Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:49 PM GMT

PDB ID	:	1VCW
Title	:	Crystal structure of DegS after backsoaking the activating peptide
Authors	:	Wilken, C.; Kitzing, K.; Kurzbauer, R.; Ehrmann, M.; Clausen, T.
Deposited on	:	2004-03-16
Resolution	:	3.05 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:

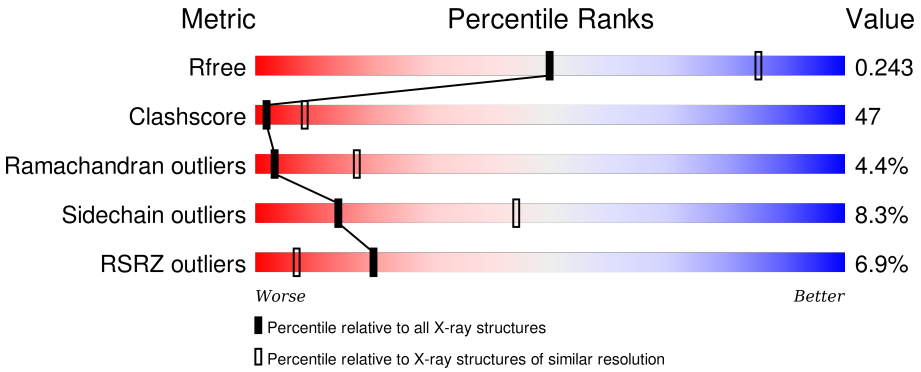
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	314	5% 41% 44% 7% • 7%
1	B	314	4% 41% 44% 6% • 7%
1	C	314	10% 40% 45% 6% • 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6384 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 Protease degS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2128	1329	380	414	5			
1	B	291	Total	C	N	O	S	51	0	0
			2128	1329	380	414	5			
1	C	291	Total	C	N	O	S	0	0	0
			2128	1329	380	414	5			

There are 3 discrepancies between the modelled and reference sequences:

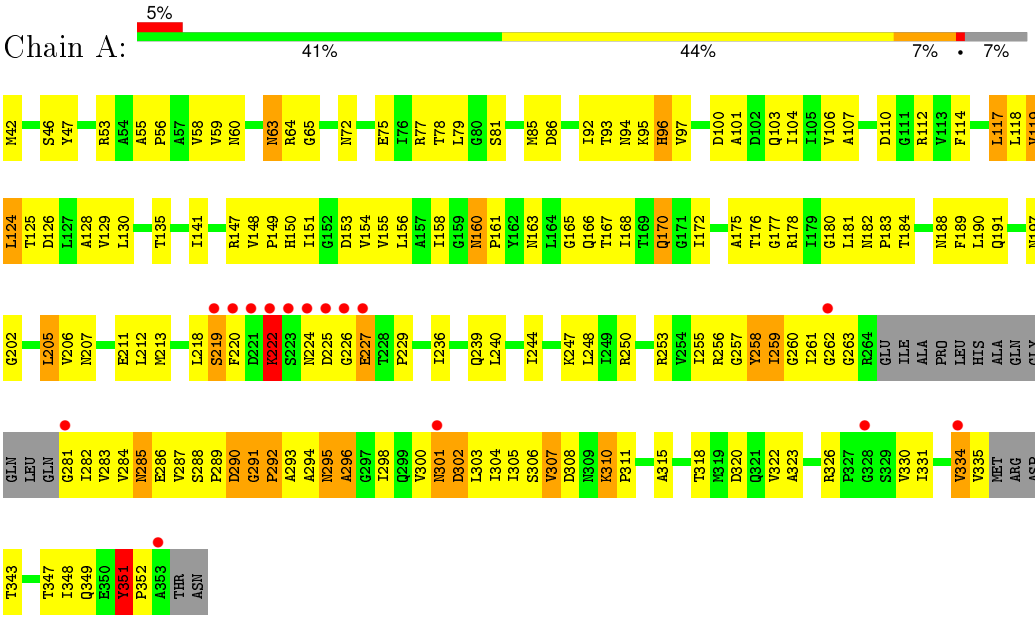
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	INITIATING METHIONINE	UNP P31137
B	42	MET	-	INITIATING METHIONINE	UNP P31137
C	42	MET	-	INITIATING METHIONINE	UNP P31137

3 Residue-property plots (i)

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

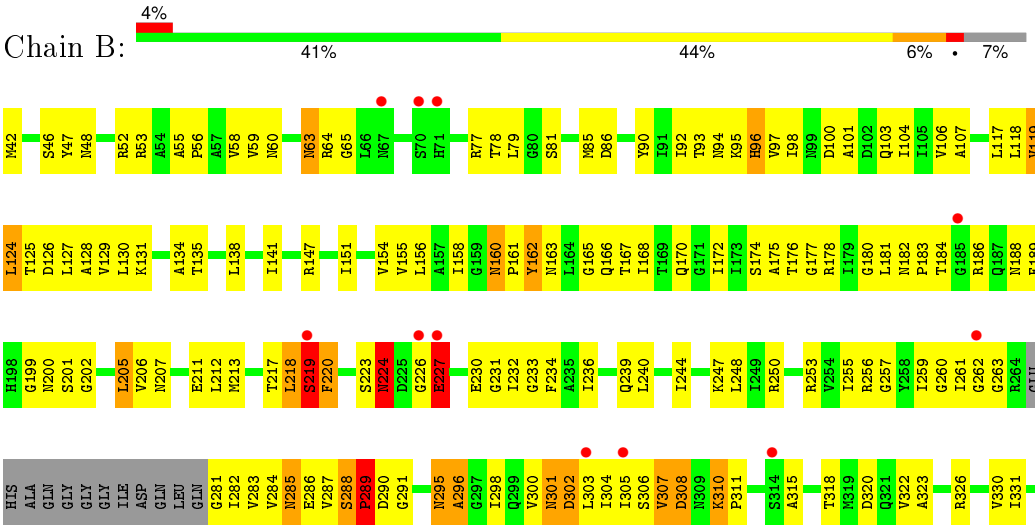
- Molecule 1: Protease degS

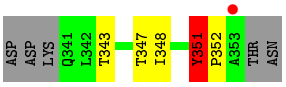
Chain A:



- Molecule 1: Protease degS

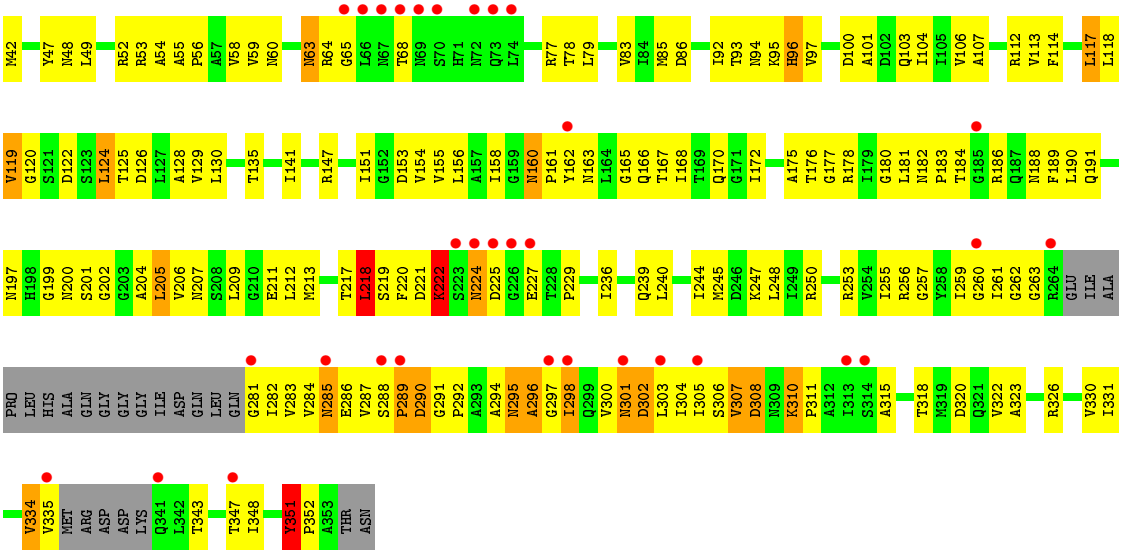
Chain B:





• Molecule 1: Protease degS

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.99Å 142.73Å 41.23Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 19.90 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.05) 96.4 (19.90-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 3.04Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.301 0.243 , 0.243	Depositor DCC
R_{free} test set	1106 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 78.5	EDS
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 21871 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6384	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

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	0.58	1/2155 (0.0%)	0.88	5/2935 (0.2%)
1	B	0.71	2/2155 (0.1%)	1.02	10/2935 (0.3%)
1	C	0.50	0/2155	0.91	8/2935 (0.3%)
All	All	0.60	3/6465 (0.0%)	0.94	23/8805 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	ASN	C-N	-19.82	0.88	1.34
1	B	227	GLU	C-N	10.94	1.59	1.34
1	A	219	SER	N-CA	-5.58	1.35	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	224	ASN	O-C-N	-22.37	86.90	122.70
1	C	334	VAL	CB-CA-C	-11.74	89.10	111.40
1	B	334	VAL	CB-CA-C	-11.35	89.84	111.40
1	B	224	ASN	CA-C-N	-9.92	95.37	117.20
1	B	224	ASN	C-N-CA	-8.62	100.16	121.70
1	B	219	SER	CA-C-N	-8.10	99.39	117.20
1	B	219	SER	C-N-CA	7.98	141.66	121.70
1	C	220	PHE	CB-CG-CD1	-7.76	115.37	120.80
1	C	220	PHE	CB-CG-CD2	7.55	126.08	120.80
1	C	218	LEU	CA-C-N	-7.36	101.00	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	ILE	N-CA-C	-7.25	91.43	111.00
1	B	289	PRO	N-CA-C	-7.14	93.54	112.10
1	C	289	PRO	CA-N-CD	-7.02	101.67	111.50
1	B	220	PHE	N-CA-CB	-7.00	98.01	110.60
1	A	259	ILE	CB-CA-C	-6.75	98.09	111.60
1	B	220	PHE	CB-CG-CD2	-6.34	116.36	120.80
1	C	285	ASN	CB-CA-C	-5.96	98.48	110.40
1	A	292	PRO	CA-N-CD	-5.52	103.77	111.50
1	B	219	SER	O-C-N	5.50	131.50	122.70
1	C	218	LEU	O-C-N	5.39	131.32	122.70
1	C	222	LYS	C-N-CA	5.37	135.13	121.70
1	A	258	TYR	C-N-CA	5.14	134.54	121.70
1	A	219	SER	CA-C-N	-5.07	106.05	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	224	ASN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2128	0	2124	209	5
1	B	2128	0	2124	207	4
1	C	2128	0	2127	205	1
All	All	6384	0	6375	598	5

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 47.

All (598) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:HD13	1:B:219:SER:N	1.41	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PRO:HD3	1:A:349:GLN:OE1	1.32	1.30
1:C:218:LEU:HD13	1:C:218:LEU:O	1.18	1.27
1:C:334:VAL:O	1:C:335:VAL:CB	1.95	1.13
1:C:334:VAL:O	1:C:334:VAL:HG12	1.36	1.11
1:B:59:VAL:HG11	1:B:106:VAL:HG13	1.24	1.10
1:C:59:VAL:HG11	1:C:106:VAL:HG13	1.30	1.09
1:A:292:PRO:CD	1:A:349:GLN:OE1	2.00	1.08
1:C:218:LEU:HD22	1:C:219:SER:O	1.53	1.07
1:C:218:LEU:HD13	1:C:218:LEU:C	1.74	1.07
1:A:59:VAL:HG11	1:A:106:VAL:HG13	1.12	1.07
1:B:260:GLY:O	1:B:289:PRO:HG2	1.55	1.07
1:B:78:THR:HG22	1:B:79:LEU:H	1.18	1.05
1:B:226:GLY:O	1:B:227:GLU:HB3	1.51	1.04
1:B:147:ARG:HD2	1:B:211:GLU:OE2	1.55	1.04
1:C:147:ARG:HD2	1:C:211:GLU:OE2	1.57	1.04
1:C:218:LEU:CD1	1:C:218:LEU:O	2.06	1.02
1:B:334:VAL:O	1:B:335:VAL:CB	2.04	1.02
1:B:218:LEU:HD13	1:B:218:LEU:C	1.77	1.00
1:C:334:VAL:O	1:C:334:VAL:CG1	1.98	1.00
1:C:217:THR:O	1:C:218:LEU:HB3	1.61	0.99
1:B:334:VAL:HG12	1:B:334:VAL:O	1.61	0.99
1:A:295:ASN:O	1:A:296:ALA:HB2	1.59	0.98
1:B:218:LEU:HD23	1:B:233:GLY:HA2	1.45	0.98
1:A:220:PHE:O	1:A:229:PRO:HG2	1.65	0.95
1:C:221:ASP:HB3	1:C:229:PRO:HG2	1.47	0.95
1:A:197:ASN:H	1:A:200:ASN:HD22	1.09	0.94
1:A:182:ASN:HD22	1:A:183:PRO:HD2	1.31	0.94
1:B:197:ASN:H	1:B:200:ASN:HD22	1.17	0.93
1:A:78:THR:HG22	1:A:79:LEU:H	1.34	0.92
1:A:147:ARG:HD2	1:A:211:GLU:OE2	1.68	0.92
1:B:218:LEU:C	1:B:218:LEU:CD1	2.35	0.92
1:A:290:ASP:O	1:A:291:GLY:O	1.87	0.92
1:B:260:GLY:C	1:B:289:PRO:HG2	1.90	0.91
1:A:292:PRO:HD3	1:A:349:GLN:CD	1.89	0.91
1:A:259:ILE:CG2	1:A:259:ILE:O	2.17	0.91
1:C:59:VAL:HG13	1:C:107:ALA:O	1.71	0.90
1:C:78:THR:HG22	1:C:79:LEU:H	1.34	0.90
1:C:221:ASP:HB3	1:C:229:PRO:CG	2.02	0.90
1:C:197:ASN:H	1:C:200:ASN:HD22	1.17	0.89
1:B:308:ASP:OD2	1:B:331:ILE:CG2	2.21	0.89
1:C:182:ASN:HD22	1:C:183:PRO:HD2	1.36	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:CD2	1:C:219:SER:O	2.21	0.89
1:A:161:PRO:HA	1:A:199:GLY:HA3	1.56	0.88
1:B:59:VAL:HG13	1:B:107:ALA:O	1.73	0.88
1:A:330:VAL:HG22	1:A:347:THR:HG22	1.53	0.88
1:B:182:ASN:HD22	1:B:183:PRO:HD2	1.36	0.87
1:B:226:GLY:O	1:B:227:GLU:CB	2.22	0.87
1:A:259:ILE:HG23	1:A:259:ILE:O	1.74	0.87
1:C:330:VAL:HG22	1:C:347:THR:HG22	1.57	0.87
1:B:218:LEU:CD1	1:B:219:SER:N	2.36	0.86
1:B:178:ARG:HB3	1:B:178:ARG:HH11	1.43	0.83
1:B:330:VAL:HG22	1:B:347:THR:HG22	1.57	0.83
1:A:259:ILE:HD11	1:A:261:ILE:HD12	1.58	0.83
1:C:178:ARG:NH1	1:C:178:ARG:HB3	1.94	0.83
1:B:118:LEU:HD23	1:B:120:GLY:H	1.43	0.83
1:B:63:ASN:HD22	1:B:63:ASN:C	1.82	0.82
1:A:63:ASN:HD22	1:A:63:ASN:C	1.81	0.82
1:A:197:ASN:H	1:A:200:ASN:ND2	1.77	0.82
1:C:125:THR:HG21	1:C:244:ILE:HD11	1.61	0.82
1:C:118:LEU:HD23	1:C:120:GLY:H	1.45	0.81
1:A:124:LEU:HD12	1:A:256:ARG:NH1	1.96	0.81
1:B:334:VAL:CG1	1:B:334:VAL:O	2.15	0.80
1:C:63:ASN:C	1:C:63:ASN:HD22	1.85	0.80
1:B:161:PRO:HA	1:B:199:GLY:HA3	1.63	0.80
1:B:217:THR:O	1:B:234:PHE:O	2.00	0.80
1:A:197:ASN:N	1:A:200:ASN:HD22	1.80	0.80
1:C:178:ARG:HH11	1:C:178:ARG:HB3	1.45	0.80
1:C:124:LEU:HD13	1:C:183:PRO:HG3	1.64	0.79
1:B:178:ARG:HB3	1:B:178:ARG:NH1	1.96	0.79
1:A:285:ASN:O	1:A:285:ASN:ND2	2.16	0.79
1:C:253:ARG:NH1	1:C:255:ILE:HG12	1.98	0.79
1:A:182:ASN:HD22	1:A:183:PRO:CD	1.96	0.78
1:C:285:ASN:ND2	1:C:285:ASN:O	2.16	0.78
1:B:125:THR:HG21	1:B:244:ILE:CD1	2.14	0.78
1:A:59:VAL:CG1	1:A:106:VAL:HG13	2.05	0.78
1:B:308:ASP:OD2	1:B:331:ILE:HG21	1.83	0.78
1:C:295:ASN:O	1:C:296:ALA:HB2	1.83	0.77
1:A:178:ARG:HH11	1:A:178:ARG:HB3	1.50	0.77
1:C:222:LYS:HG2	1:C:224:ASN:O	1.85	0.77
1:C:260:GLY:O	1:C:289:PRO:HG2	1.84	0.77
1:B:253:ARG:NH1	1:B:255:ILE:HG12	2.01	0.76
1:C:161:PRO:HA	1:C:199:GLY:HA3	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:HD2	1:B:162:TYR:CD2	2.18	0.76
1:A:178:ARG:HB3	1:A:178:ARG:NH1	2.00	0.76
1:C:129:VAL:HG23	1:C:248:LEU:HD12	1.67	0.76
1:A:255:ILE:HD12	1:A:326:ARG:HH12	1.50	0.76
1:A:125:THR:HG21	1:A:244:ILE:HD11	1.68	0.76
1:C:94:ASN:HA	1:C:126:ASP:O	1.85	0.75
1:A:59:VAL:HG11	1:A:106:VAL:CG1	2.06	0.75
1:C:260:GLY:C	1:C:289:PRO:HG2	2.07	0.75
1:B:78:THR:HG22	1:B:79:LEU:N	1.99	0.75
1:C:259:ILE:HD11	1:C:261:ILE:HD12	1.67	0.74
1:A:288:SER:N	1:A:289:PRO:HD3	2.03	0.74
1:A:295:ASN:O	1:A:296:ALA:CB	2.28	0.74
1:A:118:LEU:HD23	1:A:120:GLY:H	1.51	0.74
1:A:253:ARG:NH1	1:A:255:ILE:HG12	2.02	0.74
1:B:124:LEU:HD13	1:B:183:PRO:HG3	1.69	0.74
1:B:129:VAL:HG23	1:B:248:LEU:HD12	1.70	0.74
1:B:218:LEU:HD13	1:B:219:SER:CA	2.18	0.74
1:B:257:GLY:H	1:B:323:ALA:HA	1.53	0.73
1:C:289:PRO:HD2	1:C:289:PRO:O	1.86	0.73
1:B:310:LYS:HG3	1:B:311:PRO:HD2	1.71	0.73
1:B:160:ASN:HD21	1:B:165:GLY:H	1.36	0.73
1:A:220:PHE:HD1	1:A:229:PRO:CB	2.01	0.73
1:C:197:ASN:H	1:C:200:ASN:ND2	1.87	0.73
1:B:295:ASN:O	1:B:296:ALA:HB2	1.88	0.73
1:B:197:ASN:H	1:B:200:ASN:ND2	1.88	0.72
1:B:94:ASN:HA	1:B:126:ASP:O	1.90	0.72
1:A:181:LEU:HD22	1:A:247:LYS:HE3	1.72	0.72
1:A:334:VAL:HG12	1:A:335:VAL:H	1.55	0.71
1:B:182:ASN:HD22	1:B:183:PRO:CD	2.03	0.71
1:A:59:VAL:HG13	1:A:107:ALA:O	1.89	0.71
1:A:191:GLN:HE22	1:B:167:THR:HG21	1.53	0.71
1:A:260:GLY:C	1:A:289:PRO:HG2	2.10	0.71
1:A:160:ASN:HD21	1:A:165:GLY:H	1.35	0.71
1:B:125:THR:HG21	1:B:244:ILE:HD11	1.73	0.71
1:C:305:ILE:HB	1:C:334:VAL:HB	1.73	0.71
1:C:182:ASN:HD22	1:C:183:PRO:CD	2.04	0.71
1:C:125:THR:HG21	1:C:244:ILE:CD1	2.21	0.70
1:C:294:ALA:O	1:C:296:ALA:N	2.24	0.70
1:A:94:ASN:HA	1:A:126:ASP:O	1.91	0.70
1:A:257:GLY:H	1:A:323:ALA:HA	1.56	0.70
1:B:191:GLN:HE22	1:C:167:THR:HG21	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLY:HA3	1:A:189:PHE:O	1.92	0.70
1:C:257:GLY:H	1:C:323:ALA:HA	1.55	0.70
1:C:250:ARG:HB2	1:C:250:ARG:HH11	1.56	0.70
1:B:305:ILE:HB	1:B:334:VAL:HB	1.72	0.70
1:C:255:ILE:HD12	1:C:326:ARG:HH12	1.57	0.69
1:A:172:ILE:HG23	1:B:170:GLN:HG2	1.74	0.69
1:B:261:ILE:HG22	1:B:262:GLY:N	2.07	0.69
1:A:125:THR:HG21	1:A:244:ILE:CD1	2.24	0.68
1:C:310:LYS:HG3	1:C:311:PRO:HD2	1.74	0.68
1:A:170:GLN:HG2	1:C:172:ILE:HG23	1.74	0.68
1:B:155:VAL:HG22	1:B:205:LEU:HD22	1.76	0.68
1:A:310:LYS:HG3	1:A:311:PRO:HD2	1.76	0.67
1:B:124:LEU:HD12	1:B:256:ARG:NH1	2.09	0.67
1:A:180:GLY:HA3	1:A:320:ASP:OD2	1.95	0.67
1:A:288:SER:N	1:A:289:PRO:CD	2.57	0.67
1:A:226:GLY:C	1:A:227:GLU:HG3	2.14	0.66
1:B:218:LEU:HD22	1:B:234:PHE:HD1	1.60	0.66
1:C:263:GLY:HA2	1:C:285:ASN:HB3	1.78	0.66
1:A:250:ARG:HH11	1:A:250:ARG:HB2	1.61	0.66
1:B:259:ILE:HD11	1:B:261:ILE:HD12	1.75	0.66
1:A:334:VAL:HG12	1:A:335:VAL:N	2.09	0.66
1:B:81:SER:O	1:B:202:GLY:HA3	1.96	0.66
1:C:259:ILE:HG23	1:C:260:GLY:H	1.61	0.66
1:B:255:ILE:HD12	1:B:326:ARG:HH12	1.60	0.65
1:B:288:SER:C	1:B:289:PRO:O	2.30	0.65
1:B:177:GLY:HA3	1:B:189:PHE:O	1.97	0.65
1:A:285:ASN:C	1:A:285:ASN:ND2	2.50	0.65
1:B:180:GLY:HA3	1:B:320:ASP:OD2	1.98	0.64
1:B:260:GLY:O	1:B:289:PRO:CG	2.41	0.64
1:B:59:VAL:HG12	1:B:60:ASN:N	2.11	0.64
1:C:118:LEU:HD23	1:C:120:GLY:N	2.13	0.64
1:A:292:PRO:HD2	1:A:349:GLN:OE1	1.95	0.64
1:C:261:ILE:HG22	1:C:262:GLY:N	2.11	0.64
1:A:225:ASP:CG	1:A:226:GLY:H	2.01	0.64
1:C:250:ARG:HB2	1:C:250:ARG:NH1	2.12	0.64
1:A:155:VAL:HG22	1:A:205:LEU:HD22	1.80	0.64
1:C:217:THR:O	1:C:218:LEU:CB	2.39	0.63
1:C:308:ASP:OD2	1:C:331:ILE:CG2	2.46	0.63
1:A:59:VAL:HG12	1:A:60:ASN:N	2.13	0.63
1:C:177:GLY:HA3	1:C:189:PHE:O	1.98	0.63
1:C:180:GLY:HA3	1:C:320:ASP:OD2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASP:OD2	1:A:331:ILE:CG2	2.48	0.62
1:B:78:THR:CG2	1:B:79:LEU:H	2.01	0.62
1:A:220:PHE:CD1	1:A:229:PRO:CB	2.83	0.62
1:A:222:LYS:CD	1:B:162:TYR:CD2	2.67	0.62
1:B:160:ASN:ND2	1:B:165:GLY:H	1.97	0.62
1:B:207:ASN:HB3	1:B:213:MET:HE2	1.82	0.62
1:A:259:ILE:HB	1:A:322:VAL:HG11	1.81	0.61
1:C:94:ASN:OD1	1:C:201:SER:HB3	2.00	0.61
1:A:227:GLU:OE1	1:B:162:TYR:OH	2.17	0.61
1:C:290:ASP:CG	1:C:290:ASP:O	2.37	0.61
1:B:250:ARG:HB2	1:B:250:ARG:HH11	1.65	0.61
1:A:220:PHE:HD1	1:A:229:PRO:HB2	1.65	0.61
1:A:160:ASN:ND2	1:A:165:GLY:H	1.98	0.61
1:A:65:GLY:HA3	1:A:77:ARG:HD3	1.82	0.61
1:C:289:PRO:CD	1:C:289:PRO:O	2.49	0.61
1:B:261:ILE:HG22	1:B:262:GLY:H	1.63	0.61
1:B:178:ARG:CB	1:B:178:ARG:HH11	2.12	0.61
1:C:285:ASN:ND2	1:C:285:ASN:C	2.52	0.61
1:B:94:ASN:HB2	1:B:97:VAL:HG23	1.82	0.61
1:A:239:GLN:HA	1:A:239:GLN:NE2	2.16	0.61
1:B:93:THR:HG23	1:B:128:ALA:HB3	1.83	0.61
1:C:59:VAL:HG12	1:C:60:ASN:N	2.15	0.61
1:A:96:HIS:ND1	1:A:126:ASP:OD2	2.29	0.61
1:A:307:VAL:HG11	1:A:318:THR:HG23	1.83	0.61
1:B:55:ALA:HB1	1:B:166:GLN:HE22	1.66	0.61
1:C:259:ILE:HG23	1:C:260:GLY:N	2.16	0.60
1:A:207:ASN:HB3	1:A:213:MET:HE2	1.83	0.60
1:C:207:ASN:HB3	1:C:213:MET:HE2	1.83	0.60
1:A:282:ILE:HD12	1:A:315:ALA:HA	1.83	0.60
1:A:81:SER:O	1:A:202:GLY:HA3	2.02	0.60
1:C:306:SER:OG	1:C:334:VAL:HG23	2.02	0.60
1:C:96:HIS:ND1	1:C:126:ASP:OD2	2.32	0.60
1:C:281:GLY:HA3	1:C:303:LEU:HD21	1.84	0.60
1:A:307:VAL:CG1	1:A:318:THR:HG23	2.30	0.60
1:A:124:LEU:HD13	1:A:183:PRO:HG3	1.82	0.60
1:C:49:LEU:HD11	1:C:53:ARG:NE	2.17	0.60
1:A:288:SER:O	1:A:289:PRO:C	2.40	0.60
1:C:178:ARG:CB	1:C:178:ARG:HH11	2.12	0.59
1:B:118:LEU:HD23	1:B:120:GLY:N	2.14	0.59
1:A:124:LEU:HD12	1:A:256:ARG:CZ	2.31	0.59
1:A:155:VAL:HG21	1:A:205:LEU:HD13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:THR:HG23	1:C:128:ALA:HB3	1.84	0.59
1:B:259:ILE:HG23	1:B:260:GLY:N	2.18	0.59
1:C:221:ASP:HB3	1:C:229:PRO:HG3	1.83	0.59
1:B:120:GLY:HA3	1:B:248:LEU:HD22	1.84	0.59
1:C:55:ALA:HB1	1:C:166:GLN:NE2	2.17	0.59
1:B:257:GLY:N	1:B:323:ALA:HA	2.18	0.59
1:A:125:THR:O	1:A:236:ILE:HD11	2.02	0.59
1:C:58:VAL:HG21	1:C:158:ILE:HG22	1.83	0.59
1:A:281:GLY:HA3	1:A:303:LEU:HD21	1.84	0.59
1:B:63:ASN:ND2	1:B:63:ASN:C	2.55	0.59
1:A:94:ASN:HB2	1:A:97:VAL:HG23	1.83	0.59
1:B:65:GLY:HA3	1:B:77:ARG:HD3	1.85	0.59
1:C:287:VAL:C	1:C:289:PRO:HD3	2.23	0.59
1:B:259:ILE:HG23	1:B:260:GLY:H	1.68	0.58
1:C:160:ASN:HD21	1:C:165:GLY:H	1.51	0.58
1:C:282:ILE:HD12	1:C:315:ALA:HA	1.85	0.58
1:A:94:ASN:OD1	1:A:201:SER:HB3	2.03	0.58
1:B:300:VAL:HG22	1:B:300:VAL:O	2.04	0.58
1:A:225:ASP:C	1:A:227:GLU:H	2.06	0.58
1:C:197:ASN:N	1:C:200:ASN:HD22	1.97	0.58
1:A:300:VAL:O	1:A:300:VAL:HG22	2.04	0.58
1:A:42:MET:HE1	1:C:53:ARG:HH12	1.69	0.58
1:A:46:SER:HB2	1:C:153:ASP:HA	1.83	0.58
1:B:260:GLY:C	1:B:289:PRO:CG	2.70	0.58
1:A:257:GLY:N	1:A:323:ALA:HA	2.18	0.58
1:B:181:LEU:HD22	1:B:247:LYS:HE3	1.86	0.58
1:A:85:MET:HG3	1:A:92:ILE:HG13	1.85	0.58
1:C:257:GLY:N	1:C:323:ALA:HA	2.18	0.58
1:A:220:PHE:O	1:A:229:PRO:CG	2.47	0.58
1:B:63:ASN:HD22	1:B:64:ARG:N	2.01	0.58
1:A:253:ARG:HH12	1:A:255:ILE:HG12	1.69	0.58
1:B:124:LEU:HD12	1:B:256:ARG:CZ	2.34	0.57
1:A:63:ASN:HD22	1:A:64:ARG:N	2.02	0.57
1:B:282:ILE:HD12	1:B:315:ALA:HA	1.85	0.57
1:B:305:ILE:HG12	1:B:335:VAL:CB	2.33	0.57
1:C:78:THR:HG22	1:C:79:LEU:N	2.13	0.57
1:B:77:ARG:HH22	1:B:100:ASP:HB2	1.69	0.57
1:B:218:LEU:HD23	1:B:233:GLY:CA	2.27	0.57
1:B:348:ILE:HD12	1:B:348:ILE:N	2.19	0.57
1:A:63:ASN:ND2	1:A:63:ASN:C	2.54	0.57
1:C:103:GLN:HG2	1:C:104:ILE:N	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:CG2	1:B:284:VAL:HG13	2.35	0.57
1:C:155:VAL:HG22	1:C:205:LEU:HD22	1.87	0.57
1:C:305:ILE:HB	1:C:334:VAL:CB	2.34	0.57
1:A:263:GLY:HA3	1:A:283:VAL:O	2.05	0.57
1:C:112:ARG:HB3	1:C:114:PHE:CE1	2.39	0.57
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.69	0.56
1:B:55:ALA:HB1	1:B:166:GLN:NE2	2.20	0.56
1:A:260:GLY:O	1:A:289:PRO:HG2	2.04	0.56
1:C:124:LEU:HB3	1:C:183:PRO:HB3	1.86	0.56
1:C:305:ILE:HG12	1:C:335:VAL:CB	2.35	0.56
1:A:290:ASP:O	1:A:294:ALA:HB3	2.04	0.56
1:A:239:GLN:CA	1:A:239:GLN:HE21	2.19	0.56
1:A:178:ARG:HH11	1:A:178:ARG:CB	2.17	0.56
1:A:122:ASP:CG	1:A:256:ARG:HH22	2.09	0.56
1:C:94:ASN:HB2	1:C:97:VAL:HG23	1.87	0.56
1:C:300:VAL:O	1:C:300:VAL:HG22	2.06	0.56
1:B:197:ASN:N	1:B:200:ASN:HD22	1.97	0.56
1:A:225:ASP:CG	1:A:226:GLY:N	2.58	0.56
1:A:118:LEU:HD23	1:A:120:GLY:N	2.17	0.56
1:B:191:GLN:HE22	1:C:167:THR:CG2	2.18	0.56
1:A:288:SER:C	1:A:289:PRO:O	2.42	0.55
1:B:308:ASP:OD2	1:B:331:ILE:HB	2.06	0.55
1:C:295:ASN:O	1:C:296:ALA:CB	2.50	0.55
1:A:348:ILE:N	1:A:348:ILE:HD12	2.21	0.55
1:C:79:LEU:HD12	1:C:79:LEU:O	2.07	0.55
1:B:85:MET:HG3	1:B:92:ILE:HG13	1.88	0.55
1:A:92:ILE:HG22	1:A:93:THR:N	2.20	0.55
1:A:263:GLY:HA2	1:A:285:ASN:H	1.72	0.55
1:B:124:LEU:HB3	1:B:183:PRO:HB3	1.88	0.55
1:A:282:ILE:CD1	1:A:315:ALA:HA	2.35	0.55
1:B:282:ILE:CD1	1:B:315:ALA:HA	2.36	0.55
1:B:351:TYR:CG	1:B:352:PRO:HD2	2.41	0.55
1:B:288:SER:N	1:B:289:PRO:HD3	2.22	0.55
1:C:176:THR:O	1:C:190:LEU:HD12	2.07	0.55
1:A:129:VAL:HG23	1:A:248:LEU:HD12	1.89	0.55
1:B:288:SER:N	1:B:289:PRO:CD	2.70	0.55
1:C:288:SER:N	1:C:289:PRO:HD3	2.22	0.54
1:A:124:LEU:HB3	1:A:183:PRO:HB3	1.89	0.54
1:A:305:ILE:HB	1:A:334:VAL:HB	1.90	0.54
1:C:290:ASP:O	1:C:290:ASP:OD1	2.25	0.54
1:A:259:ILE:HG22	1:A:259:ILE:O	2.04	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:HD3	1:B:162:TYR:CD2	2.42	0.54
1:A:78:THR:HG22	1:A:79:LEU:N	2.13	0.54
1:A:181:LEU:CD2	1:A:247:LYS:HE3	2.36	0.54
1:C:351:TYR:CG	1:C:352:PRO:HD2	2.42	0.54
1:B:239:GLN:NE2	1:B:239:GLN:HA	2.23	0.54
1:C:259:ILE:O	1:C:292:PRO:HG2	2.08	0.54
1:C:96:HIS:HD1	1:C:126:ASP:CG	2.10	0.54
1:B:155:VAL:HG21	1:B:205:LEU:HD13	1.90	0.54
1:C:282:ILE:CD1	1:C:315:ALA:HA	2.37	0.54
1:C:48:ASN:OD1	1:C:52:ARG:NH1	2.40	0.54
1:C:124:LEU:HD12	1:C:256:ARG:NH1	2.23	0.54
1:C:306:SER:OG	1:C:334:VAL:CG2	2.56	0.54
1:B:308:ASP:OD2	1:B:331:ILE:CB	2.55	0.54
1:C:63:ASN:HD22	1:C:64:ARG:N	2.05	0.54
1:B:58:VAL:HG21	1:B:158:ILE:HG22	1.90	0.54
1:B:259:ILE:HB	1:B:322:VAL:HG11	1.89	0.53
1:C:63:ASN:C	1:C:63:ASN:ND2	2.57	0.53
1:C:253:ARG:HH12	1:C:255:ILE:HG12	1.70	0.53
1:A:103:GLN:HG2	1:A:104:ILE:N	2.23	0.53
1:C:259:ILE:HB	1:C:322:VAL:HG11	1.90	0.53
1:A:255:ILE:CD1	1:A:326:ARG:HH12	2.20	0.53
1:A:182:ASN:ND2	1:A:183:PRO:HD2	2.13	0.53
1:A:55:ALA:HB1	1:A:166:GLN:HE22	1.74	0.53
1:B:103:GLN:HG2	1:B:104:ILE:N	2.24	0.53
1:A:172:ILE:CG2	1:B:170:GLN:HG2	2.38	0.53
1:B:305:ILE:HB	1:B:334:VAL:CB	2.38	0.53
1:A:147:ARG:NH1	1:A:211:GLU:OE1	2.42	0.53
1:C:348:ILE:HD12	1:C:348:ILE:N	2.23	0.53
1:A:94:ASN:HB2	1:A:97:VAL:CG2	2.37	0.53
1:C:125:THR:O	1:C:236:ILE:HD11	2.08	0.53
1:A:305:ILE:HB	1:A:334:VAL:CB	2.39	0.52
1:A:291:GLY:O	1:A:295:ASN:ND2	2.41	0.52
1:B:53:ARG:HH12	1:C:42:MET:HE1	1.73	0.52
1:A:65:GLY:H	1:A:77:ARG:HG3	1.74	0.52
1:C:181:LEU:HD22	1:C:247:LYS:HE3	1.90	0.52
1:C:65:GLY:HA3	1:C:77:ARG:HD3	1.91	0.52
1:C:255:ILE:CD1	1:C:326:ARG:HH12	2.23	0.52
1:C:94:ASN:OD1	1:C:202:GLY:N	2.42	0.52
1:B:263:GLY:HA3	1:B:283:VAL:O	2.09	0.52
1:C:284:VAL:HB	1:C:302:ASP:O	2.09	0.52
1:B:306:SER:OG	1:B:334:VAL:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASP:CG	1:B:256:ARG:HH22	2.13	0.52
1:B:47:TYR:CE2	1:B:154:VAL:HG11	2.45	0.52
1:C:83:VAL:CG2	1:C:204:ALA:HB2	2.40	0.52
1:A:351:TYR:CG	1:A:352:PRO:HD2	2.45	0.52
1:A:284:VAL:HB	1:A:302:ASP:O	2.10	0.51
1:A:153:ASP:HA	1:B:46:SER:HB2	1.90	0.51
1:C:206:VAL:HG12	1:C:212:LEU:HA	1.91	0.51
1:C:284:VAL:HG12	1:C:284:VAL:O	2.10	0.51
1:C:305:ILE:HB	1:C:334:VAL:CG1	2.39	0.51
1:A:58:VAL:HG21	1:A:158:ILE:HG22	1.91	0.51
1:C:65:GLY:H	1:C:77:ARG:HG3	1.75	0.51
1:C:261:ILE:HG22	1:C:262:GLY:H	1.73	0.51
1:B:261:ILE:CG2	1:B:262:GLY:N	2.74	0.51
1:C:92:ILE:HG22	1:C:93:THR:N	2.25	0.51
1:C:288:SER:N	1:C:289:PRO:CD	2.73	0.51
1:B:59:VAL:CG1	1:B:60:ASN:N	2.73	0.51
1:C:47:TYR:HB3	1:C:156:LEU:HD11	1.92	0.51
1:A:47:TYR:HB3	1:A:156:LEU:HD11	1.91	0.51
1:A:161:PRO:HB2	1:A:197:ASN:HB2	1.92	0.51
1:B:303:LEU:O	1:B:335:VAL:C	2.49	0.51
1:A:104:ILE:HG21	1:A:130:LEU:HD13	1.92	0.51
1:A:55:ALA:HB1	1:A:166:GLN:NE2	2.25	0.51
1:B:96:HIS:ND1	1:B:126:ASP:OD2	2.39	0.51
1:A:95:LYS:O	1:A:97:VAL:N	2.44	0.51
1:A:260:GLY:O	1:A:293:ALA:HB2	2.11	0.51
1:B:162:TYR:HE1	1:B:197:ASN:HB3	1.75	0.50
1:B:181:LEU:CD2	1:B:247:LYS:HE3	2.40	0.50
1:A:250:ARG:HB2	1:A:250:ARG:NH1	2.25	0.50
1:B:59:VAL:CG1	1:B:106:VAL:HG13	2.18	0.50
1:A:290:ASP:O	1:A:291:GLY:C	2.49	0.50
1:A:263:GLY:HA2	1:A:285:ASN:HB3	1.94	0.50
1:B:250:ARG:HB2	1:B:250:ARG:NH1	2.26	0.50
1:C:77:ARG:HH22	1:C:100:ASP:HB2	1.77	0.50
1:A:161:PRO:CB	1:A:197:ASN:HB2	2.40	0.50
1:C:83:VAL:HG21	1:C:204:ALA:HB2	1.92	0.50
1:B:48:ASN:OD1	1:B:52:ARG:NH1	2.45	0.50
1:B:230:GLU:HG2	1:B:231:GLY:N	2.27	0.50
1:B:281:GLY:HA3	1:B:303:LEU:HD21	1.92	0.50
1:A:330:VAL:CG2	1:A:347:THR:HG22	2.34	0.50
1:B:92:ILE:HG22	1:B:93:THR:N	2.27	0.50
1:A:95:LYS:C	1:A:97:VAL:H	2.14	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CD1	1:A:229:PRO:HG3	2.47	0.49
1:B:125:THR:O	1:B:236:ILE:HD11	2.11	0.49
1:B:261:ILE:CG2	1:B:262:GLY:H	2.25	0.49
1:B:186:ARG:HA	1:B:189:PHE:CE2	2.47	0.49
1:C:55:ALA:HB1	1:C:166:GLN:HE22	1.77	0.49
1:A:85:MET:CG	1:A:92:ILE:HG13	2.42	0.49
1:B:147:ARG:NH1	1:B:211:GLU:OE1	2.44	0.49
1:C:263:GLY:HA3	1:C:283:VAL:O	2.12	0.49
1:A:96:HIS:HD1	1:A:126:ASP:CG	2.14	0.49
1:C:288:SER:O	1:C:289:PRO:C	2.46	0.49
1:B:284:VAL:HB	1:B:302:ASP:O	2.12	0.49
1:A:120:GLY:HA3	1:A:248:LEU:HD22	1.94	0.49
1:A:191:GLN:HE22	1:B:167:THR:CG2	2.25	0.49
1:C:307:VAL:CG1	1:C:318:THR:HG23	2.41	0.49
1:C:92:ILE:CG2	1:C:93:THR:N	2.75	0.49
1:A:334:VAL:CG1	1:A:335:VAL:H	2.18	0.49
1:A:79:LEU:O	1:A:79:LEU:HD12	2.13	0.49
1:A:63:ASN:CG	1:A:101:ALA:HB2	2.33	0.49
1:C:119:VAL:HG23	1:C:119:VAL:O	2.13	0.49
1:B:284:VAL:CG2	1:B:304:ILE:HG12	2.43	0.49
1:C:94:ASN:HB2	1:C:97:VAL:CG2	2.43	0.49
1:B:92:ILE:CG2	1:B:93:THR:N	2.76	0.49
1:B:295:ASN:O	1:B:296:ALA:CB	2.53	0.49
1:B:104:ILE:HG21	1:B:130:LEU:HD13	1.94	0.49
1:C:63:ASN:HD21	1:C:101:ALA:HA	1.78	0.48
1:B:174:SER:HB3	1:C:168:ILE:H	1.77	0.48
1:C:261:ILE:CG2	1:C:262:GLY:N	2.77	0.48
1:B:330:VAL:CG2	1:B:347:THR:HG22	2.38	0.48
1:C:151:ILE:CD1	1:C:175:ALA:HA	2.44	0.48
1:A:92:ILE:CG2	1:A:93:THR:N	2.75	0.48
1:B:253:ARG:HH12	1:B:255:ILE:HG12	1.76	0.48
1:C:104:ILE:HG21	1:C:130:LEU:HD13	1.94	0.48
1:C:239:GLN:HA	1:C:239:GLN:NE2	2.28	0.48
1:A:206:VAL:HG12	1:A:212:LEU:HA	1.96	0.48
1:C:261:ILE:CG2	1:C:284:VAL:HG13	2.43	0.48
1:B:263:GLY:HA2	1:B:285:ASN:CB	2.44	0.48
1:C:147:ARG:NH1	1:C:211:GLU:OE1	2.47	0.48
1:C:308:ASP:OD2	1:C:331:ILE:HB	2.13	0.48
1:A:55:ALA:N	1:A:56:PRO:CD	2.76	0.48
1:B:182:ASN:ND2	1:B:183:PRO:HD2	2.18	0.48
1:A:220:PHE:CE1	1:A:222:LYS:HD3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:SER:CB	1:C:153:ASP:HA	2.44	0.47
1:C:112:ARG:HB3	1:C:114:PHE:HE1	1.79	0.47
1:B:263:GLY:HA2	1:B:285:ASN:HB2	1.96	0.47
1:A:47:TYR:CE2	1:A:154:VAL:HG11	2.49	0.47
1:C:257:GLY:H	1:C:323:ALA:CA	2.27	0.47
1:B:257:GLY:HA3	1:B:322:VAL:O	2.14	0.47
1:B:260:GLY:CA	1:B:289:PRO:HG2	2.43	0.47
1:C:85:MET:HG3	1:C:92:ILE:HG13	1.94	0.47
1:A:305:ILE:HB	1:A:334:VAL:HG11	1.97	0.47
1:B:104:ILE:HG21	1:B:130:LEU:CD1	2.45	0.47
1:C:141:ILE:O	1:C:141:ILE:HG23	2.13	0.47
1:C:284:VAL:CG2	1:C:304:ILE:HG12	2.44	0.47
1:C:59:VAL:CG1	1:C:60:ASN:N	2.78	0.47
1:A:300:VAL:O	1:A:301:ASN:HB2	2.15	0.47
1:A:112:ARG:HB3	1:A:114:PHE:CE1	2.50	0.47
1:C:218:LEU:CD1	1:C:218:LEU:C	2.51	0.47
1:A:304:ILE:HA	1:A:335:VAL:C	2.35	0.47
1:A:120:GLY:O	1:A:248:LEU:HD13	2.15	0.47
1:B:94:ASN:HB2	1:B:97:VAL:CG2	2.45	0.47
1:C:297:GLY:O	1:C:298:ILE:O	2.33	0.47
1:B:59:VAL:HG11	1:B:106:VAL:CG1	2.18	0.47
1:B:95:LYS:N	1:B:126:ASP:O	2.45	0.47
1:A:93:THR:HG23	1:A:128:ALA:HB3	1.97	0.47
1:A:121:SER:O	1:A:248:LEU:HD21	2.15	0.46
1:C:250:ARG:NH1	1:C:250:ARG:CB	2.75	0.46
1:C:117:LEU:HD13	1:C:119:VAL:HG12	1.96	0.46
1:B:218:LEU:HD13	1:B:219:SER:H	1.64	0.46
1:B:239:GLN:CA	1:B:239:GLN:HE21	2.27	0.46
1:A:58:VAL:HG22	1:A:166:GLN:OE1	2.15	0.46
1:A:59:VAL:CG1	1:A:60:ASN:N	2.77	0.46
1:A:220:PHE:CD1	1:A:229:PRO:CG	2.98	0.46
1:B:121:SER:O	1:B:248:LEU:HD21	2.15	0.46
1:B:239:GLN:HA	1:B:239:GLN:HE21	1.79	0.46
1:C:181:LEU:CD2	1:C:247:LYS:HE3	2.45	0.46
1:B:304:ILE:HA	1:B:335:VAL:C	2.35	0.46
1:B:129:VAL:HG23	1:B:248:LEU:CD1	2.42	0.46
1:B:94:ASN:OD1	1:B:201:SER:HB3	2.15	0.46
1:C:49:LEU:HD11	1:C:53:ARG:HE	1.80	0.46
1:C:93:THR:O	1:C:128:ALA:N	2.41	0.46
1:B:230:GLU:O	1:B:232:ILE:HG13	2.16	0.46
1:A:86:ASP:OD2	1:A:86:ASP:C	2.54	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:CG	1:A:225:ASP:N	2.69	0.46
1:B:55:ALA:N	1:B:56:PRO:CD	2.79	0.46
1:A:261:ILE:HG23	1:A:284:VAL:HG13	1.98	0.46
1:B:161:PRO:HA	1:B:199:GLY:CA	2.41	0.46
1:C:55:ALA:N	1:C:56:PRO:CD	2.78	0.46
1:C:224:ASN:CG	1:C:225:ASP:N	2.70	0.46
1:B:307:VAL:CG1	1:B:318:THR:HG23	2.45	0.46
1:A:220:PHE:HD1	1:A:229:PRO:CG	2.29	0.46
1:B:93:THR:O	1:B:128:ALA:N	2.45	0.46
1:C:141:ILE:CG2	1:C:141:ILE:O	2.64	0.46
1:B:206:VAL:HG12	1:B:212:LEU:HA	1.98	0.45
1:B:284:VAL:O	1:B:284:VAL:HG12	2.15	0.45
1:A:261:ILE:HG22	1:A:262:GLY:N	2.31	0.45
1:B:218:LEU:HD22	1:B:234:PHE:CD1	2.45	0.45
1:C:124:LEU:HD12	1:C:256:ARG:CZ	2.45	0.45
1:B:158:ILE:HG23	1:B:168:ILE:CD1	2.47	0.45
1:A:117:LEU:HD13	1:A:119:VAL:HG12	1.98	0.45
1:A:184:THR:CB	1:A:188:ASN:HD22	2.29	0.45
1:B:305:ILE:HB	1:B:334:VAL:CG1	2.46	0.45
1:A:304:ILE:HD13	1:A:335:VAL:C	2.37	0.45
1:B:65:GLY:H	1:B:77:ARG:HG3	1.81	0.45
1:C:257:GLY:HA3	1:C:322:VAL:O	2.17	0.45
1:C:300:VAL:O	1:C:301:ASN:HB2	2.16	0.45
1:A:258:TYR:CZ	1:A:260:GLY:HA3	2.52	0.45
1:B:257:GLY:O	1:B:322:VAL:HG12	2.16	0.45
1:B:287:VAL:C	1:B:289:PRO:HD3	2.37	0.45
1:C:122:ASP:CG	1:C:256:ARG:HH22	2.21	0.45
1:C:103:GLN:HG2	1:C:104:ILE:H	1.82	0.45
1:A:239:GLN:CA	1:A:239:GLN:NE2	2.79	0.45
1:A:158:ILE:HG12	1:A:168:ILE:HD12	1.97	0.45
1:B:134:ALA:HB3	1:B:138:LEU:HG	1.98	0.45
1:C:307:VAL:O	1:C:308:ASP:C	2.53	0.45
1:B:65:GLY:N	1:B:77:ARG:HG3	2.31	0.45
1:B:263:GLY:HA2	1:B:285:ASN:H	1.82	0.44
1:C:122:ASP:OD2	1:C:125:THR:HG23	2.17	0.44
1:B:63:ASN:CG	1:B:101:ALA:HB2	2.38	0.44
1:C:93:THR:CG2	1:C:128:ALA:HB3	2.46	0.44
1:B:127:LEU:HG	1:B:236:ILE:HD13	1.99	0.44
1:C:95:LYS:O	1:C:97:VAL:N	2.50	0.44
1:B:308:ASP:OD2	1:B:331:ILE:HG22	2.14	0.44
1:A:117:LEU:HD22	1:A:118:LEU:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:CD1	1:B:175:ALA:HA	2.47	0.44
1:C:222:LYS:C	1:C:224:ASN:H	2.20	0.44
1:C:218:LEU:HD22	1:C:219:SER:N	2.32	0.44
1:C:47:TYR:CE2	1:C:154:VAL:HG11	2.53	0.44
1:B:141:ILE:O	1:B:141:ILE:HG23	2.16	0.44
1:B:122:ASP:OD2	1:B:125:THR:HG23	2.17	0.44
1:C:304:ILE:HA	1:C:335:VAL:C	2.38	0.44
1:A:305:ILE:HB	1:A:334:VAL:CG1	2.48	0.44
1:C:78:THR:O	1:C:79:LEU:HB3	2.18	0.44
1:B:300:VAL:O	1:B:301:ASN:HB2	2.18	0.44
1:C:158:ILE:HG12	1:C:168:ILE:HD12	2.00	0.43
1:C:182:ASN:ND2	1:C:183:PRO:HD2	2.18	0.43
1:B:165:GLY:O	1:B:167:THR:HG23	2.17	0.43
1:A:170:GLN:HG3	1:A:170:GLN:O	2.17	0.43
1:B:218:LEU:CD2	1:B:234:PHE:HD1	2.30	0.43
1:C:308:ASP:OD2	1:C:331:ILE:HG22	2.18	0.43
1:A:153:ASP:HA	1:B:46:SER:CB	2.48	0.43
1:A:292:PRO:O	1:A:293:ALA:C	2.55	0.43
1:B:78:THR:O	1:B:79:LEU:HB3	2.18	0.43
1:A:148:VAL:HA	1:A:149:PRO:HD3	1.85	0.43
1:A:219:SER:OG	1:A:220:PHE:N	2.52	0.43
1:C:95:LYS:C	1:C:97:VAL:H	2.22	0.43
1:B:176:THR:O	1:B:190:LEU:HD12	2.18	0.43
1:A:63:ASN:ND2	1:A:101:ALA:CB	2.82	0.43
1:B:218:LEU:CD2	1:B:233:GLY:HA2	2.31	0.43
1:B:170:GLN:HE22	1:C:170:GLN:HE22	1.67	0.43
1:C:308:ASP:H	1:C:331:ILE:HD12	1.84	0.43
1:A:151:ILE:CD1	1:A:175:ALA:HA	2.49	0.43
1:A:250:ARG:CB	1:A:250:ARG:NH1	2.82	0.43
1:C:68:THR:OG1	1:C:77:ARG:HG2	2.18	0.43
1:C:303:LEU:O	1:C:335:VAL:C	2.58	0.42
1:A:331:ILE:O	1:A:331:ILE:HG13	2.17	0.42
1:A:331:ILE:HG12	1:A:348:ILE:HD11	2.00	0.42
1:B:351:TYR:CD2	1:B:352:PRO:HD2	2.54	0.42
1:A:58:VAL:HG11	1:A:158:ILE:HB	2.01	0.42
1:C:261:ILE:CG2	1:C:262:GLY:H	2.31	0.42
1:C:287:VAL:C	1:C:289:PRO:CD	2.88	0.42
1:B:160:ASN:C	1:B:160:ASN:HD22	2.22	0.42
1:C:186:ARG:HA	1:C:189:PHE:CE2	2.55	0.42
1:B:98:ILE:HG21	1:B:104:ILE:HD13	2.02	0.42
1:C:162:TYR:HE1	1:C:197:ASN:HB3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:VAL:C	1:C:114:PHE:CD1	2.93	0.42
1:A:141:ILE:O	1:A:141:ILE:HG23	2.19	0.42
1:A:167:THR:HG21	1:C:191:GLN:HE22	1.84	0.42
1:A:306:SER:OG	1:A:334:VAL:HG23	2.20	0.42
1:A:63:ASN:HD21	1:A:101:ALA:HA	1.83	0.42
1:C:291:GLY:O	1:C:295:ASN:ND2	2.52	0.42
1:A:176:THR:O	1:A:190:LEU:HD12	2.19	0.42
1:C:65:GLY:N	1:C:77:ARG:HG3	2.34	0.42
1:C:263:GLY:HA2	1:C:285:ASN:H	1.85	0.42
1:A:308:ASP:OD2	1:A:331:ILE:HG21	2.19	0.42
1:C:58:VAL:HG11	1:C:158:ILE:HB	2.02	0.42
1:B:47:TYR:HB3	1:B:156:LEU:HD11	2.01	0.42
1:B:134:ALA:CB	1:B:138:LEU:HG	2.50	0.42
1:A:182:ASN:HD22	1:A:183:PRO:N	2.17	0.41
1:A:42:MET:CE	1:C:209:LEU:HD22	2.50	0.41
1:C:184:THR:OG1	1:C:188:ASN:HB2	2.20	0.41
1:A:53:ARG:HH12	1:B:42:MET:HE1	1.85	0.41
1:A:284:VAL:O	1:A:284:VAL:HG12	2.19	0.41
1:C:54:ALA:HB1	1:C:141:ILE:HD11	2.02	0.41
1:C:307:VAL:CG2	1:C:318:THR:HG23	2.50	0.41
1:C:158:ILE:HG23	1:C:168:ILE:CD1	2.50	0.41
1:A:148:VAL:HG13	1:A:150:HIS:CE1	2.56	0.41
1:B:257:GLY:H	1:B:323:ALA:CA	2.28	0.41
1:B:287:VAL:C	1:B:289:PRO:CD	2.89	0.41
1:B:147:ARG:HH11	1:B:211:GLU:CD	2.23	0.41
1:A:259:ILE:CD1	1:A:261:ILE:HD12	2.38	0.41
1:C:94:ASN:O	1:C:97:VAL:HG23	2.19	0.41
1:C:239:GLN:HE21	1:C:239:GLN:CA	2.34	0.41
1:A:284:VAL:CG2	1:A:304:ILE:HG12	2.51	0.41
1:B:172:ILE:HG23	1:C:170:GLN:HG2	2.03	0.41
1:C:331:ILE:HG12	1:C:348:ILE:HD11	2.03	0.41
1:A:65:GLY:N	1:A:77:ARG:HG3	2.34	0.41
1:A:77:ARG:HH22	1:A:100:ASP:HB2	1.84	0.41
1:B:90:TYR:CE2	1:B:131:LYS:HD2	2.54	0.41
1:A:95:LYS:C	1:A:97:VAL:N	2.72	0.41
1:C:86:ASP:C	1:C:86:ASP:OD2	2.59	0.41
1:C:218:LEU:HD22	1:C:218:LEU:C	2.41	0.41
1:A:64:ARG:HA	1:A:75:GLU:O	2.21	0.41
1:C:248:LEU:HD23	1:C:248:LEU:HA	1.87	0.41
1:B:95:LYS:C	1:B:97:VAL:H	2.23	0.41
1:A:110:ASP:OD1	1:A:110:ASP:C	2.57	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:HG23	1:B:284:VAL:HG13	2.02	0.41
1:B:155:VAL:CG2	1:B:205:LEU:HD22	2.48	0.41
1:B:186:ARG:HA	1:B:189:PHE:CD2	2.56	0.41
1:C:85:MET:HG3	1:C:245:MET:SD	2.60	0.41
1:A:184:THR:OG1	1:A:188:ASN:HB2	2.21	0.41
1:A:79:LEU:C	1:A:79:LEU:HD12	2.41	0.41
1:B:122:ASP:OD2	1:B:256:ARG:NH2	2.48	0.41
1:B:175:ALA:HB3	1:B:191:GLN:HB3	2.03	0.41
1:B:58:VAL:HG11	1:B:158:ILE:HB	2.03	0.41
1:B:86:ASP:C	1:B:86:ASP:OD2	2.60	0.41
1:C:125:THR:O	1:C:236:ILE:CD1	2.68	0.40
1:B:184:THR:OG1	1:B:188:ASN:HB2	2.21	0.40
1:A:287:VAL:C	1:A:289:PRO:HD3	2.41	0.40
1:B:158:ILE:HG23	1:B:168:ILE:HD13	2.03	0.40
1:A:161:PRO:HA	1:A:199:GLY:CA	2.38	0.40
1:C:79:LEU:HD12	1:C:79:LEU:C	2.41	0.40
1:A:257:GLY:H	1:A:323:ALA:CA	2.28	0.40
1:C:310:LYS:HG3	1:C:311:PRO:CD	2.45	0.40
1:A:220:PHE:HE1	1:A:222:LYS:HD3	1.87	0.40
1:B:119:VAL:O	1:B:119:VAL:HG23	2.20	0.40
1:B:94:ASN:CA	1:B:126:ASP:O	2.67	0.40
1:C:55:ALA:HB3	1:C:56:PRO:HD3	2.03	0.40
1:B:119:VAL:HG22	1:B:129:VAL:HB	2.04	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:C	1:B:53:ARG:NH2[1_556]	1.48	0.72
1:A:225:ASP:N	1:B:53:ARG:NH2[1_556]	1.75	0.45
1:A:224:ASN:O	1:B:53:ARG:NH2[1_556]	1.86	0.34
1:A:225:ASP:OD1	1:C:42:MET:CE[1_556]	1.94	0.26
1:A:225:ASP:CB	1:B:53:ARG:NH1[1_556]	2.03	0.17

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	285/314 (91%)	234 (82%)	39 (14%)	12 (4%)	3 18
1	B	285/314 (91%)	233 (82%)	37 (13%)	15 (5%)	2 14
1	C	285/314 (91%)	235 (82%)	39 (14%)	11 (4%)	4 20
All	All	855/942 (91%)	702 (82%)	115 (14%)	38 (4%)	3 17

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLY
1	A	295	ASN
1	A	296	ALA
1	A	298	ILE
1	A	334	VAL
1	B	220	PHE
1	B	227	GLU
1	B	285	ASN
1	B	298	ILE
1	C	295	ASN
1	C	296	ALA
1	C	298	ILE
1	A	222	LYS
1	A	301	ASN
1	B	223	SER
1	B	291	GLY
1	B	296	ALA
1	B	301	ASN
1	C	96	HIS
1	C	301	ASN
1	A	96	HIS
1	A	124	LEU
1	C	124	LEU
1	C	222	LYS
1	B	96	HIS
1	B	124	LEU
1	B	162	TYR
1	C	218	LEU
1	A	351	TYR
1	B	343	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	351	TYR
1	C	343	THR
1	A	72	ASN
1	A	343	THR
1	B	295	ASN
1	C	308	ASP
1	B	288	SER
1	C	351	TYR

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	225/253 (89%)	206 (92%)	19 (8%)	14	43
1	B	225/253 (89%)	205 (91%)	20 (9%)	12	39
1	C	225/253 (89%)	208 (92%)	17 (8%)	16	49
All	All	675/759 (89%)	619 (92%)	56 (8%)	14	44

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	117	LEU
1	A	119	VAL
1	A	135	THR
1	A	160	ASN
1	A	163	ASN
1	A	170	GLN
1	A	205	LEU
1	A	218	LEU
1	A	222	LYS
1	A	227	GLU
1	A	240	LEU
1	A	285	ASN
1	A	286	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	290	ASP
1	A	302	ASP
1	A	307	VAL
1	A	310	LYS
1	A	351	TYR
1	B	63	ASN
1	B	117	LEU
1	B	119	VAL
1	B	135	THR
1	B	160	ASN
1	B	163	ASN
1	B	205	LEU
1	B	218	LEU
1	B	219	SER
1	B	224	ASN
1	B	227	GLU
1	B	240	LEU
1	B	286	GLU
1	B	289	PRO
1	B	290	ASP
1	B	302	ASP
1	B	307	VAL
1	B	308	ASP
1	B	310	LYS
1	B	351	TYR
1	C	63	ASN
1	C	117	LEU
1	C	119	VAL
1	C	135	THR
1	C	160	ASN
1	C	163	ASN
1	C	205	LEU
1	C	218	LEU
1	C	224	ASN
1	C	227	GLU
1	C	240	LEU
1	C	286	GLU
1	C	290	ASP
1	C	302	ASP
1	C	307	VAL
1	C	310	LYS
1	C	351	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	63	ASN
1	A	73	GLN
1	A	160	ASN
1	A	163	ASN
1	A	170	GLN
1	A	182	ASN
1	A	191	GLN
1	A	197	ASN
1	A	200	ASN
1	A	216	ASN
1	A	239	GLN
1	A	295	ASN
1	A	299	GLN
1	A	345	GLN
1	B	60	ASN
1	B	63	ASN
1	B	73	GLN
1	B	160	ASN
1	B	163	ASN
1	B	182	ASN
1	B	191	GLN
1	B	197	ASN
1	B	200	ASN
1	B	216	ASN
1	B	239	GLN
1	B	285	ASN
1	B	295	ASN
1	B	299	GLN
1	B	345	GLN
1	C	60	ASN
1	C	63	ASN
1	C	73	GLN
1	C	160	ASN
1	C	163	ASN
1	C	170	GLN
1	C	182	ASN
1	C	191	GLN
1	C	200	ASN
1	C	216	ASN
1	C	239	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	295	ASN
1	C	299	GLN
1	C	309	ASN
1	C	345	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	291/314 (92%)	-0.12	15 (5%) 31 13	17, 55, 156, 176	0
1	B	285/314 (90%)	-0.00	13 (4%) 36 16	22, 71, 167, 179	1 (0%)
1	C	291/314 (92%)	0.31	32 (10%) 7 2	27, 81, 179, 191	0
All	All	867/942 (92%)	0.06	60 (6%) 20 7	17, 70, 172, 191	1 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	67	ASN	9.0
1	C	66	LEU	8.8
1	C	74	LEU	6.1
1	C	305	ILE	5.3
1	C	68	THR	5.1
1	C	298	ILE	5.1
1	C	226	GLY	5.0
1	C	65	GLY	4.8
1	B	219	SER	4.7
1	A	221	ASP	4.6
1	A	262	GLY	4.4
1	B	185	GLY	4.3
1	A	225	ASP	4.3
1	C	285	ASN	4.2
1	C	227	GLU	4.2
1	B	226	GLY	4.0
1	A	226	GLY	3.9
1	C	72	ASN	3.9
1	C	301	ASN	3.9
1	C	223	SER	3.8
1	C	224	ASN	3.8
1	C	260	GLY	3.6
1	C	69	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	264	ARG	3.5
1	B	227	GLU	3.5
1	B	353	ALA	3.5
1	A	219	SER	3.5
1	C	314	SER	3.3
1	C	73	GLN	3.3
1	C	289	PRO	3.2
1	A	223	SER	3.2
1	B	262	GLY	3.2
1	A	227	GLU	3.1
1	B	67	ASN	3.1
1	C	347	THR	3.1
1	B	305	ILE	3.0
1	A	334	VAL	3.0
1	B	334	VAL	3.0
1	C	288	SER	3.0
1	C	185	GLY	2.9
1	A	220	PHE	2.9
1	B	303	LEU	2.9
1	B	71	HIS	2.9
1	C	335	VAL	2.9
1	A	301	ASN	2.9
1	C	297	GLY	2.8
1	C	70	SER	2.8
1	B	70	SER	2.5
1	A	353	ALA	2.5
1	C	281	GLY	2.5
1	A	281	GLY	2.4
1	C	313	ILE	2.2
1	C	225	ASP	2.2
1	C	341	GLN	2.1
1	A	222	LYS	2.1
1	C	162	TYR	2.1
1	A	224	ASN	2.1
1	A	328	GLY	2.1
1	B	314	SER	2.0
1	C	303	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.