Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:29 AM GMT

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
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:

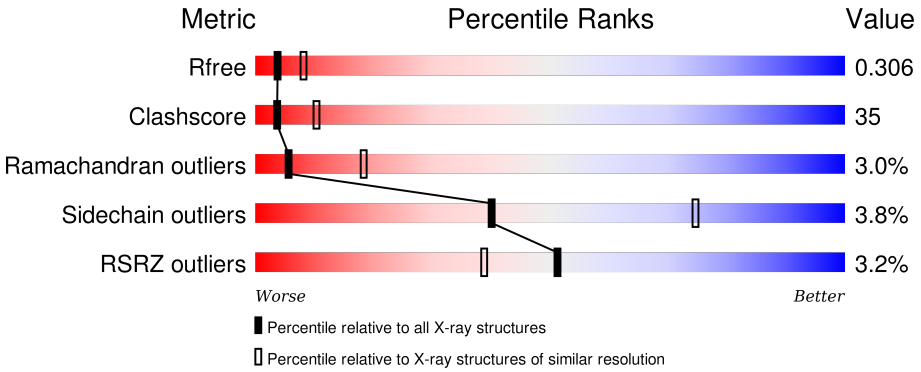
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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.



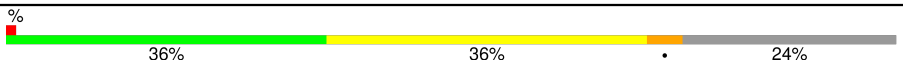
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 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	493	4% 32% 40% • 24%
1	B	493	3% 33% 39% • 25%
1	C	493	6% 26% 44% 5% 25%
1	D	493	% 36% 38% • 24%
1	E	493	% 40% 34% • 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	493	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	B	502	-	-	-	X

2 Entry composition

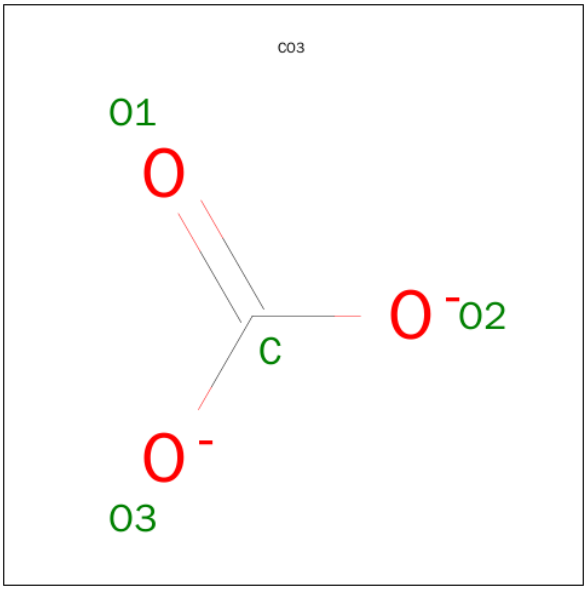
There are 3 unique types of molecules in this entry. The entry contains 17703 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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

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

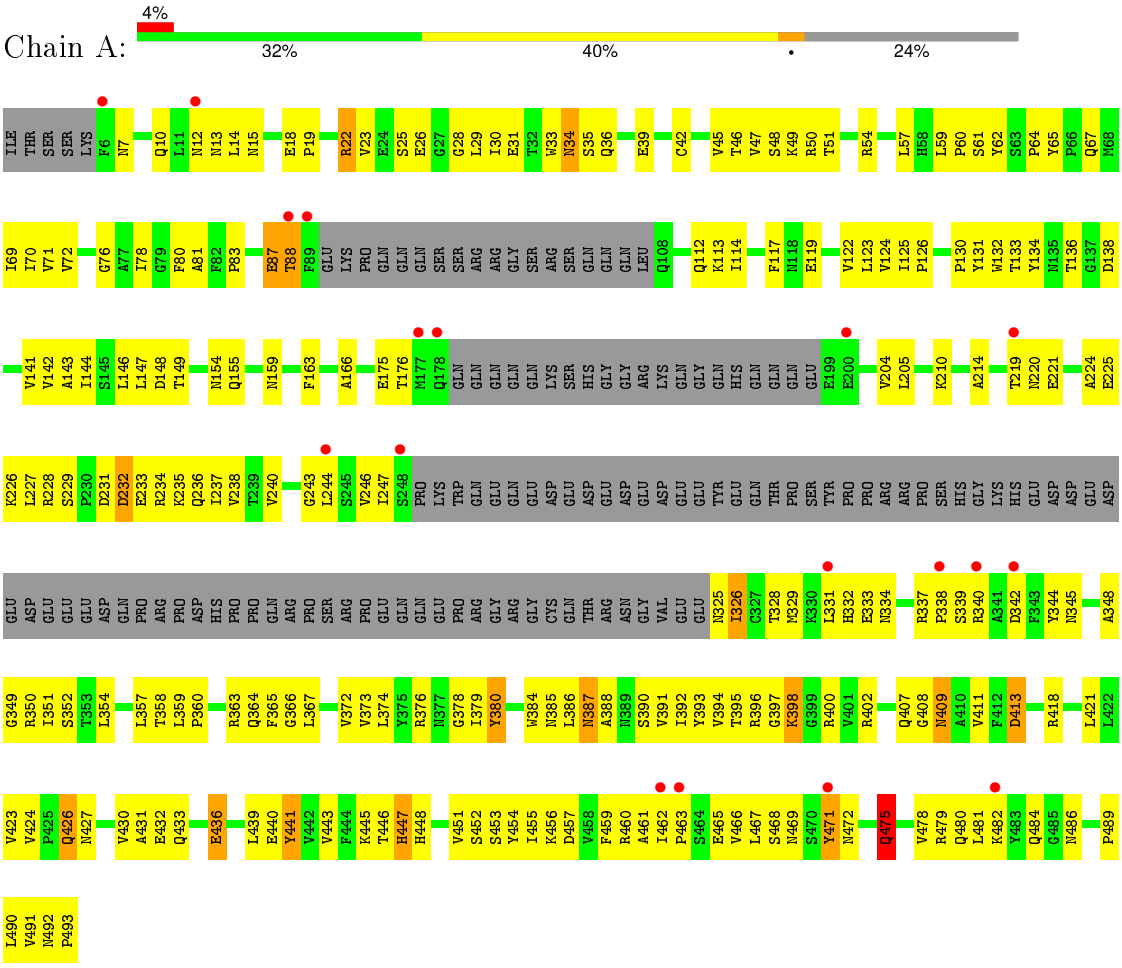
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

3 Residue-property plots

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.

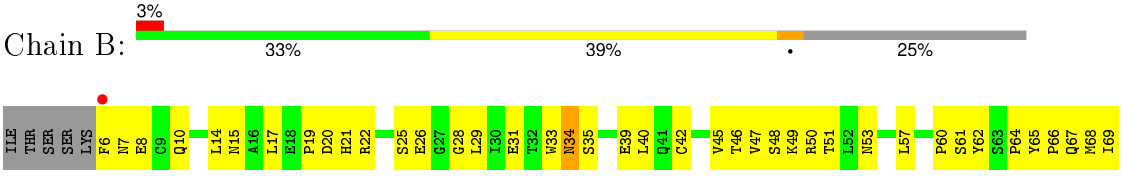
- Molecule 1: glycinin A3B4 subunit

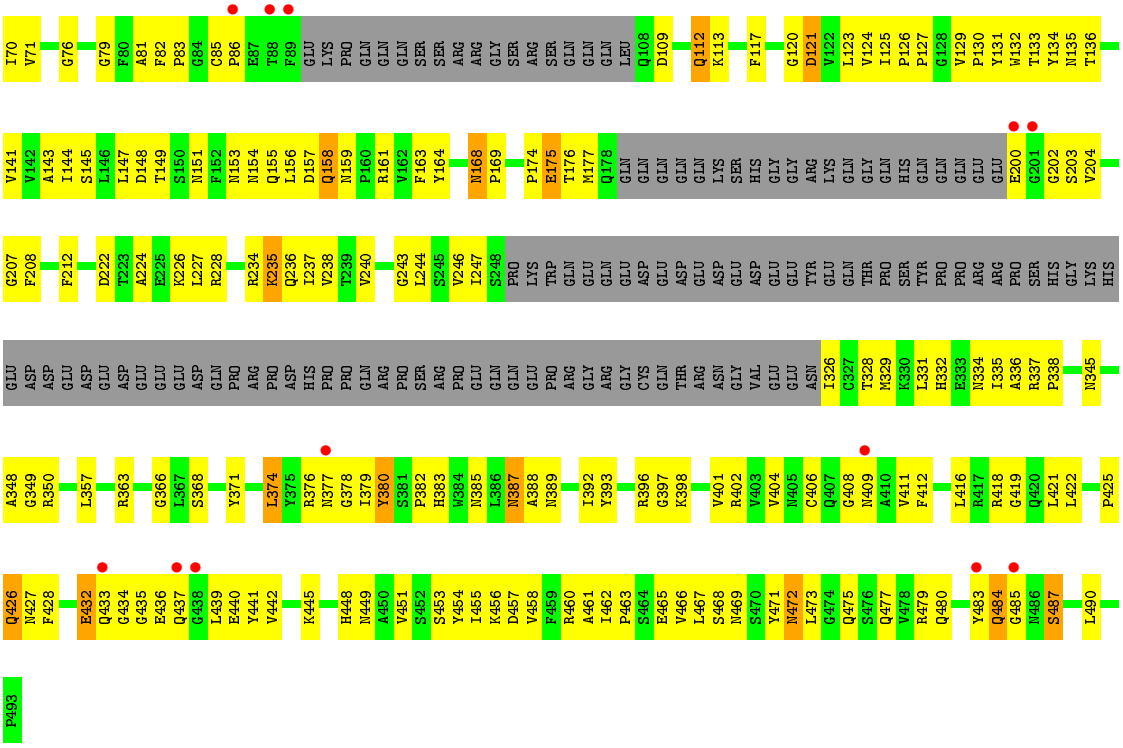
Chain A:



- Molecule 1: glycinin A3B4 subunit

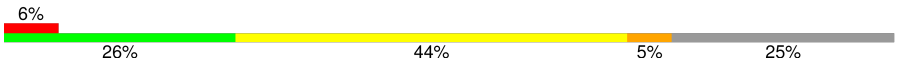
Chain B:

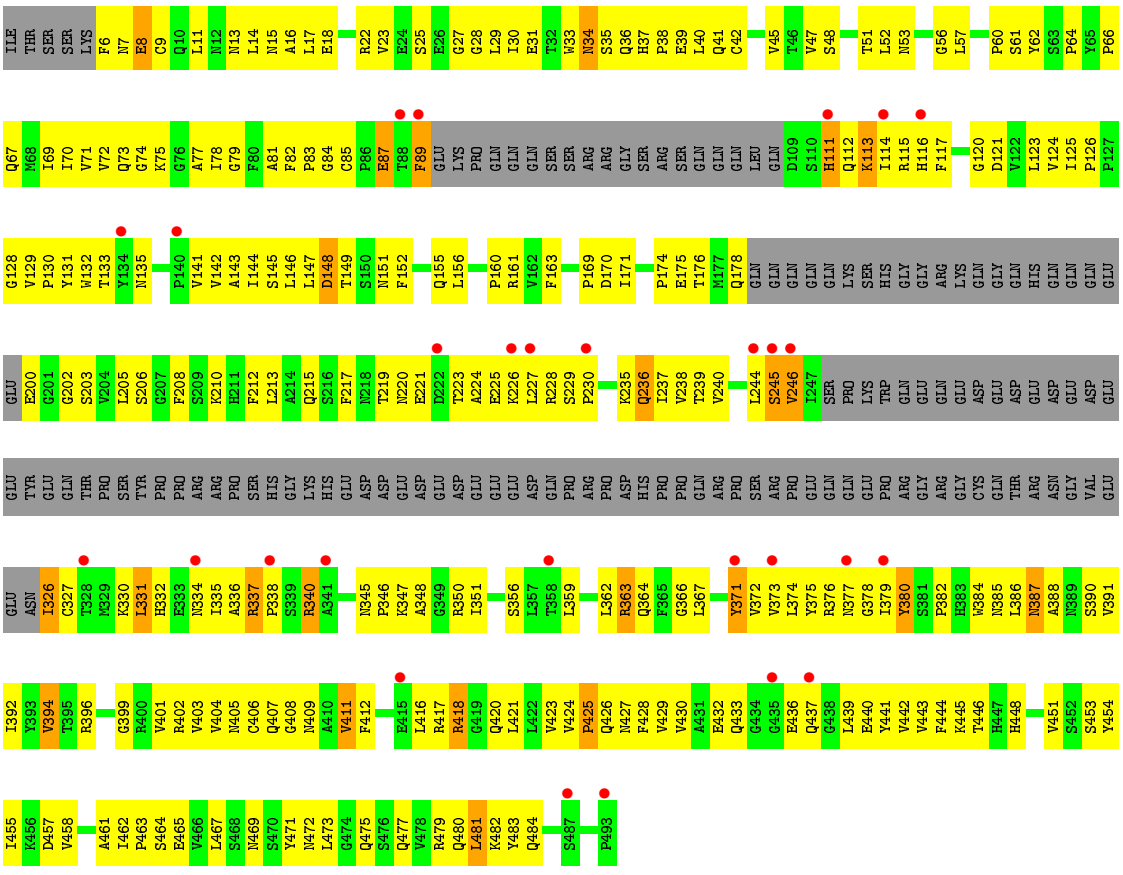




• Molecule 1: glycinin A3B4 subunit

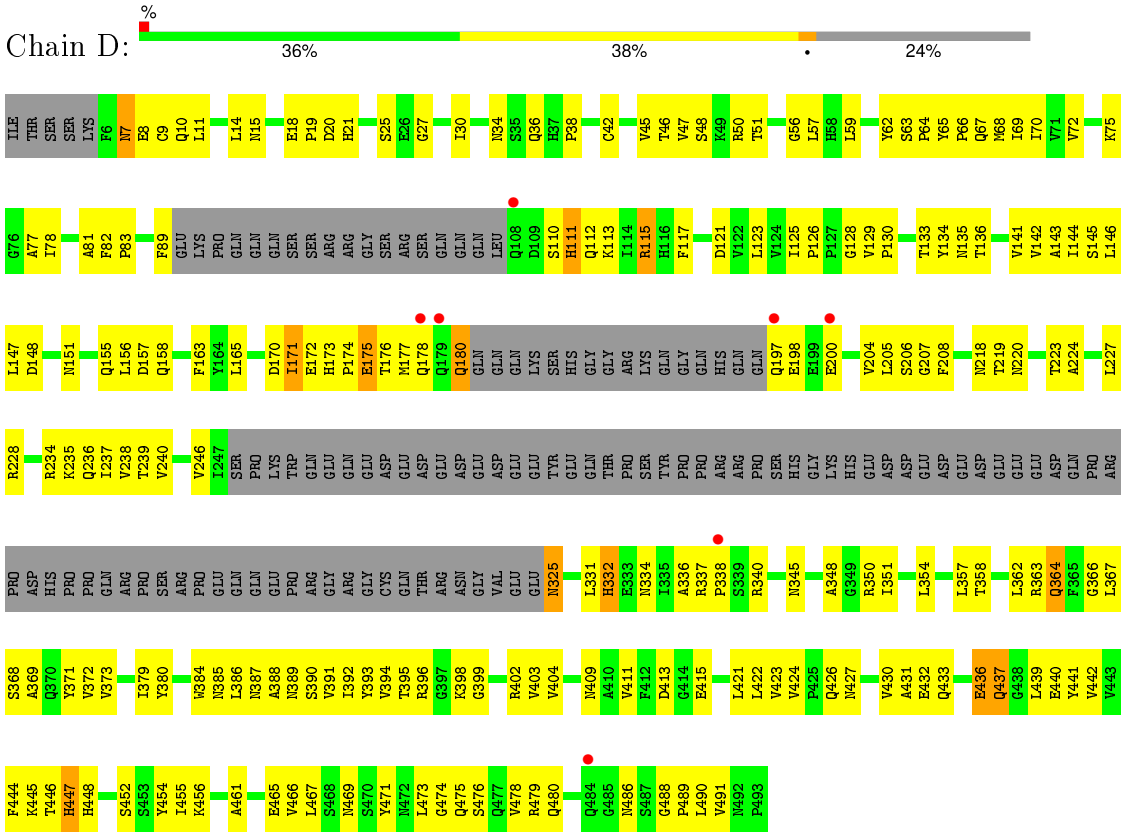
Chain C:





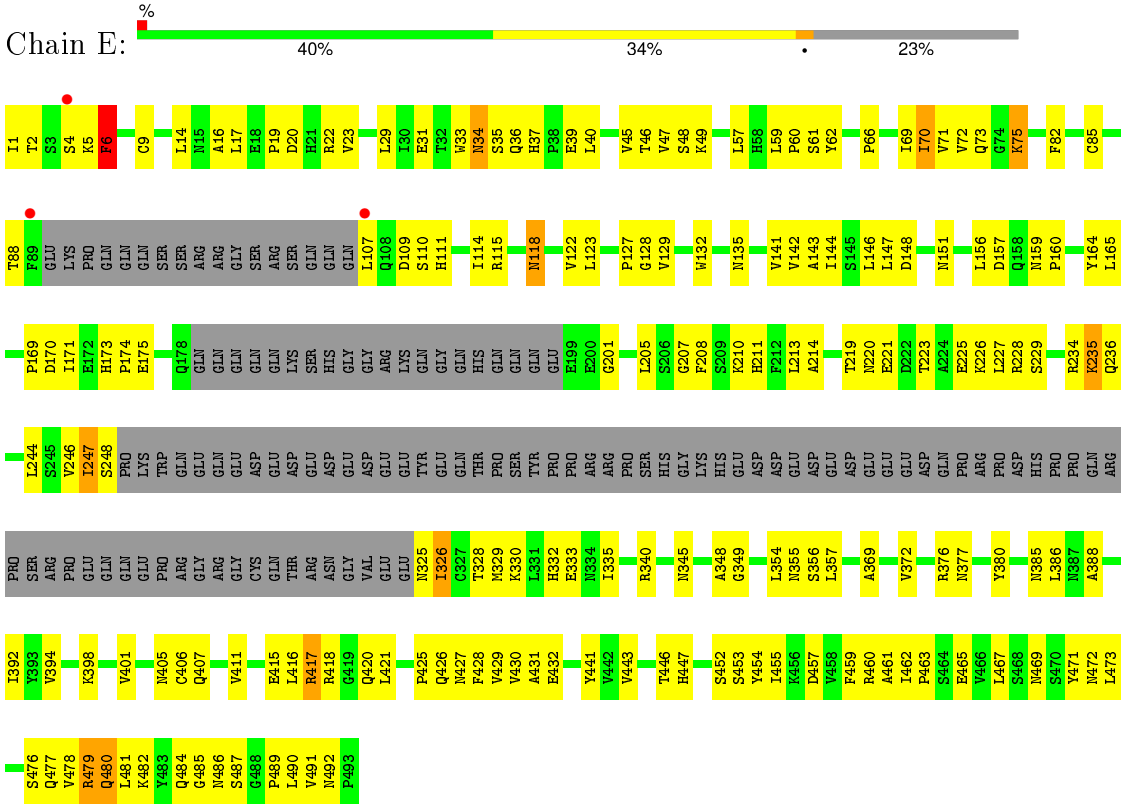
• Molecule 1: glycinin A3B4 subunit

Chain D:



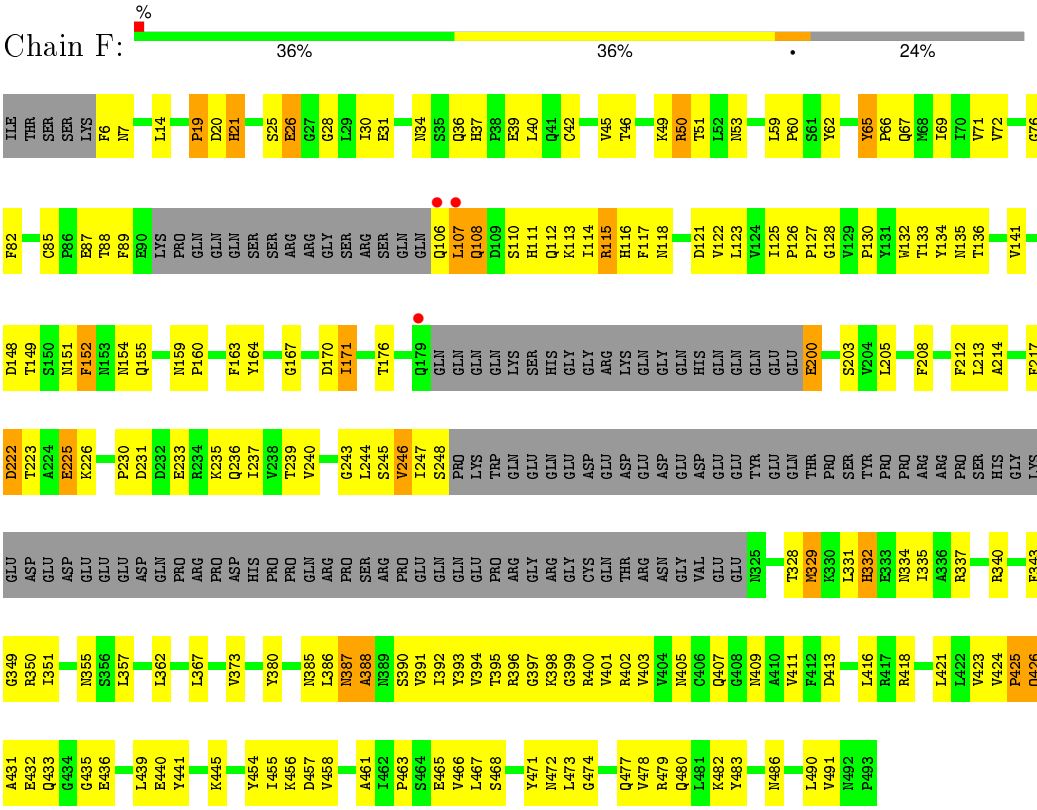
• Molecule 1: glycinin A3B4 subunit

Chain E:



• 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 0.231 , 0.306	Depositor DCC
R_{free} test set	5961 reflections (10.13%)	DCC
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
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
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 63184 reflections	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, 0.375 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: CSD, CO3, MG

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

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

Continued on next page...

Continued from previous page...

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:H	1:E:247:ILE:HD13	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:HH11	1:A:340:ARG:HB3	1.34	0.87
1:D:364:GLN:HE21	1:D:364:GLN:H	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:HD2	1:D:115:ARG:H	1.41	0.85
1:C:124:VAL:H	1:C:331:LEU:HD12	1.42	0.84

Continued on next page...

Continued from previous page...

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:F:171:ILE:H	1:F:171:ILE:HD12	1.45	0.81
1:D:68:MET:HE1	1:D:369:ALA:HB2	1.62	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: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:C:477:GLN:O	1:C:480:GLN:HB3	1.82	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:NH1	1:E:376:ARG:HB3	2.01	0.75

Continued on next page...

Continued from previous page...

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:H	1:B:387:ASN:HD22	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:HE3	1:E:235:LYS:HA	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:F:135:ASN:ND2	1:F:141:VAL:HG23	2.04	0.72
1:C:391:VAL:HG23	1:C:444:PHE:HB2	1.70	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:NE2	1:D:364:GLN:H	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:B:156:LEU:HB3	1:B:161:ARG:NH2	2.05	0.70
1:A:459:PHE:HE2	1:A:471:TYR:HH	1.37	0.70
1:C:124:VAL:H	1:C:331:LEU:CD1	2.03	0.70
1:D:390:SER:HB2	1:D:424:VAL:HB	1.74	0.70
1:D:240:VAL:HG13	1:E:469:ASN:HD21	1.57	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:B:401:VAL:HG21	1:B:416:LEU:HD22	1.74	0.69
1:A:46:THR:HG23	1:A:147:LEU:HD12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:VAL:CG2	1:C:444:PHE:HB2	2.23	0.69
1:B:113:LYS:HD2	1:B:113:LYS:H	1.55	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:123:LEU:HD23	1:B:332:HIS:CB	2.22	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:D:50:ARG:HH12	1:D:67:GLN:HE22	1.39	0.69
1:B:83:PRO:HB3	1:C:453:SER:HB2	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: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: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:D:394:VAL:HA	1:D:441:TYR:HB3	1.76	0.68
1:A:357:LEU:HD12	1:A:357:LEU:H	1.57	0.68
1:A:367:LEU:O	1:A:448:HIS:HA	1.93	0.68
1:E:385:ASN:HD22	1:E:452:SER:HB3	1.59	0.68
1:A:409:ASN:N	1:A:409:ASN:HD22	1.92	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:F:66:PRO:HG3	1:F:151:ASN:ND2	2.10	0.67
1:E:345:ASN:HB3	1:E:348:ALA:HB3	1.77	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:159:ASN:ND2	1:B:176:THR:HG22	2.07	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:C	1:B:15:ASN:HD22	1.99	0.66
1:C:463:PRO:O	1:C:467:LEU:HD13	1.95	0.66
1:B:120:GLY:O	1:B:335:ILE:HG22	1.96	0.66
1:C:169:PRO:HA	1:C:236:GLN:OE1	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:D:334:ASN:ND2	1:D:337:ARG:HB2	2.09	0.66
1:B:40:LEU:HD21	1:B:46:THR:HA	1.77	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:F:159:ASN:ND2	1:F:176:THR:HG22	2.03	0.66
1:E:75:LYS:HB3	1:E:118:ASN:HA	1.77	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:C:229:SER:N	1:C:230:PRO:HD3	2.10	0.65
1:A:481:LEU:HD22	1:C:217:PHE:HB3	1.77	0.65
1:F:115:ARG:NH2	1:F:331:LEU:HD12	2.02	0.65
1:F:30:ILE:HG12	1:F:50:ARG:HG3	1.78	0.65
1:F:401:VAL:HG22	1:F:432:GLU:HG3	1.77	0.65
1:A:31:GLU:OE1	1:A:49:LYS:HD2	1.95	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:F:14:LEU:HD13	1:F:411:VAL:HB	1.77	0.65
1:B:393:TYR:HB3	1:B:442:VAL:CG1	2.28	0.65
1:A:205:LEU:HD21	1:B:455:ILE:HD13	1.79	0.65
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:382:PRO:HB2	1:C:455:ILE:HD12	1.78	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:F:19:PRO:HB3	1:F:31:GLU:HB3	1.78	0.64
1:C:51:THR:HG23	1:C:142:VAL:HG22	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

Continued on next page...

Continued from previous page...

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:C:208:PHE:HB2	1:C:213:LEU:HD21	1.80	0.64
1:B:22:ARG:NH2	1:B:29:LEU:HD21	2.13	0.64
1:F:25:SER:HB3	1:F:235:LYS:HB2	1.81	0.63
1:B:475:GLN:NE2	1:B:479:ARG:HB2	2.13	0.63
1:A:326:ILE:O	1:A:326:ILE:HD13	1.98	0.63
1:C:124:VAL:HG21	1:C:362:LEU:HD23	1.81	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:235:LYS:HB3	1:A:236:GLN:OE1	1.99	0.63
1:C:205:LEU:HD13	1:C:227:LEU:HB3	1.79	0.63
1:A:112:GLN:NE2	1:B:461:ALA:HB1	2.14	0.63
1:D:224:ALA:HA	1:D:227:LEU:HD12	1.81	0.63
1:B:456:LYS:HG2	1:B:460:ARG:NH2	2.13	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:D:176:THR:O	1:D:177:MET:HE2	1.99	0.63
1:A:363:ARG:HE	1:A:448:HIS:CD2	2.16	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: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:A:392:ILE:HG12	1:A:443:VAL:HG22	1.79	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: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:A:471:TYR:HB3	1:C:226:LYS:O	1.99	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:454:TYR:CE1	1:F:457:ASP:HB2	2.35	0.61
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: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:136:THR:HG22	1:B:247:ILE:HG21	1.82	0.61
1:B:46:THR:CG2	1:B:147:LEU:HB2	2.30	0.61
1:E:144:ILE:HD12	1:E:144:ILE:N	2.16	0.61
1:E:135:ASN:ND2	1:E:141:VAL:HG23	2.14	0.61
1:F:170:ASP:HB2	1:F:235:LYS:HD2	1.82	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: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:C:52:LEU:CD2	1:C:237:ILE:HD13	2.31	0.60
1:B:31:GLU:HB2	1:B:49:LYS:HB3	1.83	0.60
1:F:28:GLY:HA3	1:F:237:ILE:HG21	1.84	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:A:234:ARG:CB	1:A:238:VAL:HG12	2.31	0.60
1:D:338:PRO:HG3	1:D:350:ARG:NH1	2.16	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: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:D:489:PRO:O	1:D:491:VAL:HG23	2.02	0.60
1:B:387:ASN:C	1:B:426:GLN:HE21	2.04	0.60
1:B:240:VAL:HG13	1:C:469:ASN:HD21	1.67	0.60
1:A:409:ASN:ND2	1:A:409:ASN:N	2.49	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:B:69:ILE:HG12	1:B:145:SER:HA	1.84	0.59
1:A:33:TRP:CE3	1:A:47:VAL:HB	2.37	0.59
1:D:34:ASN:HD21	1:D:36:GLN:HB2	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLN:HB2	1:A:409:ASN:HD21	1.67	0.59
1:B:376:ARG:HD3	1:B:436:GLU:O	2.02	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:350:ARG:HG3	1:C:350:ARG:HH21	1.68	0.59
1:C:363:ARG:HE	1:C:448:HIS:CG	2.21	0.59
1:C:213:LEU:HD12	1:C:217:PHE:HE1	1.66	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: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:A:123:LEU:HD23	1:A:332:HIS:HB3	1.83	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:F:395:THR:O	1:F:418:ARG:HG3	2.02	0.58
1:D:123:LEU:HD23	1:D:332:HIS:HB3	1.84	0.58
1:C:399:GLY:HA3	1:C:439:LEU:HD22	1.86	0.58
1:F:107:LEU:H	1:F:107:LEU:CD2	2.16	0.58
1:B:348:ALA:O	1:B:374:LEU:HD22	2.03	0.58
1:A:159:ASN:ND2	1:A:176:THR:HA	2.19	0.58
1:C:23:VAL:HG11	1:C:170:ASP:HB3	1.85	0.58
1:B:338:PRO:HG3	1:B:350:ARG:HH21	1.68	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:D:386:LEU:HG	1:F:128:GLY:HA3	1.84	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: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:F:164:TYR:O	1:F:203:SER:HB2	2.04	0.58
1:E:62:TYR:HE2	1:F:427:ASN:HB3	1.67	0.58
1:D:368:SER:HB3	1:D:445:LYS:HB2	1.85	0.58
1:B:393:TYR:HB3	1:B:442:VAL:HG12	1.85	0.57
1:A:22:ARG:HH12	1:A:29:LEU:HD21	1.69	0.57
1:D:480:GLN:OE1	1:F:219:THR:HA	2.04	0.57
1:A:378:GLY:O	1:A:433:GLN: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:PRO:CG	1:C:350:ARG:HH11	2.17	0.57
1:B:387:ASN:HD22	1:B:387:ASN:N	1.98	0.57
1:A:326:ILE:HA	1:A:329:MET:CE	2.34	0.57
1:A:144:ILE:N	1:A:144:ILE:HD12	2.20	0.57
1:A:354:LEU:HD12	1:A:358:THR:OG1	2.04	0.57
1:F:456:LYS:NZ	1:F:486:ASN:HD21	2.02	0.57
1:B:124:VAL:HG12	1:B:331:LEU:O	2.05	0.57
1:B:34:ASN:HD22	1:B:35:SER:N	2.03	0.57
1:F:71:VAL:HG21	1:F:117:PHE:CD2	2.39	0.57
1:E:73:GLN:HE21	1:E:142:VAL:HG12	1.69	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:F:219:THR:OG1	1:F:223:THR:HB	2.04	0.57
1:C:345:ASN:HD22	1:C:348:ALA:HB3	1.68	0.57
1:A:71:VAL:HG21	1:A:117:PHE:CD2	2.40	0.57
1:D:391:VAL:O	1:D:391:VAL:HG13	2.05	0.57
1:D:175:GLU:O	1:D:178:GLN:HG3	2.05	0.57
1:A:22:ARG:HB2	1:A:22:ARG:NH1	2.19	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:C:386:LEU:HD12	1:C:386:LEU:H	1.70	0.57
1:A:357:LEU:CD1	1:A:357:LEU:H	2.17	0.57
1:D:379:ILE:HG13	1:D:433:GLN:HB2	1.87	0.57
1:A:234:ARG:HB2	1:A:238:VAL:HG12	1.86	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:NH1	1:B:22:ARG:HB3	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:34:ASN:OD1	1:D:175:GLU:HB3	2.06	0.56
1:D:14:LEU:HD23	1:D:423:VAL:O	2.05	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:B:28:GLY:HA3	1:B:237:ILE:HG21	1.87	0.56
1:A:396:ARG:HH11	1:A:396:ARG:HG2	1.71	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:F:51:THR:HA	1:F:141:VAL:O	2.05	0.56

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:HD12	1:A:357:LEU:N	2.22	0.55
1:A:23:VAL:HB	1:A:30:ILE:HB	1.89	0.55
1:A:395:THR:C	1:A:418:ARG:HG3	2.27	0.55
1:B:385:ASN:HD21	1:B:445:LYS:HZ2	1.53	0.54
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:E:2:THR:HA	1:E:5:LYS:NZ	2.22	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:B:479:ARG:HE	1:B:483:TYR:HD2	1.53	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:F:235:LYS:HB3	1:F:236:GLN:OE1	2.08	0.54
1:E:208:PHE:CD1	1:F:402:ARG:HD3	2.43	0.54
1:D:156:LEU:HA	1:E:9:CYS:SG	2.46	0.54
1:F:25:SER:OG	1:F:237:ILE:HB	2.07	0.54
1:C:30:ILE:HD12	1:C:236:GLN:HG3	1.90	0.54
1:C:206:SER:HA	1:C:228:ARG:HG2	1.90	0.54
1:B:387:ASN:HA	1:B:426:GLN:HE21	1.72	0.54
1:C:403:VAL:HG22	1:C:430:VAL:HG23	1.89	0.54
1:B:65:TYR:CE2	1:B:147:LEU:HB3	2.43	0.54
1:A:358:THR:O	1:A:360:PRO:HD3	2.07	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:135:ASN:ND2	1:C:141:VAL:HG23	2.22	0.54
1:E:478:VAL:O	1:E:482:LYS:HB2	2.08	0.54
1:C:11:LEU:HD21	1:C:38:PRO:HB3	1.89	0.54
1:E:36:GLN:HE21	1:E:175:GLU:HB2	1.73	0.54
1:A:46:THR:HG23	1:A:147:LEU:HB2	1.90	0.54
1:B:67:GLN:HE21	1:B:147:LEU:CD2	2.20	0.54
1:A:400:ARG:HG2	1:A:402:ARG:HH22	1.72	0.54
1:D:69:ILE:CG2	1:D:143:ALA:HB1	2.38	0.54
1:F:334:ASN:HB3	1:F:340:ARG:NH1	2.22	0.54
1:F:25:SER:CB	1:F:235:LYS:HB2	2.38	0.54
1:C:210:LYS:HD3	1:C:225:GLU:CG	2.35	0.54
1:C:60:PRO:HA	1:C:131:TYR:O	2.08	0.54
1:D:466:VAL:HG22	1:F:244:LEU:CD2	2.38	0.54
1:A:325:ASN:HA	1:A:328:THR:HG22	1.89	0.54
1:D:246:VAL:HG13	1:E:465:GLU:CD	2.28	0.54
1:B:35:SER:OG	1:B:175:GLU:HG3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:N	1:C:386:LEU:HD12	2.23	0.54
1:A:25:SER:OG	1:A:237:ILE:HB	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:124:VAL:O	1:A:126:PRO:HD3	2.08	0.54
1:A:350:ARG:HH12	1:A:373:VAL:HG21	1.73	0.53
1:E:376:ARG:CB	1:E:376:ARG:HH11	2.18	0.53
1:F:402:ARG:NH2	1:F:413:ASP:OD1	2.41	0.53
1:F:34:ASN:ND2	1:F:36:GLN:HB2	2.14	0.53
1:D:50:ARG:HH12	1:D:67:GLN:NE2	2.05	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:394:VAL:HA	1:D:441:TYR:CB	2.38	0.53
1:A:122:VAL:O	1:A:332:HIS:HA	2.08	0.53
1:F:343:PHE:HB2	1:F:351:ILE:HB	1.89	0.53
1:E:16:ALA:HB1	1:E:420:GLN:NE2	2.22	0.53
1:C:326:ILE:HD13	1:C:326:ILE:C	2.28	0.53
1:D:218:ASN:OD1	1:E:485:GLY:HA3	2.08	0.53
1:D:180:GLN:N	1:D:180:GLN:NE2	2.56	0.53
1:D:171:ILE:HG12	1:D:198:GLU:O	2.08	0.53
1:D:115:ARG:HD2	1:D:115:ARG:N	2.20	0.53
1:A:391:VAL:CG1	1:A:421:LEU:HD11	2.37	0.53
1:A:15:ASN:HB2	1:A:39:GLU:OE2	2.09	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:425:PRO:HB2	1:B:428:PHE:CD2	2.44	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:F:171:ILE:HD13	1:F:200:GLU:N	2.24	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:E:170:ASP:OD2	1:E:235:LYS:HE2	2.09	0.53
1:A:391:VAL:HG12	1:A:421:LEU:HD11	1.90	0.53
1:F:20:ASP:O	1:F:21:HIS:HB2	2.08	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:B:396:ARG:HA	1:B:418:ARG:HG3	1.91	0.53
1:D:430:VAL:HG22	1:D:431:ALA:N	2.24	0.53
1:C:454:TYR:CE1	1:C:457:ASP:HB2	2.44	0.53
1:C:87:GLU:HG3	1:C:112:GLN:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:CG2	1:B:143:ALA:HB1	2.39	0.53
1:F:405:ASN:OD1	1:F:407:GLN:HG3	2.08	0.53
1:E:247:ILE:CD1	1:E:247:ILE:H	2.16	0.52
1:E:376:ARG:O	1:E:377:ASN:HB2	2.10	0.52
1:B:31:GLU:OE1	1:B:49:LYS:HD3	2.08	0.52
1:C:372:VAL:HB	1:C:441:TYR:CZ	2.44	0.52
1:F:107:LEU:N	1:F:107:LEU:HD22	2.20	0.52
1:A:461:ALA:HA	1:C:87:GLU:CG	2.39	0.52
1:A:70:ILE:O	1:A:70:ILE:HG23	2.09	0.52
1:B:15:ASN:N	1:B:15:ASN:HD22	2.05	0.52
1:C:146:LEU:HB2	1:C:444:PHE:CD1	2.43	0.52
1:F:244:LEU:O	1:F:247:ILE:HD13	2.09	0.52
1:E:40:LEU:HD12	1:E:45:VAL:O	2.10	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:A:386:LEU:HD13	1:A:452:SER:HA	1.90	0.52
1:A:387:ASN:HD21	1:A:451:VAL:H	1.57	0.52
1:B:81:ALA:HA	1:B:112:GLN:NE2	2.24	0.52
1:C:240:VAL:HG11	1:C:244:LEU:HD13	1.91	0.52
1:B:240:VAL:HG11	1:B:244:LEU:CD1	2.39	0.52
1:C:213:LEU:H	1:C:213:LEU:HD22	1.75	0.52
1:B:69:ILE:HA	1:B:144:ILE:O	2.09	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: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:D:62:TYR:HE2	1:E:427:ASN:HB3	1.74	0.52
1:E:244:LEU:HD11	1:F:465:GLU:HB3	1.91	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:F:152:PHE:HD1	1:F:152:PHE:H	1.56	0.52
1:A:61:SER:O	1:A:130:PRO:HA	2.10	0.52
1:B:85:CYS:HB3	1:B:113:LYS:NZ	2.24	0.52
1:B:76:GLY:HA2	1:B:136:THR:H	1.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:CSD:C	1:C:408:GLY:H	2.23	0.52
1:C:170:ASP:H	1:C:236:GLN:CD	2.13	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:335:ILE:HD11	1:B:371:TYR:N	2.25	0.51
1:F:46:THR:CG2	1:F:147:LEU:HB2	2.41	0.51
1:B:204:VAL:HB	1:C:429:VAL:HG21	1.93	0.51
1:D:21:HIS:HE1	1:D:197:GLN:HG3	1.75	0.51
1:F:170:ASP:H	1:F:236:GLN:HE22	1.58	0.51
1:C:392:ILE:O	1:C:421:LEU:HD12	2.11	0.51
1:E:462:ILE:HB	1:E:467:LEU:HD21	1.92	0.51
1:E:128:GLY:O	1:F:386:LEU:HG	2.09	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:C:225:GLU:HA	1:C:225:GLU:OE1	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:E:62:TYR:CE2	1:F:427:ASN:HB3	2.44	0.51
1:C:378:GLY:O	1:C:433:GLN:HA	2.11	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:D:469:ASN:ND2	1:F:240:VAL:HG13	2.26	0.51
1:B:240:VAL:HG11	1:B:244:LEU:HD12	1.92	0.51
1:A:14:LEU:HD23	1:A:423:VAL:O	2.10	0.51
1:D:126:PRO:HB2	1:D:129:VAL:CG2	2.40	0.51
1:A:18:GLU:CA	1:A:33:TRP:HE1	2.24	0.51
1:D:57:LEU:HD12	1:D:133:THR:O	2.11	0.51
1:B:357:LEU:HD23	1:B:449:ASN:ND2	2.25	0.51
1:A:462:ILE:HG22	1:A:466:VAL:HB	1.91	0.51
1:A:480:GLN:NE2	1:A:480:GLN:HA	2.24	0.51
1:E:227:LEU:HA	1:F:471:TYR:HD2	1.75	0.51
1:A:69:ILE:HG22	1:A:143:ALA:HB1	1.93	0.51
1:C:223:THR:O	1:C:227:LEU:HD22	2.11	0.51
1:B:164:TYR:CD1	1:B:169:PRO:HG3	2.45	0.51
1:A:166:ALA:HB2	1:B:471:TYR:CZ	2.45	0.51
1:C:27:GLY:HA3	1:C:237:ILE:HG22	1.92	0.51
1:A:344:TYR:CE1	1:F:233:GLU:HB2	2.46	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:C:338:PRO:HG3	1:C:350:ARG:NH1	2.21	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:VAL:HG22	1:F:430:VAL:HG23	1.92	0.50
1:D:475:GLN:O	1:D:479:ARG:HG2	2.11	0.50
1:A:475:GLN:CG	1:A:479:ARG:HH12	2.23	0.50
1:B:408:GLY:C	1:B:409:ASN:HD22	2.14	0.50
1:F:144:ILE:N	1:F:144:ILE:HD12	2.26	0.50
1:B:200:GLU:OE1	1:B:200:GLU:N	2.44	0.50
1:F:40:LEU:N	1:F:40:LEU:HD12	2.26	0.50
1:A:76:GLY:HA2	1:A:136:THR:H	1.76	0.50
1:D:115:ARG:H	1:D:115:ARG:CD	2.17	0.50
1:C:221:GLU:O	1:C:224:ALA:HB3	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:A:134:TYR:OH	1:A:243:GLY:HA2	2.12	0.50
1:F:220:ASN:OD1	1:F:222:ASP:HB2	2.11	0.50
1:F:114:ILE:HD12	1:F:132:TRP:HZ2	1.74	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:D:8:GLU:O	1:D:42:CYS:HB2	2.11	0.50
1:C:79:GLY:HA3	1:C:132:TRP:CE2	2.47	0.50
1:B:134:TYR:CZ	1:B:244:LEU:HD13	2.46	0.50
1:C:213:LEU:HD12	1:C:217:PHE:CE1	2.46	0.50
1:C:418:ARG:HG3	1:C:418:ARG:HH21	1.76	0.50
1:B:404:VAL:HA	1:B:409:ASN:O	2.12	0.50
1:D:473:LEU:HD21	1:F:226:LYS:HB2	1.94	0.50
1:D:219:THR:OG1	1:D:220:ASN:N	2.44	0.50
1:E:157:ASP:OD2	1:E:159:ASN:HB2	2.11	0.50
1:F:236:GLN:N	1:F:236:GLN:OE1	2.39	0.50
1:B:345:ASN:CG	1:B:348:ALA:HB3	2.31	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:F:474:GLY:O	1:F:478:VAL:HG23	2.11	0.50
1:C:114:ILE:HD12	1:C:132:TRP:CZ2	2.47	0.50
1:C:57:LEU:HD22	1:C:240:VAL:HG22	1.94	0.50
1:E:326:ILE:O	1:E:329:MET:HG2	2.12	0.50
1:B:34:ASN:HD21	1:B:175:GLU:HB3	1.76	0.50
1:F:385:ASN:HD21	1:F:445:LYS:CE	2.25	0.50
1:C:36:GLN:HE21	1:C:175:GLU:HB2	1.76	0.50
1:C:479:ARG:HG2	1:C:479:ARG:HH11	1.77	0.50
1:A:379:ILE:HB	1:A:491:VAL:O	2.12	0.50

Continued on next page...

Continued from previous page...

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:E:476:SER:O	1:E:479:ARG:HB2	2.11	0.50
1:D:389:ASN:ND2	1:F:155:GLN:HB3	2.27	0.50
1:F:65:TYR:CE1	1:F:149:THR:HG22	2.47	0.50
1:D:66:PRO:HG3	1:D:151:ASN:ND2	2.26	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:E:372:VAL:HB	1:E:441:TYR:CE1	2.47	0.50
1:C:9:CYS:C	1:C:11:LEU:H	2.16	0.50
1:A:226:LYS:HE3	1:A:231:ASP:OD1	2.11	0.50
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:B:67:GLN:O	1:B:124:VAL:HA	2.12	0.49
1:D:402:ARG:HG3	1:D:402:ARG:HH11	1.76	0.49
1:F:50:ARG:NH2	1:F:67:GLN:NE2	2.57	0.49
1:A:331:LEU:O	1:A:359:LEU:HD21	2.12	0.49
1:B:70:ILE:CG2	1:B:144:ILE:HB	2.42	0.49
1:B:17:LEU:HB2	1:B:421:LEU:HB3	1.94	0.49
1:E:205:LEU:HD21	1:F:455:ILE:HD13	1.93	0.49
1:D:404:VAL:HG13	1:D:409:ASN:O	2.13	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:B:374:LEU:HD11	1:B:378:GLY:O	2.12	0.49
1:A:124:VAL:HG11	1:A:365:PHE:CD2	2.47	0.49
1:F:386:LEU:N	1:F:386:LEU:HD12	2.27	0.49
1:F:59:LEU:HD13	1:F:167:GLY:HA3	1.94	0.49
1:E:247:ILE:N	1:E:247:ILE:HD13	2.17	0.49
1:C:386:LEU:HD13	1:C:451:VAL:HG23	1.93	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:396:ARG:C	1:C:396:ARG:HD2	2.33	0.49
1:A:480:GLN:CD	1:A:484:GLN:HG3	2.32	0.49
1:D:146:LEU:HB2	1:D:444:PHE:CD2	2.48	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:E:349:GLY:O	1:E:490:LEU:HD13	2.11	0.49
1:A:247:ILE:N	1:A:247:ILE:HD12	2.27	0.49
1:B:109:ASP:HA	1:C:483:TYR:OH	2.12	0.49
1:D:68:MET:HB2	1:D:367:LEU:HD13	1.94	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

Continued on next page...

Continued from previous page...

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:E:88:THR:O	1:E:110:SER:HA	2.13	0.49
1:B:363:ARG:HA	1:B:448:HIS:CB	2.43	0.49
1:B:396:ARG:HA	1:B:418:ARG:CD	2.43	0.49
1:A:155:GLN:HB3	1:B:389:ASN:ND2	2.28	0.49
1:F:46:THR:CG2	1:F:147:LEU:HD12	2.42	0.49
1:A:329:MET:HG3	1:A:329:MET:O	2.11	0.49
1:C:34:ASN:HD22	1:C:35:SER:H	1.59	0.49
1:C:376:ARG:HB2	1:C:376:ARG:NH1	2.28	0.49
1:B:402:ARG:HG3	1:B:402:ARG:HH11	1.78	0.49
1:C:404:VAL:HA	1:C:409:ASN:O	2.13	0.49
1:C:236:GLN:N	1:C:236:GLN:OE1	2.46	0.49
1:E:57:LEU:HD13	1:E:57:LEU:C	2.33	0.49
1:C:385:ASN:HD21	1:C:445:LYS:CE	2.26	0.49
1:E:46:THR:HG23	1:E:147:LEU:HD12	1.94	0.49
1:A:72:VAL:HG22	1:A:142:VAL:O	2.13	0.49
1:A:166:ALA:HB2	1:B:471:TYR:CE2	2.48	0.49
1:F:401:VAL:HG21	1:F:416:LEU:HD23	1.95	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:F:45:VAL:HG21	1:F:146:LEU:HD21	1.94	0.49
1:D:357:LEU:N	1:D:357:LEU:HD12	2.27	0.49
1:F:394:VAL:HG21	1:F:416:LEU:HG	1.94	0.48
1:A:471:TYR:HE2	1:C:205:LEU:HD12	1.79	0.48
1:F:409:ASN:HD22	1:F:409:ASN:N	2.11	0.48
1:A:159:ASN:HB3	1:A:176:THR:CG2	2.41	0.48
1:F:400:ARG:O	1:F:432:GLU:HA	2.13	0.48
1:A:46:THR:CG2	1:A:147:LEU:HB2	2.43	0.48
1:F:31:GLU:OE1	1:F:49:LYS:HD2	2.12	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:328:THR:HG23	1:F:329:MET:N	2.22	0.48
1:B:67:GLN:HB2	1:B:125:ILE:HB	1.95	0.48
1:A:481:LEU:CD2	1:C:217:PHE:HB3	2.42	0.48
1:B:383:HIS:HB3	1:B:454:TYR:HB3	1.96	0.48
1:A:234:ARG:HB3	1:A:238:VAL:HG12	1.95	0.48
1:F:218:ASN:ND2	1:F:218:ASN:N	2.61	0.48
1:A:475:GLN:HG2	1:A:479:ARG:HH22	1.78	0.48
1:A:240:VAL:HG13	1:B:469:ASN:ND2	2.29	0.48
1:E:398:LYS:HE2	1:E:415:GLU:OE1	2.12	0.48
1:E:22:ARG:HH11	1:E:22:ARG:HB3	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:LEU:CD1	1:F:465:GLU:HB3	2.42	0.48
1:D:469:ASN:HD21	1:F:240:VAL:HG13	1.78	0.48
1:F:134:TYR:CE1	1:F:244:LEU:HD13	2.49	0.48
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:A:337:ARG:HH11	1:A:337:ARG:HG3	1.78	0.48
1:F:123:LEU:HD23	1:F:332:HIS:CB	2.40	0.48
1:D:47:VAL:HG12	1:D:48:SER:N	2.28	0.48
1:A:475:GLN:HG2	1:A:479:ARG:HH12	1.78	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:D:9:CYS:C	1:D:11:LEU:H	2.16	0.48
1:E:486:ASN:HD21	1:E:491:VAL:CG2	2.20	0.48
1:C:350:ARG:NH2	1:C:350:ARG:HG3	2.27	0.48
1:A:12:ASN:O	1:A:411:VAL:HG12	2.14	0.48
1:B:65:TYR:OH	1:B:147:LEU:HD13	2.13	0.48
1:A:454:TYR:HD1	1:A:456:LYS:HB2	1.77	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:57:LEU:HD22	1:C:240:VAL:CG2	2.43	0.48
1:C:40:LEU:HD12	1:C:45:VAL:HG23	1.94	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:F:337:ARG:HH21	1:F:337:ARG:HG3	1.78	0.48
1:B:387:ASN:CA	1:B:426:GLN:HE21	2.27	0.48
1:B:374:LEU:HD12	1:B:434:GLY:HA3	1.95	0.48
1:D:325:ASN:N	1:D:325:ASN:ND2	2.62	0.48
1:D:205:LEU:HD21	1:E:455:ILE:HD13	1.96	0.48
1:A:348:ALA:O	1:A:374:LEU:HA	2.14	0.48
1:D:51:THR:HA	1:D:141:VAL:O	2.14	0.48
1:D:21:HIS:CE1	1:D:197:GLN:HG3	2.49	0.48
1:A:87:GLU:O	1:A:88:THR:C	2.53	0.48
1:B:335:ILE:CD1	1:B:371:TYR:HB2	2.44	0.47
1:A:326:ILE:HA	1:A:329:MET:HE3	1.96	0.47
1:C:62:TYR:HD1	1:C:130:PRO:HB3	1.78	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: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:F:170:ASP:H	1:F:236:GLN:NE2	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HD3	1:B:396:ARG:C	2.34	0.47
1:C:392:ILE:HG23	1:C:441:TYR:CD2	2.50	0.47
1:C:111:HIS:CD2	1:C:111:HIS:H	2.32	0.47
1:E:75:LYS:CB	1:E:118:ASN:HA	2.42	0.47
1:A:402:ARG:NH1	1:C:212:PHE:HE2	2.12	0.47
1:A:392:ILE:O	1:A:421:LEU:HD12	2.15	0.47
1:E:5:LYS:HB3	1:E:6:PHE:H	1.51	0.47
1:C:396:ARG:HH11	1:C:396:ARG:HG3	1.79	0.47
1:C:362:LEU:HD22	1:C:367:LEU:O	2.14	0.47
1:E:405:ASN:OD1	1:E:407:GLN:HB2	2.14	0.47
1:E:61:SER:HB3	1:E:164:TYR:CD2	2.49	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:E:392:ILE:HG23	1:E:441:TYR:CD2	2.49	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:F:480:GLN:HA	1:F:480:GLN:HE21	1.78	0.47
1:D:476:SER:O	1:D:479:ARG:HB2	2.15	0.47
1:A:351:ILE:HG23	1:A:372:VAL:HG22	1.96	0.47
1:E:394:VAL:HA	1:E:441:TYR:HB3	1.97	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:B:387:ASN:ND2	1:B:387:ASN:H	2.07	0.47
1:C:112:GLN:O	1:C:114:ILE:N	2.47	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:394:VAL:HB	1:A:418:ARG:HA	1.96	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:D:78:ILE:HG23	1:D:78:ILE:O	2.14	0.47
1:F:334:ASN:HD22	1:F:337:ARG:H	1.59	0.47
1:F:170:ASP:O	1:F:171:ILE:C	2.52	0.47
1:B:426:GLN:HG2	1:B:427:ASN:N	2.29	0.47
1:F:148:ASP:OD2	1:F:151:ASN:HB2	2.14	0.47
1:A:47:VAL:HG12	1:A:48:SER:N	2.30	0.47
1:E:394:VAL:HG21	1:E:416:LEU:HG	1.96	0.47
1:A:380:TYR:HB3	1:A:432:GLU:H	1.80	0.47
1:D:56:GLY:O	1:D:134:TYR:HA	2.15	0.47
1:A:83:PRO:HB3	1:B:453:SER:OG	2.13	0.47
1:B:159:ASN:HD22	1:B:176:THR:CG2	2.12	0.47
1:F:454:TYR:HD1	1:F:456:LYS:HB3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:LEU:HB3	1:B:477:GLN:HB2	1.96	0.47
1:B:387:ASN:ND2	1:B:387:ASN:N	2.63	0.47
1:B:388:ALA:H	1:B:426:GLN:HG3	1.80	0.47
1:A:210:LYS:HD3	1:A:225:GLU:HG2	1.97	0.47
1:A:144:ILE:HG12	1:A:393:TYR:CE2	2.50	0.47
1:C:6:PHE:CD2	1:C:6:PHE:N	2.81	0.47
1:F:40:LEU:HD12	1:F:40:LEU:H	1.80	0.47
1:C:401:VAL:HG13	1:C:432:GLU:HG3	1.97	0.47
1:C:340:ARG:H	1:C:340:ARG:HD2	1.80	0.47
1:E:489:PRO:O	1:E:491:VAL:HG23	2.15	0.47
1:E:107:LEU:HA	1:F:479:ARG:HH21	1.79	0.47
1:E:228:ARG:NH1	1:E:228:ARG:HB3	2.30	0.47
1:C:22:ARG:NH1	1:C:31:GLU:HG2	2.29	0.47
1:B:437:GLN:HA	1:B:437:GLN:NE2	2.30	0.47
1:B:60:PRO:HG3	1:B:132:TRP:HB3	1.97	0.47
1:A:363:ARG:CZ	1:A:363:ARG:O	2.64	0.46
1:B:134:TYR:CE2	1:B:244:LEU:HD13	2.51	0.46
1:A:22:ARG:NH2	1:A:29:LEU:HD11	2.31	0.46
1:F:392:ILE:HG23	1:F:441:TYR:CD2	2.51	0.46
1:B:398:LYS:N	1:B:439:LEU:HD13	2.30	0.46
1:A:396:ARG:HG2	1:A:396:ARG:NH1	2.29	0.46
1:E:223:THR:O	1:E:227:LEU:HG	2.15	0.46
1:D:223:THR:OG1	1:E:477:GLN:NE2	2.48	0.46
1:B:371:TYR:OH	1:B:440:GLU:HB3	2.15	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:B:33:TRP:CD2	1:B:421:LEU:HD22	2.51	0.46
1:B:382:PRO:HB2	1:B:455:ILE:HD12	1.98	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:E:244:LEU:HD21	1:F:466:VAL:HG22	1.98	0.46
1:C:114:ILE:HG22	1:C:115:ARG:N	2.29	0.46
1:D:336:ALA:HA	1:D:371:TYR:CD1	2.50	0.46
1:C:394:VAL:HG22	1:C:420:GLN:O	2.16	0.46
1:D:388:ALA:HA	1:F:155:GLN:OE1	2.16	0.46
1:D:206:SER:C	1:D:208:PHE:H	2.19	0.46
1:E:418:ARG:HH21	1:E:418:ARG:HG2	1.81	0.46
1:B:15:ASN:ND2	1:B:15:ASN:N	2.63	0.46
1:C:225:GLU:OE1	1:C:228:ARG:HD3	2.15	0.46
1:B:338:PRO:HG3	1:B:350:ARG:NH2	2.30	0.46
1:A:50:ARG:HH22	1:A:67:GLN:HE22	1.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:C	1:B:57:LEU:HD23	2.36	0.46
1:B:174:PRO:C	1:B:176:THR:H	2.18	0.46
1:D:171:ILE:HG21	1:D:174:PRO:HA	1.97	0.46
1:F:171:ILE:N	1:F:171:ILE:HD12	2.23	0.46
1:B:46:THR:HG23	1:B:147:LEU:HD12	1.96	0.46
1:D:235:LYS:N	1:D:235:LYS:HD2	2.31	0.46
1:D:8:GLU:OE2	1:D:8:GLU:N	2.48	0.46
1:B:20:ASP:O	1:B:21:HIS:HB2	2.16	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:D:36:GLN:NE2	1:D:178:GLN:NE2	2.64	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:D:70:ILE:HG22	1:D:144:ILE:O	2.16	0.46
1:C:376:ARG:HG3	1:C:376:ARG:O	2.15	0.46
1:F:108:GLN:O	1:F:108:GLN:HG2	2.16	0.46
1:F:108:GLN:N	1:F:108:GLN:OE1	2.49	0.46
1:C:351:ILE:CG2	1:C:372:VAL:HG22	2.46	0.45
1:B:387:ASN:O	1:B:388:ALA:HB2	2.16	0.45
1:C:57:LEU:HD12	1:C:133:THR:O	2.16	0.45
1:F:240:VAL:HG21	1:F:244:LEU:HD11	1.98	0.45
1:C:169:PRO:HD2	1:C:202:GLY:HA2	1.98	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:213:LEU:HD22	1:C:213:LEU:N	2.30	0.45
1:B:376:ARG:C	1:B:378:GLY:H	2.18	0.45
1:B:460:ARG:CZ	1:B:487:SER:HA	2.46	0.45
1:D:455:ILE:CD1	1:F:205:LEU:HD21	2.45	0.45
1:A:71:VAL:O	1:A:119:GLU:HA	2.15	0.45
1:B:425:PRO:HB2	1:B:428:PHE:CG	2.51	0.45
1:E:201:GLY:HA2	1:F:407:GLN:O	2.16	0.45
1:E:471:TYR:HB2	1:E:473:LEU:HG	1.97	0.45
1:E:388:ALA:HB2	1:E:447:HIS:HB2	1.97	0.45
1:F:159:ASN:HB3	1:F:176:THR:CG2	2.45	0.45
1:A:340:ARG:NE	1:A:350:ARG:HB2	2.31	0.45
1:E:326:ILE:C	1:E:326:ILE:HD13	2.36	0.45
1:D:157:ASP:HB2	1:E:5:LYS:O	2.16	0.45
1:A:163:PHE:CE1	1:B:406:CSD:HB2	2.52	0.45
1:F:479:ARG:HH11	1:F:479:ARG:HG2	1.81	0.45
1:C:417:ARG:HG2	1:C:417:ARG:NH1	2.31	0.45
1:B:228:ARG:NH1	1:B:228:ARG:HB3	2.31	0.45

Continued on next page...

Continued from previous page...

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:340:ARG:HH11	1:A:340:ARG:CB	2.17	0.45
1:C:148:ASP:OD2	1:C:367:LEU:HD21	2.17	0.45
1:C:418:ARG:NH2	1:C:418:ARG:HG3	2.32	0.45
1:A:384:TRP:O	1:A:452:SER:HB2	2.17	0.45
1:F:222:ASP:O	1:F:226:LYS:HG2	2.16	0.45
1:A:54:ARG:HG3	1:A:54:ARG:HH11	1.82	0.45
1:F:76:GLY:HA2	1:F:136:THR:HG23	1.98	0.45
1:E:246:VAL:HG11	1:F:463:PRO:HB3	1.98	0.45
1:A:155:GLN:HB3	1:B:389:ASN:HD21	1.81	0.45
1:C:146:LEU:HD13	1:C:146:LEU:C	2.37	0.45
1:A:402:ARG:O	1:A:430:VAL:HG23	2.15	0.45
1:F:343:PHE:O	1:F:350:ARG:HA	2.17	0.45
1:A:7:ASN:N	1:A:7:ASN:HD22	2.14	0.45
1:C:471:TYR:CB	1:C:473:LEU:HD13	2.47	0.45
1:D:34:ASN:C	1:D:36:GLN:H	2.20	0.45
1:C:67:GLN:HE21	1:C:147:LEU:HD22	1.80	0.45
1:B:480:GLN:O	1:B:484:GLN:N	2.49	0.45
1:C:391:VAL:O	1:C:391:VAL:HG23	2.17	0.45
1:B:454:TYR:CE1	1:B:457:ASP:HB2	2.52	0.45
1:E:480:GLN:O	1:E:484:GLN:HB2	2.17	0.45
1:E:471:TYR:O	1:E:472:ASN:C	2.55	0.45
1:A:446:THR:O	1:A:447:HIS:HB2	2.17	0.45
1:D:81:ALA:HB3	1:D:130:PRO:HB2	1.98	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:C:22:ARG:NH1	1:C:22:ARG:HB3	2.32	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:F:34:ASN:HB3	1:F:37:HIS:CD2	2.52	0.45
1:B:247:ILE:HD12	1:B:247:ILE:N	2.32	0.45
1:B:70:ILE:HG23	1:B:70:ILE:O	2.17	0.45
1:F:349:GLY:HA3	1:F:373:VAL:O	2.17	0.45
1:F:72:VAL:HG11	1:F:144:ILE:HD13	1.99	0.45
1:B:8:GLU:O	1:B:42:CYS:HB2	2.16	0.45
1:F:424:VAL:O	1:F:425:PRO:O	2.35	0.45
1:D:46:THR:HG23	1:D:147:LEU:HB2	1.99	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:F:144:ILE:HG12	1:F:393:TYR:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

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:A:229:SER:C	1:A:231:ASP:H	2.20	0.45
1:E:114:ILE:HD12	1:E:132:TRP:CZ2	2.52	0.45
1:D:30:ILE:HD12	1:D:236:GLN:HG3	1.97	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: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:A:325:ASN:HA	1:A:328:THR:CG2	2.47	0.44
1:D:461:ALA:O	1:F:111:HIS:HB2	2.17	0.44
1:F:77:ALA:HB2	1:F:116:HIS:CE1	2.52	0.44
1:E:165:LEU:HD13	1:F:458:VAL:HG11	1.99	0.44
1:C:337:ARG:CA	1:C:337:ARG:HH21	2.29	0.44
1:F:334:ASN:ND2	1:F:337:ARG:N	2.61	0.44
1:C:404:VAL:CG1	1:C:408:GLY:HA2	2.46	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:B:6:PHE:N	1:B:6:PHE:CD1	2.84	0.44
1:D:171:ILE:HG21	1:D:177:MET:HG3	1.99	0.44
1:A:385:ASN:HD21	1:A:445:LYS:HE2	1.82	0.44
1:D:402:ARG:HG2	1:D:413:ASP:OD1	2.17	0.44
1:A:240:VAL:HG11	1:A:244:LEU:HD12	1.99	0.44
1:C:147:LEU:O	1:C:149:THR:N	2.49	0.44
1:C:67:GLN:O	1:C:124:VAL:HA	2.16	0.44
1:D:403:VAL:O	1:D:411:VAL:HG22	2.18	0.44
1:D:240:VAL:HG22	1:E:469:ASN:ND2	2.33	0.44
1:B:401:VAL:HG11	1:B:422:LEU:CD2	2.48	0.44
1:E:47:VAL:HG12	1:E:48:SER:N	2.33	0.44
1:C:120:GLY:O	1:C:335:ILE:HG22	2.18	0.44
1:E:235:LYS:HB3	1:E:236:GLN:OE1	2.18	0.44
1:A:363:ARG:NE	1:A:448:HIS:CD2	2.86	0.44
1:A:65:TYR:HD1	1:A:154:ASN:HD22	1.66	0.44
1:D:354:LEU:HD12	1:D:358:THR:OG1	2.18	0.44
1:A:224:ALA:HA	1:A:227:LEU:CD1	2.43	0.44
1:D:15:ASN:N	1:D:15:ASN:HD22	2.16	0.44
1:C:23:VAL:O	1:C:29:LEU:HD12	2.16	0.44
1:A:491:VAL:HG12	1:A:492:ASN:H	1.82	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:SER:HA	1:C:359:LEU:O	2.18	0.44
1:B:158:GLN:N	1:B:158:GLN:OE1	2.50	0.44
1:D:340:ARG:HG2	1:D:340:ARG:O	2.18	0.44
1:F:247:ILE:HG22	1:F:248:SER:N	2.32	0.44
1:D:218:ASN:N	1:D:218:ASN:HD22	2.15	0.44
1:F:425:PRO:HG2	1:F:428:PHE:CE1	2.52	0.44
1:D:200:GLU:O	1:D:200:GLU:HG3	2.18	0.44
1:D:436:GLU:OE1	1:D:436:GLU:HA	2.18	0.44
1:F:113:LYS:HD3	1:F:115:ARG:HE	1.82	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:A:28:GLY:HA3	1:A:237:ILE:HG21	2.00	0.44
1:D:11:LEU:HD22	1:D:38:PRO:HB3	1.99	0.44
1:D:461:ALA:HA	1:F:87:GLU:OE1	2.17	0.44
1:C:200:GLU:OE1	1:C:200:GLU:N	2.50	0.44
1:D:228:ARG:CZ	1:D:228:ARG:HB3	2.48	0.44
1:F:456:LYS:NZ	1:F:486:ASN:ND2	2.65	0.44
1:D:148:ASP:OD2	1:D:151:ASN:HB2	2.18	0.44
1:A:13:ASN:C	1:A:14:LEU:HD12	2.38	0.44
1:C:405:ASN:HD22	1:C:411:VAL:CG1	2.31	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:A:69:ILE:CG2	1:A:143:ALA:HB1	2.47	0.44
1:D:163:PHE:CD2	1:E:406:CSD:HB2	2.52	0.44
1:B:7:ASN:ND2	1:B:10:GLN:NE2	2.66	0.43
1:D:146:LEU:HD21	1:D:391:VAL:HG11	2.00	0.43
1:B:234:ARG:HB3	1:B:238:VAL:HG12	1.99	0.43
1:A:22:ARG:CZ	1:A:29:LEU:HD11	2.48	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:F:398:LYS:NZ	1:F:398:LYS:CB	2.82	0.43
1:C:384:TRP:HH2	1:C:458:VAL:HG21	1.83	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:C:340:ARG:HH11	1:C:340:ARG:HG2	1.83	0.43
1:F:334:ASN:HB3	1:F:340:ARG:HH11	1.84	0.43
1:C:16:ALA:HA	1:C:421:LEU:O	2.18	0.43
1:B:124:VAL:HG13	1:B:124:VAL:O	2.18	0.43
1:A:22:ARG:NH1	1:A:22:ARG:CB	2.81	0.43
1:E:114:ILE:HD12	1:E:132:TRP:HZ2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:478:VAL:HG12	1:E:478:VAL:O	2.18	0.43
1:B:379:ILE:HG22	1:B:380:TYR:N	2.34	0.43
1:A:18:GLU:HA	1:A:33:TRP:HE1	1.83	0.43
1:C:38:PRO:HA	1:C:41:GLN:HB2	2.00	0.43
1:B:357:LEU:HD22	1:B:357:LEU:N	2.33	0.43
1:A:65:TYR:CE1	1:A:149:THR:HG22	2.53	0.43
1:D:399:GLY:HA3	1:D:439:LEU:HD22	1.99	0.43
1:F:244:LEU:N	1:F:244:LEU:HD12	2.34	0.43
1:B:401:VAL:HA	1:B:432:GLU:HB3	2.01	0.43
1:F:373:VAL:HG13	1:F:440:GLU:HG2	1.98	0.43
1:F:348:ALA:CB	1:F:490:LEU:HB3	2.49	0.43
1:B:228:ARG:HB3	1:B:228:ARG:CZ	2.49	0.43
1:C:121:ASP:OD2	1:C:332:HIS:HE1	2.01	0.43
1:B:335:ILE:HD11	1:B:371:TYR:H	1.84	0.43
1:B:47:VAL:HG12	1:B:48:SER:N	2.34	0.43
1:A:326:ILE:HA	1:A:329:MET:HE2	2.00	0.43
1:E:340:ARG:HH22	1:E:354:LEU:HD13	1.84	0.43
1:E:227:LEU:HA	1:F:471:TYR:CD2	2.53	0.43
1:A:240:VAL:HG11	1:A:244:LEU:CD1	2.48	0.43
1:C:471:TYR:HB2	1:C:473:LEU:HD13	1.99	0.43
1:F:230:PRO:HG2	1:F:231:ASP:H	1.82	0.43
1:F:53:ASN:HD22	1:F:53:ASN:N	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:H	1:C:387:ASN:ND2	2.17	0.43
1:F:46:THR:HG23	1:F:147:LEU:HB2	2.00	0.43
1:A:345:ASN:HD22	1:A:486:ASN:ND2	2.16	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:C:210:LYS:HE2	1:C:221:GLU:OE2	2.18	0.43
1:C:79:GLY:HA3	1:C:132:TRP:NE1	2.34	0.43
1:D:391:VAL:HG12	1:D:444:PHE:HB2	1.98	0.43
1:C:70:ILE:O	1:C:70:ILE:HG23	2.19	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:A:64:PRO:O	1:A:154:ASN:HA	2.18	0.43
1:D:340:ARG:HG3	1:D:340:ARG:HH11	1.83	0.43
1:C:219:THR:OG1	1:C:220:ASN:N	2.51	0.43
1:C:373:VAL:HG22	1:C:440:GLU:CG	2.41	0.43
1:D:489:PRO:HG2	1:D:490:LEU:H	1.83	0.43
1:F:395:THR:C	1:F:418:ARG:HG3	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:CD1	1:C:386:LEU:H	2.31	0.43
1:F:362:LEU:HB3	1:F:367:LEU:O	2.19	0.43
1:C:367:LEU:CD2	1:C:446:THR:HA	2.44	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:F:122:VAL:O	1:F:332:HIS:HA	2.19	0.43
1:B:437:GLN:HA	1:B:437:GLN:HE21	1.83	0.43
1:A:64:PRO:HG2	1:A:65:TYR:CD1	2.54	0.43
1:A:340:ARG:CD	1:A:350:ARG:HB2	2.49	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:B:61:SER:HA	1:B:163:PHE:O	2.18	0.43
1:A:78:ILE:HG13	1:A:133:THR:HG22	2.00	0.43
1:F:213:LEU:H	1:F:213:LEU:HD22	1.83	0.43
1:C:34:ASN:HB3	1:C:37:HIS:CD2	2.53	0.43
1:E:22:ARG:CB	1:E:22:ARG:HH11	2.32	0.43
1:A:337:ARG:C	1:A:339:SER:H	2.23	0.42
1:E:236:GLN:H	1:E:236:GLN:CD	2.20	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:B:47:VAL:HA	1:B:145:SER:O	2.19	0.42
1:E:175:GLU:OE1	1:E:175:GLU:N	2.50	0.42
1:D:228:ARG:NH1	1:D:228:ARG:HB3	2.34	0.42
1:E:82:PHE:HB2	1:E:85:CYS:SG	2.59	0.42
1:A:387:ASN:O	1:A:388:ALA:HB2	2.18	0.42
1:C:87:GLU:HA	1:C:112:GLN:HA	2.01	0.42
1:B:86:PRO:O	1:B:113:LYS:HE3	2.19	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:B:79:GLY:O	1:B:131:TYR:HA	2.19	0.42
1:C:471:TYR:O	1:C:472:ASN:HB2	2.19	0.42
1:A:408:GLY:HA2	1:C:203:SER:O	2.19	0.42
1:E:376:ARG:O	1:E:377:ASN:CB	2.67	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:A:244:LEU:HD12	1:A:244:LEU:N	2.34	0.42
1:E:171:ILE:HG21	1:E:174:PRO:HA	2.01	0.42
1:E:73:GLN:HE21	1:E:142:VAL:HG11	1.84	0.42
1:B:169:PRO:HA	1:B:236:GLN:OE1	2.19	0.42
1:C:348:ALA:O	1:C:374:LEU:HA	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:HD12	1:C:40:LEU:CD2	2.49	0.42
1:B:366:GLY:HA2	1:B:448:HIS:H	1.84	0.42
1:E:22:ARG:CB	1:E:22:ARG:NH1	2.83	0.42
1:F:225:GLU:O	1:F:230:PRO:HD3	2.19	0.42
1:E:246:VAL:HG23	1:F:465:GLU:CD	2.40	0.42
1:C:151:ASN:OD1	1:C:152:PHE:N	2.52	0.42
1:E:14:LEU:HD13	1:E:411:VAL:HB	2.01	0.42
1:B:396:ARG:HA	1:B:418:ARG:HD2	2.02	0.42
1:A:46:THR:CG2	1:A:147:LEU:HD12	2.43	0.42
1:E:417:ARG:HG2	1:E:417:ARG:HH11	1.85	0.42
1:A:454:TYR:CD2	1:A:489:PRO:HB3	2.55	0.42
1:E:69:ILE:HB	1:E:123:LEU:HB2	2.00	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:A:7:ASN:N	1:A:7:ASN:ND2	2.66	0.42
1:B:133:THR:HG21	2:B:502:CO3:O1	2.20	0.42
1:C:148:ASP:CG	1:C:151:ASN:HB2	2.40	0.42
1:E:72:VAL:HG23	1:E:142:VAL:HG13	2.01	0.42
1:C:70:ILE:HG22	1:C:144:ILE:O	2.19	0.42
1:D:363:ARG:HH21	1:D:363:ARG:HG3	1.84	0.42
1:F:152:PHE:CD1	1:F:152:PHE:N	2.81	0.42
1:C:72:VAL:HG23	1:C:73:GLN:H	1.84	0.42
1:E:228:ARG:O	1:E:229:SER:C	2.57	0.42
1:C:405:ASN:OD1	1:C:406:CSD:N	2.53	0.42
1:C:326:ILE:CG2	1:C:327:CYS:N	2.82	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:146:LEU:C	1:A:146:LEU:HD13	2.40	0.42
1:A:148:ASP:OD1	1:A:367:LEU:HD21	2.19	0.42
1:D:350:ARG:HG3	1:D:350:ARG:HH21	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:E:72:VAL:HG22	1:E:142:VAL:O	2.20	0.42
1:C:363:ARG:HH21	1:C:448:HIS:CD2	2.38	0.42
1:A:430:VAL:HG22	1:A:431:ALA:N	2.34	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:D:234:ARG:HB3	1:D:238:VAL:HG12	2.00	0.42
1:C:7:ASN:O	1:C:9:CYS:N	2.53	0.42
1:B:392:ILE:HG23	1:B:441:TYR:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ASN:CG	1:D:10:GLN:HB2	2.40	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:C:148:ASP:HB2	1:C:367:LEU:HD11	2.01	0.42
1:F:134:TYR:CZ	1:F:244:LEU:HD13	2.55	0.42
1:A:402:ARG:O	1:A:430:VAL:HA	2.20	0.42
1:C:345:ASN:O	1:C:347:LYS:N	2.53	0.42
1:F:355:ASN:OD1	1:F:357:LEU:HB2	2.20	0.42
1:E:164:TYR:CD1	1:E:169:PRO:HG3	2.54	0.41
1:C:47:VAL:HG12	1:C:48:SER:H	1.85	0.41
1:D:402:ARG:HB2	1:F:208:PHE:HE1	1.84	0.41
1:F:72:VAL:CG1	1:F:144:ILE:HD13	2.50	0.41
1:E:31:GLU:OE1	1:E:49:LYS:HD3	2.19	0.41
1:A:376:ARG:HH12	1:A:436:GLU:HG2	1.85	0.41
1:E:111:HIS:HB2	1:F:461:ALA:O	2.19	0.41
1:D:25:SER:OG	1:D:237:ILE:HB	2.20	0.41
1:A:80:PHE:CD1	1:A:80:PHE:N	2.87	0.41
1:A:387:ASN:HD22	1:A:387:ASN:C	2.24	0.41
1:A:426:GLN:HG2	1:A:427:ASN:N	2.36	0.41
1:C:67:GLN:O	1:C:125:ILE:N	2.53	0.41
1:B:397:GLY:HA3	1:B:439:LEU:HA	2.02	0.41
1:B:151:ASN:OD1	1:B:153:ASN: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:51:THR:HA	1:A:141:VAL:O	2.20	0.41
1:A:12:ASN:O	1:A:411:VAL:HA	2.20	0.41
1:B:479:ARG:NE	1:B:483:TYR:HD2	2.17	0.41
1:B:337:ARG:HA	1:B:338:PRO:HD3	1.90	0.41
1:D:11:LEU:HD11	1:D:38:PRO:O	2.21	0.41
1:C:337:ARG:HB2	1:C:340:ARG:HE	1.86	0.41
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.85	0.41
1:A:386:LEU:CD1	1:A:452:SER:HA	2.50	0.41
1:E:46:THR:CG2	1:E:147:LEU:HD12	2.50	0.41
1:B:228:ARG:CB	1:B:228:ARG:NH1	2.84	0.41
1:F:398:LYS:NZ	1:F:398:LYS:HB2	2.36	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:B:176:THR:C	1:B:177:MET:HE2	2.41	0.41
1:B:156:LEU:CB	1:B:161:ARG:HH21	2.15	0.41
1:D:175:GLU:C	1:D:177:MET:H	2.23	0.41
1:B:68:MET:HA	1:B:123:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HA	1:B:130:PRO:HD3	1.91	0.41
1:B:234:ARG:CB	1:B:238:VAL:HG12	2.51	0.41
1:B:79:GLY:HA3	1:B:132:TRP:CE2	2.56	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:E:244:LEU:HD21	1:F:466:VAL:HG23	2.02	0.41
1:A:455:ILE:CD1	1:C:205:LEU:HD21	2.48	0.41
1:C:56:GLY:N	1:C:135:ASN:HB3	2.32	0.41
1:E:70:ILE:HD13	1:E:70:ILE:C	2.41	0.41
1:E:2:THR:HG22	1:E:5:LYS:HZ3	1.85	0.41
1:C:17:LEU:HD13	1:C:37:HIS:CD2	2.56	0.41
1:D:112:GLN:HE21	1:E:461:ALA:CB	2.32	0.41
1:B:363:ARG:HA	1:B:448:HIS:HB2	2.02	0.41
1:B:437:GLN:CA	1:B:437:GLN:HE21	2.33	0.41
1:F:89:PHE:CD1	1:F:110:SER:HB3	2.55	0.41
1:F:88:THR:HG22	1:F:89:PHE:N	2.35	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:A:397:GLY:O	1:A:398:LYS:HB2	2.19	0.41
1:F:335:ILE:HG12	1:F:335:ILE:O	2.21	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:B:379:ILE:CG2	1:B:380:TYR:N	2.84	0.41
1:F:59:LEU:HA	1:F:60:PRO:HD3	1.95	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:34:ASN:ND2	1:F:36:GLN:H	2.19	0.41
1:D:362:LEU:HD13	1:D:367:LEU:O	2.20	0.41
1:C:237:ILE:HG22	1:C:238:VAL:N	2.36	0.41
1:A:461:ALA:HA	1:C:87:GLU:CD	2.41	0.41
1:F:82:PHE:HB3	1:F:85:CYS:SG	2.61	0.41
1:D:366:GLY:HA2	1:D:448:HIS:N	2.34	0.41
1:D:437:GLN:N	1:D:437:GLN:NE2	2.67	0.41
1:F:390:SER:HB2	1:F:424:VAL:HB	2.02	0.41
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:A:34:ASN:ND2	1:A:36:GLN:H	2.19	0.41
1:F:328:THR:O	1:F:329:MET:C	2.59	0.41
1:C:75:LYS:O	1:C:141:VAL:HG21	2.20	0.41
1:B:208:PHE:CE2	1:C:382:PRO:HB3	2.56	0.41
1:A:326:ILE:C	1:A:326:ILE:HD13	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ILE:O	1:E:123:LEU:N	2.52	0.41
1:D:368:SER:HB2	1:D:447:HIS:O	2.21	0.41
1:C:14:LEU:HD12	1:C:14:LEU:N	2.36	0.41
1:D:206:SER:O	1:D:208:PHE:N	2.54	0.41
1:A:80:PHE:HE2	1:A:125:ILE:HD13	1.86	0.41
1:B:62:TYR:HE2	1:C:427:ASN:HB3	1.86	0.41
1:B:164:TYR:O	1:B:203:SER:HB2	2.20	0.41
1:A:454:TYR:CD1	1:A:456:LYS:HB2	2.55	0.41
1:B:456:LYS:HD2	1:B:485:GLY:CA	2.50	0.41
1:D:393:TYR:CE2	1:D:395:THR:HG22	2.56	0.41
1:A:62:TYR:CE1	1:A:163:PHE:HB2	2.56	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:E:228:ARG:HH11	1:E:228:ARG:CB	2.34	0.41
1:A:402:ARG:HG2	1:A:413:ASP:CG	2.42	0.40
1:A:54:ARG:HH11	1:A:138:ASP:HA	1.86	0.40
1:E:82:PHE:CE1	1:E:129:VAL:HG11	2.55	0.40
1:D:63:SER:C	1:D:65:TYR:H	2.23	0.40
1:F:126:PRO:HA	1:F:127:PRO:HD3	1.90	0.40
1:E:491:VAL:HG12	1:E:492:ASN:N	2.36	0.40
1:B:15:ASN:H	1:B:39:GLU:CD	2.23	0.40
1:A:480:GLN:HE21	1:A:480:GLN:CA	2.27	0.40
1:C:405:ASN:ND2	1:C:409:ASN:HB2	2.36	0.40
1:A:19:PRO:HB3	1:A:31:GLU:HB3	2.02	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:C:22:ARG:HH11	1:C:22:ARG:HB3	1.87	0.40
1:A:81:ALA:HB1	1:B:458:VAL:HG13	2.02	0.40
1:B:212:PHE:HE2	1:C:379:ILE:HG21	1.86	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:HD22	1:C:387:ASN:N	2.19	0.40
1:F:46:THR:HG22	1:F:147:LEU:HB2	2.03	0.40
1:B:50:ARG:HH12	1:B:67:GLN:NE2	2.20	0.40
1:C:14:LEU:C	1:C:15:ASN:ND2	2.72	0.40
1:E:430:VAL:CG2	1:E:431:ALA:N	2.84	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:D:89:PHE:HD2	1:D:110:SER:HA	1.86	0.40
1:B:154:ASN:ND2	1:B:157:ASP:O	2.55	0.40
1:F:468:SER:O	1:F:472:ASN:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:ASN:N	1:F:121:ASP:OD2	2.51	0.40
1:D:18:GLU:O	1:D:19:PRO:C	2.60	0.40
1:C:18:GLU:HA	1:C:33:TRP:HE1	1.85	0.40
1:B:471:TYR:O	1:B:472:ASN:CB	2.68	0.40
1:B:51:THR:HA	1:B:141:VAL:O	2.21	0.40
1:A:472:ASN:O	1:C:226:LYS:HD2	2.21	0.40
1:B:66:PRO:HG2	1:B:148:ASP:HB3	2.02	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: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:228:ARG:HH11	1:A:228:ARG:HB2	1.87	0.40
1:A:333:GLU:HG3	1:A:334:ASN:N	2.36	0.40
1:A:159:ASN:OD1	1:B:7:ASN:ND2	2.55	0.40
1:B:14:LEU:HD12	1:B:14:LEU:N	2.36	0.40
1:A:227:LEU:HA	1:B:471:TYR:CD2	2.56	0.40
1:E:75:LYS:HD2	1:E:75:LYS:O	2.22	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:115:ARG:HH21	1:E:115:ARG:HG2	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%)	7 24
1	B	363/493 (74%)	297 (82%)	54 (15%)	12 (3%)	5 16
1	C	361/493 (73%)	291 (81%)	51 (14%)	19 (5%)	2 7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	368/493 (75%)	307 (83%)	54 (15%)	7 (2%)	10 32
1	E	371/493 (75%)	311 (84%)	54 (15%)	6 (2%)	12 38
1	F	368/493 (75%)	311 (84%)	44 (12%)	13 (4%)	4 15
All	All	2196/2958 (74%)	1819 (83%)	311 (14%)	66 (3%)	5 18

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

Continued on next page...

Continued from previous page...

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%)	35 70
1	B	322/435 (74%)	313 (97%)	9 (3%)	51 84
1	C	320/435 (74%)	305 (95%)	15 (5%)	32 67
1	D	327/435 (75%)	314 (96%)	13 (4%)	38 73
1	E	330/435 (76%)	318 (96%)	12 (4%)	42 76
1	F	327/435 (75%)	316 (97%)	11 (3%)	44 78
All	All	1950/2610 (75%)	1876 (96%)	74 (4%)	40 74

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Some 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	A	406	1	3,7,8	0.61	0	3,8,10	1.35	0
1	CSD	B	406	1	3,7,8	0.63	0	3,8,10	1.53	0
1	CSD	C	406	1	3,7,8	0.55	0	3,8,10	1.29	0
1	CSD	D	406	1	3,7,8	0.61	0	3,8,10	1.49	0
1	CSD	E	406	1	3,7,8	0.55	0	3,8,10	1.37	0
1	CSD	F	406	1	3,7,8	0.60	0	3,8,10	1.56	1 (33%)

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	A	406	1	-	0/2/6/8	0/0/0/0
1	CSD	B	406	1	-	0/2/6/8	0/0/0/0
1	CSD	C	406	1	-	0/2/6/8	0/0/0/0
1	CSD	D	406	1	-	0/2/6/8	0/0/0/0
1	CSD	E	406	1	-	0/2/6/8	0/0/0/0
1	CSD	F	406	1	-	0/2/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	406	CSD	O-C-CA	-2.04	120.18	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	B	502	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	C	503	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	D	504	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	E	505	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	F	506	-	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO3	A	501	-	-	0/0/0/0	0/0/0/0
2	CO3	B	502	-	-	0/0/0/0	0/0/0/0
2	CO3	C	503	-	-	0/0/0/0	0/0/0/0
2	CO3	D	504	-	-	0/0/0/0	0/0/0/0
2	CO3	E	505	-	-	0/0/0/0	0/0/0/0
2	CO3	F	506	-	-	0/0/0/0	0/0/0/0

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

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	373/493 (75%)	0.08	18 (4%) 34 23	13, 37, 54, 62	0
1	B	371/493 (75%)	0.03	13 (3%) 48 35	6, 37, 56, 63	0
1	C	369/493 (74%)	0.28	28 (7%) 17 9	7, 39, 54, 66	0
1	D	376/493 (76%)	-0.38	7 (1%) 70 59	6, 19, 46, 57	0
1	E	379/493 (76%)	-0.43	3 (0%) 87 81	6, 13, 43, 58	0
1	F	376/493 (76%)	-0.41	3 (0%) 87 81	6, 18, 45, 57	0
All	All	2244/2958 (75%)	-0.14	72 (3%) 51 39	6, 28, 52, 66	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	THR	6.2
1	B	437	GLN	4.9
1	C	89	PHE	4.6
1	C	435	GLY	4.4
1	C	226	LYS	3.8
1	A	88	THR	3.7
1	C	328	THR	3.6
1	D	338	PRO	3.6
1	C	246	VAL	3.6
1	D	179	GLN	3.6
1	D	197	GLN	3.4
1	A	200	GLU	3.4
1	E	89	PHE	3.3
1	A	342	ASP	3.2
1	A	463	PRO	3.2
1	B	485	GLY	3.1
1	B	88	THR	3.0
1	C	358	THR	3.0
1	B	89	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	200	GLU	2.9
1	A	12	ASN	2.8
1	A	340	ARG	2.8
1	C	487	SER	2.8
1	C	111	HIS	2.8
1	C	373	VAL	2.8
1	C	437	GLN	2.8
1	C	245	SER	2.7
1	B	483	TYR	2.7
1	D	484	GLN	2.7
1	A	177	MET	2.7
1	C	227	LEU	2.7
1	F	107	LEU	2.7
1	A	6	PHE	2.7
1	F	179	GLN	2.6
1	C	114	ILE	2.6
1	C	493	PRO	2.5
1	C	244	LEU	2.5
1	E	107	LEU	2.5
1	A	471	TYR	2.5
1	A	178	GLN	2.5
1	D	178	GLN	2.5
1	A	338	PRO	2.5
1	B	438	GLY	2.5
1	C	334	ASN	2.5
1	D	108	GLN	2.5
1	C	230	PRO	2.4
1	C	140	PRO	2.4
1	A	89	PHE	2.4
1	B	377	ASN	2.4
1	B	86	PRO	2.4
1	A	244	LEU	2.4
1	C	371	TYR	2.3
1	A	331	LEU	2.3
1	C	338	PRO	2.3
1	A	248	SER	2.3
1	F	106	GLN	2.2
1	C	116	HIS	2.2
1	B	6	PHE	2.2
1	C	134	TYR	2.2
1	C	377	ASN	2.2
1	B	409	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	200	GLU	2.1
1	A	462	ILE	2.1
1	C	379	ILE	2.1
1	C	341	ALA	2.1
1	B	201	GLY	2.1
1	A	482	LYS	2.1
1	A	219	THR	2.1
1	E	4	SER	2.1
1	C	222	ASP	2.0
1	C	415	GLU	2.0
1	B	433	GLN	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. 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	CSD	B	406	8/9	0.94	0.14	-	39,44,63,73	0
1	CSD	A	406	8/9	0.91	0.16	-	30,41,46,53	0
1	CSD	D	406	8/9	0.96	0.10	-	5,13,23,38	0
1	CSD	C	406	8/9	0.88	0.16	-	31,38,58,62	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

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
2	CO3	B	502	4/4	0.88	0.22	4.20	12,22,39,45	0
2	CO3	A	501	4/4	0.88	0.24	1.57	14,35,39,41	0
3	MG	E	605	1/1	0.99	0.16	0.94	5,5,5,5	0
2	CO3	E	505	4/4	0.89	0.17	0.93	5,5,10,17	0
2	CO3	F	506	4/4	0.87	0.19	0.92	5,5,18,21	0
3	MG	D	604	1/1	0.96	0.16	-0.07	17,17,17,17	0
3	MG	B	602	1/1	0.91	0.21	-0.81	41,41,41,41	0
2	CO3	D	504	4/4	0.97	0.14	-0.82	5,19,20,21	0
2	CO3	C	503	4/4	0.91	0.15	-1.24	36,40,41,42	0
3	MG	F	606	1/1	0.97	0.14	-1.46	8,8,8,8	0
3	MG	C	603	1/1	0.93	0.13	-2.35	21,21,21,21	0
3	MG	A	601	1/1	0.94	0.08	-4.99	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.