG	2.61	0.41
1:F:390:SER:HB2	1:F:424:VAL:HB	2.02	0.41
1:A:34:ASN:ND2	1:A:36:GLN:H	2.19	0.41
1:A:80:PHE:HE2	1:A:125:ILE:HD13	1.86	0.41
1:A:326:ILE:HD13	1:A:326:ILE:C	2.41	0.41
1:B:62:TYR:HE2	1:C:427:ASN:HB3	1.86	0.41
1:B:208:PHE:CE2	1:C:382:PRO:HB3	2.56	0.41
1:C:14:LEU:N	1:C:14:LEU:HD12	2.36	0.41
1:C:75:LYS:O	1:C:141:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ARG:NH2	1:C:337:ARG:HB3	2.36	0.41
1:C:366:GLY:O	1:C:367:LEU:HG	2.20	0.41
1:D:206:SER:O	1:D:208:PHE:N	2.54	0.41
1:D:368:SER:HB2	1:D:447:HIS:O	2.21	0.41
1:E:69:ILE:O	1:E:123:LEU:N	2.52	0.41
1:F:328:THR:O	1:F:329:MET:C	2.59	0.41
1:A:62:TYR:CE1	1:A:163:PHE:HB2	2.56	0.41
1:A:454:TYR:CD1	1:A:456:LYS:HB2	2.55	0.41
1:B:164:TYR:O	1:B:203:SER:HB2	2.20	0.41
1:B:456:LYS:HD2	1:B:485:GLY:CA	2.50	0.41
1:C:36:GLN:HE21	1:C:175:GLU:CB	2.33	0.41
1:D:82:PHE:CZ	1:D:331:LEU:HD11	2.56	0.41
1:D:393:TYR:CE2	1:D:395:THR:HG22	2.56	0.41
1:E:228:ARG:CB	1:E:228:ARG:HH11	2.34	0.41
1:A:54:ARG:HH11	1:A:138:ASP:HA	1.86	0.40
1:A:402:ARG:HG2	1:A:413:ASP:CG	2.42	0.40
1:D:63:SER:C	1:D:65:TYR:H	2.23	0.40
1:E:82:PHE:CE1	1:E:129:VAL:HG11	2.55	0.40
1:F:126:PRO:HA	1:F:127:PRO:HD3	1.90	0.40
1:A:19:PRO:HB3	1:A:31:GLU:HB3	2.02	0.40
1:A:81:ALA:HB1	1:B:458:VAL:HG13	2.02	0.40
1:A:480:GLN:HE21	1:A:480:GLN:CA	2.27	0.40
1:B:15:ASN:H	1:B:39:GLU:CD	2.23	0.40
1:B:212:PHE:HE2	1:C:379:ILE:HG21	1.86	0.40
1:C:22:ARG:HB3	1:C:22:ARG:HH11	1.87	0.40
1:C:405:ASN:ND2	1:C:409:ASN:HB2	2.36	0.40
1:E:491:VAL:HG12	1:E:492:ASN:N	2.36	0.40
1:F:348:ALA:HB1	1:F:490:LEU:HB3	2.02	0.40
1:F:385:ASN:HD21	1:F:445:LYS:HZ3	1.69	0.40
1:B:50:ARG:HH12	1:B:67:GLN:NE2	2.20	0.40
1:B:154:ASN:ND2	1:B:157:ASP:O	2.55	0.40
1:C:14:LEU:C	1:C:15:ASN:ND2	2.72	0.40
1:C:18:GLU:HA	1:C:33:TRP:HE1	1.85	0.40
1:C:124:VAL:HG21	1:C:362:LEU:CD2	2.49	0.40
1:C:351:ILE:HD13	1:C:380:TYR:CE2	2.57	0.40
1:C:387:ASN:N	1:C:387:ASN:HD22	2.19	0.40
1:D:18:GLU:O	1:D:19:PRO:C	2.60	0.40
1:D:89:PHE:HD2	1:D:110:SER:HA	1.86	0.40
1:D:165:LEU:HD23	1:D:204:VAL:HG21	2.02	0.40
1:E:46:THR:HG22	1:E:147:LEU:HB2	2.03	0.40
1:E:430:VAL:CG2	1:E:431:ALA:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:THR:HG22	1:F:147:LEU:HB2	2.03	0.40
1:F:118:ASN:N	1:F:121:ASP:OD2	2.51	0.40
1:F:468:SER:O	1:F:472:ASN:N	2.54	0.40
1:A:228:ARG:HB2	1:A:228:ARG:HH11	1.87	0.40
1:A:232:ASP:CG	1:A:234:ARG:HH21	2.24	0.40
1:A:386:LEU:HG	1:C:128:GLY:O	2.21	0.40
1:A:472:ASN:O	1:C:226:LYS:HD2	2.21	0.40
1:B:51:THR:HA	1:B:141:VAL:O	2.21	0.40
1:B:66:PRO:HG2	1:B:148:ASP:HB3	2.02	0.40
1:B:471:TYR:O	1:B:472:ASN:CB	2.68	0.40
1:C:402:ARG:HA	1:C:412:PHE:O	2.22	0.40
1:D:77:ALA:O	1:D:117:PHE:HE1	2.04	0.40
1:E:401:VAL:HG22	1:E:432:GLU:HG3	2.04	0.40
1:A:159:ASN:OD1	1:B:7:ASN:ND2	2.55	0.40
1:A:227:LEU:HA	1:B:471:TYR:CD2	2.56	0.40
1:A:333:GLU:HG3	1:A:334:ASN:N	2.36	0.40
1:B:14:LEU:N	1:B:14:LEU:HD12	2.36	0.40
1:B:376:ARG:HA	1:B:435:GLY:O	2.21	0.40
1:B:380:TYR:CZ	1:B:383:HIS:NE2	2.89	0.40
1:E:66:PRO:N	1:E:127:PRO:HG3	2.35	0.40
1:E:75:LYS:HD2	1:E:75:LYS:O	2.22	0.40
1:E:115:ARG:HG2	1:E:115:ARG:HH21	1.87	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	365/493 (74%)	302 (83%)	54 (15%)	9 (2%)	5 19
1	B	363/493 (74%)	297 (82%)	54 (15%)	12 (3%)	4 13
1	C	361/493 (73%)	291 (81%)	51 (14%)	19 (5%)	2 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	368/493 (75%)	307 (83%)	54 (15%)	7 (2%)	8	26
1	E	371/493 (75%)	311 (84%)	54 (15%)	6 (2%)	9	31
1	F	368/493 (75%)	311 (84%)	44 (12%)	13 (4%)	3	12
All	All	2196/2958 (74%)	1819 (83%)	311 (14%)	66 (3%)	4	15

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	GLN
1	B	426	GLN
1	C	245	SER
1	C	418	ARG
1	D	171	ILE
1	D	436	GLU
1	D	447	HIS
1	E	426	GLN
1	F	107	LEU
1	F	171	ILE
1	F	425	PRO
1	F	482	LYS
1	A	113	LYS
1	A	232	ASP
1	B	53	ASN
1	B	472	ASN
1	C	8	GLU
1	C	53	ASN
1	C	113	LYS
1	C	330	LYS
1	C	375	TYR
1	F	21	HIS
1	F	246	VAL
1	F	329	MET
1	F	388	ALA
1	A	398	LYS
1	A	447	HIS
1	A	475	GLN
1	B	175	GLU
1	C	171	ILE
1	C	346	PRO
1	C	407	GLN
1	C	482	LYS

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Mol	Chain	Res	Type
1	D	207	GLY
1	E	6	PHE
1	E	446	THR
1	F	26	GLU
1	A	220	ASN
1	B	112	GLN
1	B	377	ASN
1	C	13	ASN
1	C	425	PRO
1	C	426	GLN
1	D	111	HIS
1	E	4	SER
1	E	35	SER
1	E	356	SER
1	F	108	GLN
1	F	243	GLY
1	F	426	GLN
1	A	88	THR
1	A	338	PRO
1	B	235	LYS
1	B	468	SER
1	B	487	SER
1	C	148	ASP
1	C	481	LEU
1	D	64	PRO
1	F	19	PRO
1	B	419	GLY
1	C	337	ARG
1	B	19	PRO
1	B	45	VAL
1	D	488	GLY
1	C	246	VAL
1	C	411	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/435 (74%)	310 (96%)	14 (4%)	29	62
1	B	322/435 (74%)	313 (97%)	9 (3%)	43	77
1	C	320/435 (74%)	305 (95%)	15 (5%)	26	59
1	D	327/435 (75%)	314 (96%)	13 (4%)	31	65
1	E	330/435 (76%)	318 (96%)	12 (4%)	35	69
1	F	327/435 (75%)	316 (97%)	11 (3%)	37	71
All	All	1950/2610 (75%)	1876 (96%)	74 (4%)	33	67

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	34	ASN
1	A	42	CYS
1	A	87	GLU
1	A	326	ILE
1	A	364	GLN
1	A	380	TYR
1	A	387	ASN
1	A	409	ASN
1	A	413	ASP
1	A	436	GLU
1	A	441	TYR
1	A	471	TYR
1	A	475	GLN
1	B	34	ASN
1	B	121	ASP
1	B	158	GLN
1	B	168	ASN
1	B	374	LEU
1	B	380	TYR
1	B	387	ASN
1	B	432	GLU
1	B	484	GLN
1	C	34	ASN
1	C	87	GLU
1	C	89	PHE
1	C	111	HIS
1	C	236	GLN
1	C	326	ILE
1	C	331	LEU

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Mol	Chain	Res	Type
1	C	340	ARG
1	C	363	ARG
1	C	364	GLN
1	C	371	TYR
1	C	380	TYR
1	C	387	ASN
1	C	394	VAL
1	C	436	GLU
1	D	7	ASN
1	D	20	ASP
1	D	115	ARG
1	D	121	ASP
1	D	158	GLN
1	D	175	GLU
1	D	180	GLN
1	D	325	ASN
1	D	332	HIS
1	D	364	GLN
1	D	380	TYR
1	D	437	GLN
1	D	467	LEU
1	E	6	PHE
1	E	34	ASN
1	E	70	ILE
1	E	75	LYS
1	E	118	ASN
1	E	235	LYS
1	E	247	ILE
1	E	326	ILE
1	E	380	TYR
1	E	417	ARG
1	E	479	ARG
1	E	480	GLN
1	F	42	CYS
1	F	50	ARG
1	F	65	TYR
1	F	115	ARG
1	F	152	PHE
1	F	200	GLU
1	F	222	ASP
1	F	225	GLU
1	F	332	HIS

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Mol	Chain	Res	Type
1	F	380	TYR
1	F	387	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	15	ASN
1	A	34	ASN
1	A	36	GLN
1	A	53	ASN
1	A	55	ASN
1	A	67	GLN
1	A	108	GLN
1	A	112	GLN
1	A	153	ASN
1	A	158	GLN
1	A	159	ASN
1	A	334	ASN
1	A	377	ASN
1	A	385	ASN
1	A	387	ASN
1	A	409	ASN
1	A	426	GLN
1	A	433	GLN
1	A	448	HIS
1	A	469	ASN
1	A	477	GLN
1	A	480	GLN
1	B	7	ASN
1	B	10	GLN
1	B	12	ASN
1	B	13	ASN
1	B	15	ASN
1	B	34	ASN
1	B	53	ASN
1	B	55	ASN
1	B	67	GLN
1	B	112	GLN
1	B	116	HIS
1	B	153	ASN
1	B	159	ASN

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Mol	Chain	Res	Type
1	B	168	ASN
1	B	218	ASN
1	B	332	HIS
1	B	334	ASN
1	B	385	ASN
1	B	387	ASN
1	B	389	ASN
1	B	409	ASN
1	B	426	GLN
1	B	433	GLN
1	B	437	GLN
1	B	449	ASN
1	B	472	ASN
1	B	475	GLN
1	B	477	GLN
1	B	480	GLN
1	C	7	ASN
1	C	15	ASN
1	C	34	ASN
1	C	36	GLN
1	C	53	ASN
1	C	67	GLN
1	C	73	GLN
1	C	154	ASN
1	C	178	GLN
1	C	211	HIS
1	C	332	HIS
1	C	334	ASN
1	C	345	ASN
1	C	385	ASN
1	C	387	ASN
1	C	407	GLN
1	C	409	ASN
1	C	437	GLN
1	C	448	HIS
1	C	469	ASN
1	C	480	GLN
1	D	7	ASN
1	D	10	GLN
1	D	12	ASN
1	D	15	ASN
1	D	21	HIS

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Mol	Chain	Res	Type
1	D	36	GLN
1	D	53	ASN
1	D	67	GLN
1	D	112	GLN
1	D	159	ASN
1	D	168	ASN
1	D	178	GLN
1	D	180	GLN
1	D	197	GLN
1	D	215	GLN
1	D	332	HIS
1	D	334	ASN
1	D	364	GLN
1	D	407	GLN
1	D	409	ASN
1	D	437	GLN
1	D	469	ASN
1	D	480	GLN
1	E	15	ASN
1	E	34	ASN
1	E	36	GLN
1	E	67	GLN
1	E	73	GLN
1	E	364	GLN
1	E	385	ASN
1	E	409	ASN
1	E	420	GLN
1	E	437	GLN
1	E	469	ASN
1	E	477	GLN
1	E	486	ASN
1	F	7	ASN
1	F	13	ASN
1	F	21	HIS
1	F	34	ASN
1	F	37	HIS
1	F	53	ASN
1	F	67	GLN
1	F	106	GLN
1	F	153	ASN
1	F	159	ASN
1	F	179	GLN

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Mol	Chain	Res	Type
1	F	215	GLN
1	F	218	ASN
1	F	332	HIS
1	F	334	ASN
1	F	364	GLN
1	F	385	ASN
1	F	387	ASN
1	F	407	GLN
1	F	409	ASN
1	F	433	GLN
1	F	437	GLN
1	F	469	ASN
1	F	480	GLN
1	F	486	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	CSD	D	406	1	4,7,8	0.60	0	1,8,10	1.36	0
1	CSD	F	406	1	4,7,8	0.61	0	1,8,10	1.37	0
1	CSD	E	406	1	4,7,8	0.56	0	1,8,10	1.16	0
1	CSD	B	406	1	4,7,8	0.62	0	1,8,10	1.41	0
1	CSD	C	406	1	4,7,8	0.59	0	1,8,10	0.75	0
1	CSD	A	406	1	4,7,8	0.60	0	1,8,10	0.98	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	D	406	1	-	0/2/6/8	-
1	CSD	F	406	1	-	1/2/6/8	-
1	CSD	E	406	1	-	1/2/6/8	-
1	CSD	B	406	1	-	1/2/6/8	-
1	CSD	C	406	1	-	1/2/6/8	-
1	CSD	A	406	1	-	0/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	406	CSD	CA-CB-SG-OD1
1	F	406	CSD	CA-CB-SG-OD1
1	B	406	CSD	CA-CB-SG-OD1
1	C	406	CSD	CA-CB-SG-OD1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	406	CSD	1	0
1	B	406	CSD	2	0
1	C	406	CSD	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CO3	A	501	-	3,3,3	0.68	0	2,3,3	0.16	0
2	CO3	C	503	-	3,3,3	0.68	0	2,3,3	0.15	0
2	CO3	B	502	-	3,3,3	0.76	0	2,3,3	0.18	0
2	CO3	E	505	-	3,3,3	0.77	0	2,3,3	0.07	0
2	CO3	D	504	-	3,3,3	0.71	0	2,3,3	0.11	0
2	CO3	F	506	-	3,3,3	0.72	0	2,3,3	0.14	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	CO3	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	373/493 (75%)	0.07	18 (4%)	30	21	13, 37, 54, 62	0
1	B	371/493 (75%)	0.01	12 (3%)	47	37	6, 37, 56, 63	0
1	C	369/493 (74%)	0.26	27 (7%)	15	8	7, 39, 54, 66	0
1	D	376/493 (76%)	-0.39	7 (1%)	66	59	6, 19, 46, 57	0
1	E	379/493 (76%)	-0.44	3 (0%)	86	81	6, 13, 43, 58	0
1	F	376/493 (76%)	-0.42	3 (0%)	86	81	6, 18, 45, 56	0
All	All	2244/2958 (75%)	-0.15	70 (3%)	49	39	6, 28, 52, 66	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	THR	6.0
1	B	437	GLN	4.7
1	C	89	PHE	4.4
1	C	435	GLY	4.4
1	C	226	LYS	3.7
1	C	246	VAL	3.6
1	A	88	THR	3.6
1	C	328	THR	3.5
1	D	338	PRO	3.5
1	D	179	GLN	3.4
1	D	197	GLN	3.3
1	E	89	PHE	3.2
1	A	200	GLU	3.2
1	A	342	ASP	3.0
1	A	463	PRO	3.0
1	A	340	ARG	3.0
1	B	485	GLY	3.0
1	B	88	THR	2.9
1	B	89	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	358	THR	2.9
1	B	200	GLU	2.8
1	C	111	HIS	2.8
1	C	373	VAL	2.8
1	C	487	SER	2.7
1	A	12	ASN	2.7
1	C	437	GLN	2.7
1	C	227	LEU	2.7
1	A	177	MET	2.6
1	C	245	SER	2.6
1	B	483	TYR	2.6
1	C	114	ILE	2.6
1	F	107	LEU	2.6
1	A	6	PHE	2.6
1	D	484	GLN	2.6
1	F	179	GLN	2.5
1	C	493	PRO	2.5
1	E	107	LEU	2.5
1	A	178	GLN	2.4
1	B	438	GLY	2.4
1	C	334	ASN	2.4
1	C	244	LEU	2.4
1	C	230	PRO	2.4
1	A	471	TYR	2.4
1	A	338	PRO	2.3
1	D	108	GLN	2.3
1	D	178	GLN	2.3
1	A	244	LEU	2.3
1	A	89	PHE	2.3
1	C	371	TYR	2.3
1	B	377	ASN	2.3
1	C	140	PRO	2.3
1	B	86	PRO	2.3
1	A	331	LEU	2.2
1	C	338	PRO	2.2
1	F	106	GLN	2.2
1	C	116	HIS	2.1
1	A	248	SER	2.1
1	B	6	PHE	2.1
1	A	462	ILE	2.1
1	C	134	TYR	2.1
1	C	341	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	201	GLY	2.1
1	C	377	ASN	2.1
1	D	200	GLU	2.1
1	A	482	LYS	2.1
1	B	409	ASN	2.1
1	C	379	ILE	2.0
1	A	219	THR	2.0
1	C	415	GLU	2.0
1	E	4	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSD	C	406	8/9	0.88	0.16	31,38,58,62	0
1	CSD	A	406	8/9	0.91	0.16	30,41,46,53	0
1	CSD	B	406	8/9	0.94	0.14	39,44,63,73	0
1	CSD	F	406	8/9	0.95	0.17	5,8,30,57	0
1	CSD	E	406	8/9	0.96	0.14	5,7,45,53	0
1	CSD	D	406	8/9	0.96	0.10	5,13,23,38	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO3	F	506	4/4	0.87	0.19	5,5,18,21	0
2	CO3	B	502	4/4	0.88	0.22	12,22,39,45	0
2	CO3	A	501	4/4	0.88	0.24	14,35,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO3	E	505	4/4	0.89	0.17	5,5,10,17	0
2	CO3	C	503	4/4	0.91	0.16	36,40,41,42	0
3	MG	B	602	1/1	0.91	0.21	41,41,41,41	0
3	MG	C	603	1/1	0.93	0.13	21,21,21,21	0
3	MG	A	601	1/1	0.94	0.08	17,17,17,17	0
3	MG	D	604	1/1	0.96	0.16	17,17,17,17	0
2	CO3	D	504	4/4	0.97	0.14	5,19,20,21	0
3	MG	F	606	1/1	0.97	0.14	8,8,8,8	0
3	MG	E	605	1/1	0.99	0.16	5,5,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.