Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:47 am BST

PDB ID	:	5M1B
Title	:	Crystal structure of C-terminally tagged apo-UbiD from E. coli
Authors	:	White, M.; Leys, D.
Deposited on	:	2016-10-07
Resolution	:	3.15 Å(reported)

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

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

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

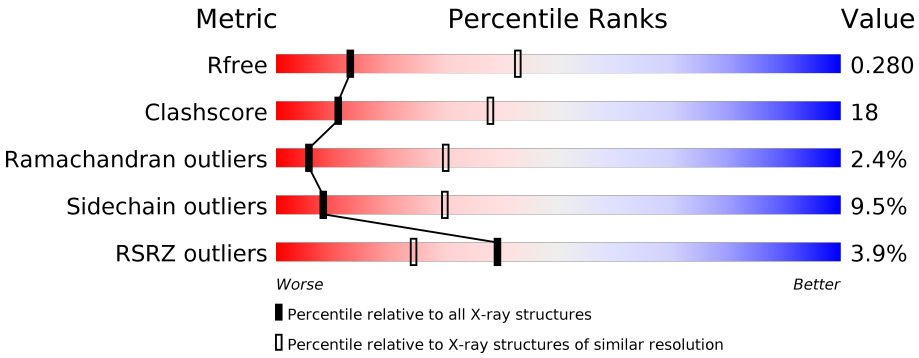
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	2% 57% 26% • 13%
1	B	505	6% 49% 36% 6% 9%
1	C	505	2% 53% 32% • 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10593 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 3-octaprenyl-4-hydroxybenzoate carboxy-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3451	2205	588	641	17			
1	B	461	Total	C	N	O	S	0	0	0
			3625	2318	617	673	17			
1	C	448	Total	C	N	O	S	0	0	0
			3517	2252	596	652	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP P0AAB5
A	499	GLU	-	expression tag	UNP P0AAB5
A	500	HIS	-	expression tag	UNP P0AAB5
A	501	HIS	-	expression tag	UNP P0AAB5
A	502	HIS	-	expression tag	UNP P0AAB5
A	503	HIS	-	expression tag	UNP P0AAB5
A	504	HIS	-	expression tag	UNP P0AAB5
A	505	HIS	-	expression tag	UNP P0AAB5
B	498	LEU	-	expression tag	UNP P0AAB5
B	499	GLU	-	expression tag	UNP P0AAB5
B	500	HIS	-	expression tag	UNP P0AAB5
B	501	HIS	-	expression tag	UNP P0AAB5
B	502	HIS	-	expression tag	UNP P0AAB5
B	503	HIS	-	expression tag	UNP P0AAB5
B	504	HIS	-	expression tag	UNP P0AAB5
B	505	HIS	-	expression tag	UNP P0AAB5
C	498	LEU	-	expression tag	UNP P0AAB5
C	499	GLU	-	expression tag	UNP P0AAB5
C	500	HIS	-	expression tag	UNP P0AAB5
C	501	HIS	-	expression tag	UNP P0AAB5
C	502	HIS	-	expression tag	UNP P0AAB5
C	503	HIS	-	expression tag	UNP P0AAB5
C	504	HIS	-	expression tag	UNP P0AAB5

Continued on next page...

Continued from previous page...

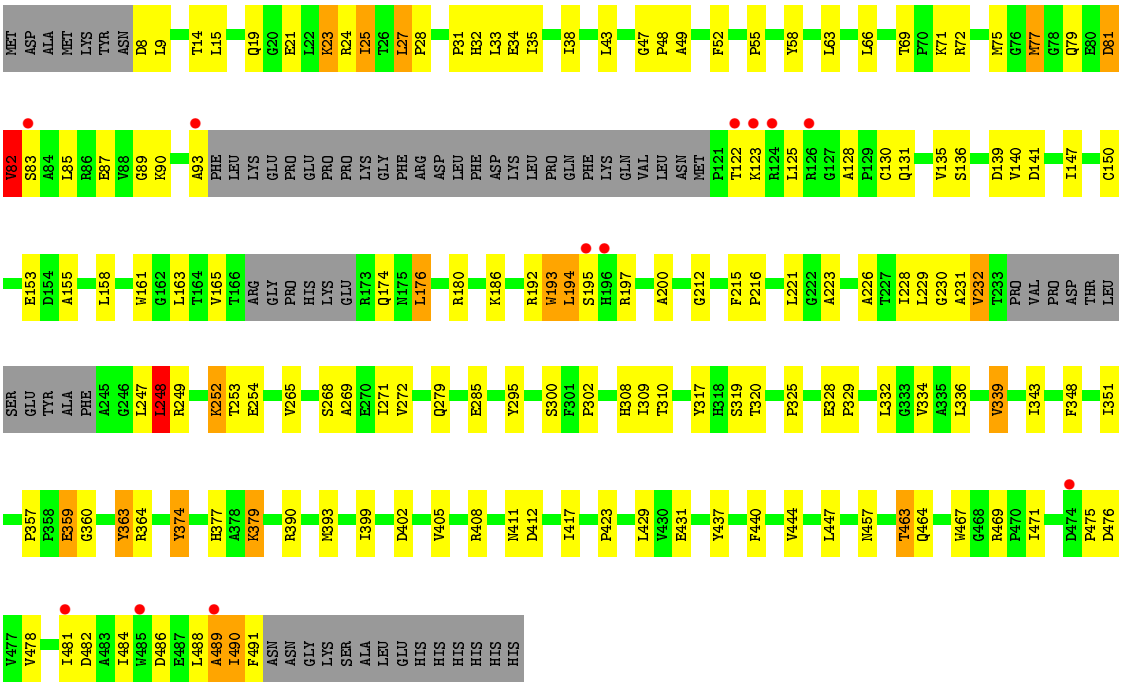
Chain	Residue	Modelled	Actual	Comment	Reference
C	505	HIS	-	expression tag	UNP P0AAB5

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

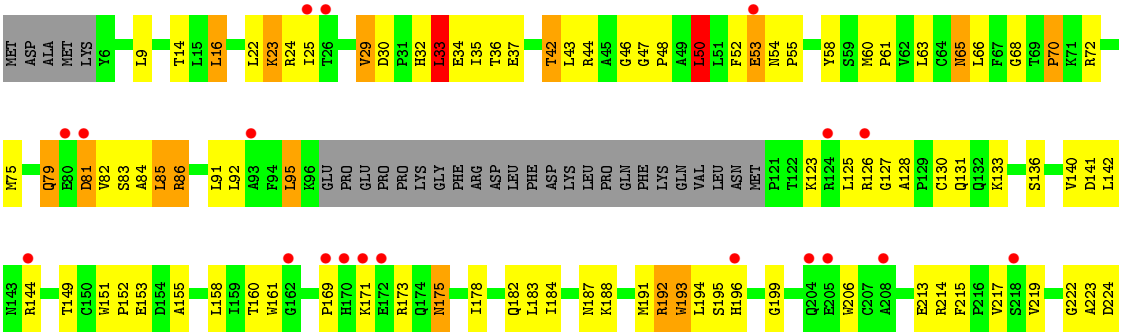
- Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

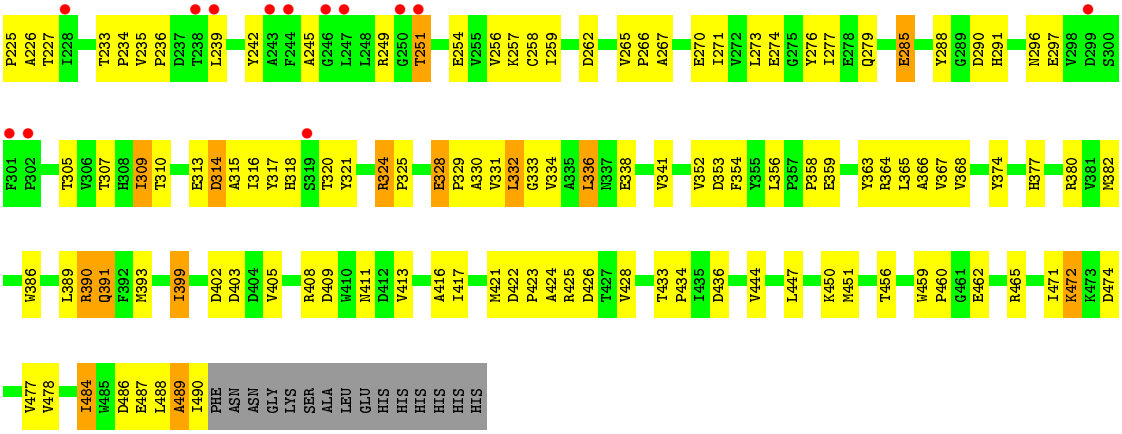
Chain A:



- Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

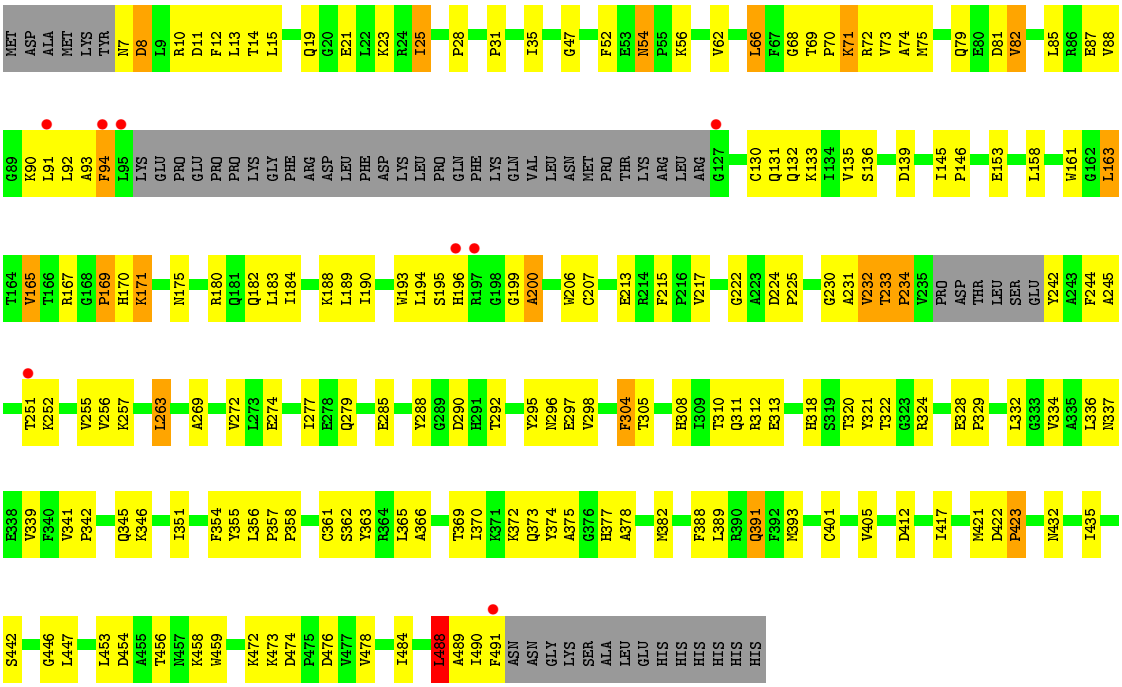
Chain B:





• Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	210.19Å 210.19Å 109.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.15 29.89 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.90-3.15) 100.0 (29.89-3.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.23 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.221 , 0.277 0.221 , 0.280	Depositor DCC
R_{free} test set	2151 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	74.2	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10593	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.54	0/3534	0.78	0/4812
1	B	0.55	0/3717	0.78	4/5065 (0.1%)
1	C	0.52	0/3606	0.77	2/4914 (0.0%)
All	All	0.54	0/10857	0.78	6/14791 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	488	LEU	CA-CB-CG	6.82	130.98	115.30
1	B	336	LEU	CA-CB-CG	5.96	129.01	115.30
1	C	66	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	399	ILE	N-CA-C	-5.43	96.34	111.00
1	B	50	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	63	LEU	CA-CB-CG	5.18	127.22	115.30

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	3451	0	3425	125	0
1	B	3625	0	3594	153	0
1	C	3517	0	3475	122	0
All	All	10593	0	10494	382	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 18.

All (382) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HD2	1:A:339:VAL:HG13	1.27	1.12
1:A:25:ILE:HD12	1:A:52:PHE:CD1	1.87	1.08
1:C:93:ALA:HB3	1:C:346:LYS:NZ	1.70	1.06
1:C:135:VAL:HG13	1:C:139:ASP:HB3	1.43	0.98
1:A:27:LEU:HD23	1:A:28:PRO:HD2	1.49	0.95
1:B:227:THR:HA	1:B:245:ALA:HB1	1.48	0.94
1:A:247:LEU:HD12	1:A:248:LEU:H	1.32	0.93
1:C:93:ALA:HB3	1:C:346:LYS:HZ3	1.26	0.92
1:B:234:PRO:HG2	1:B:391:GLN:OE1	1.69	0.91
1:A:82:VAL:H	1:A:85:LEU:HD12	1.35	0.90
1:A:131:GLN:HA	1:A:310:THR:HG23	1.51	0.90
1:C:25:ILE:HG22	1:C:52:PHE:HA	1.54	0.88
1:A:131:GLN:HA	1:A:310:THR:CG2	2.02	0.88
1:B:32:HIS:HA	1:B:149:THR:HB	1.59	0.85
1:C:355:TYR:CE2	1:C:357:PRO:HG3	2.10	0.84
1:A:90:LYS:HD2	1:A:339:VAL:CG1	2.08	0.83
1:A:158:LEU:HD11	1:A:180:ARG:HG3	1.60	0.82
1:C:69:THR:HG21	1:C:71:LYS:HE2	1.60	0.82
1:C:93:ALA:CB	1:C:346:LYS:HZ3	1.92	0.82
1:C:93:ALA:CB	1:C:346:LYS:NZ	2.42	0.82
1:A:25:ILE:HD12	1:A:52:PHE:HD1	1.41	0.81
1:C:135:VAL:CG1	1:C:139:ASP:HB3	2.13	0.79
1:B:222:GLY:O	1:B:270:GLU:HG2	1.83	0.79
1:C:188:LYS:HD3	1:C:305:THR:HG23	1.64	0.78
1:A:163:LEU:HB3	1:A:176:LEU:HD21	1.64	0.78
1:A:158:LEU:HD11	1:A:180:ARG:CG	2.14	0.78
1:B:219:VAL:HB	1:B:273:LEU:HD12	1.66	0.77
1:A:47:GLY:O	1:A:72:ARG:NH2	2.19	0.76
1:A:130:CYS:O	1:A:310:THR:HG22	1.85	0.76
1:A:247:LEU:HD12	1:A:248:LEU:N	2.01	0.76
1:B:313:GLU:C	1:B:315:ALA:H	1.85	0.76
1:B:23:LYS:HB2	1:B:48:PRO:HG2	1.69	0.74
1:C:7:ASN:O	1:C:8:ASP:HB2	1.87	0.73
1:A:249:ARG:NH2	1:A:253:THR:HA	2.03	0.73
1:B:234:PRO:CG	1:B:391:GLN:OE1	2.37	0.73
1:B:242:TYR:HE1	1:B:266:PRO:HG3	1.54	0.73
1:B:24:ARG:NH1	1:B:53:GLU:OE2	2.21	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:H	1:A:197:ARG:NH1	1.88	0.72
1:B:382:MET:SD	1:B:428:VAL:HG21	2.30	0.72
1:B:126:ARG:C	1:B:128:ALA:H	1.92	0.71
1:B:9:LEU:HD13	1:B:223:ALA:O	1.90	0.71
1:B:192:ARG:HG3	1:B:285:GLU:OE2	1.91	0.70
1:A:25:ILE:CD1	1:A:52:PHE:HD1	2.04	0.70
1:A:317:TYR:CE2	1:A:319:SER:HB2	2.27	0.70
1:B:55:PRO:HB2	1:B:58:TYR:HB2	1.74	0.70
1:A:249:ARG:HH21	1:A:253:THR:HA	1.56	0.70
1:B:125:LEU:HB2	1:B:128:ALA:HB2	1.73	0.69
1:B:356:LEU:HD22	1:B:363:TYR:HA	1.74	0.69
1:C:35:ILE:HD13	1:C:62:VAL:HG11	1.75	0.69
1:A:136:SER:O	1:A:139:ASP:HB2	1.92	0.68
1:B:290:ASP:HB2	1:B:296:ASN:HD21	1.58	0.68
1:A:489:ALA:HB1	1:A:491:PHE:CE2	2.28	0.68
1:C:230:GLY:HA2	1:C:244:PHE:CD2	2.29	0.68
1:B:408:ARG:HH11	1:B:408:ARG:HG3	1.59	0.68
1:B:486:ASP:C	1:B:488:LEU:H	1.97	0.68
1:C:435:ILE:O	1:C:446:GLY:HA2	1.93	0.67
1:A:405:VAL:HG13	1:A:412:ASP:HB3	1.76	0.67
1:A:226:ALA:HB3	1:A:249:ARG:HH11	1.59	0.67
1:B:391:GLN:HE21	1:B:391:GLN:H	1.43	0.67
1:A:471:ILE:HG21	1:B:151:TRP:CE3	2.30	0.66
1:A:25:ILE:CD1	1:A:52:PHE:CD1	2.73	0.66
1:C:230:GLY:HA3	1:C:245:ALA:HB2	1.77	0.66
1:A:63:LEU:HD21	1:A:66:LEU:HD13	1.78	0.65
1:B:47:GLY:O	1:B:72:ARG:NH2	2.29	0.65
1:C:374:TYR:O	1:C:377:HIS:HB2	1.97	0.65
1:A:226:ALA:HB3	1:A:249:ARG:NH1	2.10	0.65
1:B:188:LYS:HD3	1:B:305:THR:HG23	1.79	0.65
1:C:130:CYS:O	1:C:310:THR:HG22	1.95	0.65
1:A:194:LEU:H	1:A:197:ARG:HH11	1.43	0.64
1:B:214:ARG:HB3	1:B:276:TYR:CD2	2.32	0.64
1:A:231:ALA:O	1:A:232:VAL:O	2.16	0.64
1:B:91:LEU:O	1:B:95:LEU:HG	1.97	0.64
1:B:52:PHE:O	1:B:55:PRO:HD3	1.97	0.63
1:A:295:TYR:CE2	1:B:471:ILE:HA	2.34	0.63
1:C:167:ARG:HH11	1:C:263:LEU:HD23	1.64	0.63
1:A:247:LEU:CD1	1:A:248:LEU:H	2.09	0.63
1:C:136:SER:O	1:C:139:ASP:HB2	1.98	0.63
1:C:354:PHE:CE2	1:C:356:LEU:HD11	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:HG13	1:A:309:ILE:HD11	1.79	0.62
1:B:258:CYS:SG	1:B:265:VAL:HG13	2.39	0.62
1:B:33:LEU:N	1:B:149:THR:O	2.25	0.62
1:C:153:GLU:HB2	1:C:295:TYR:CZ	2.35	0.61
1:B:259:ILE:HD13	1:B:310:THR:HG21	1.82	0.61
1:B:29:VAL:HG21	1:B:52:PHE:CD1	2.36	0.61
1:C:69:THR:HG21	1:C:71:LYS:CE	2.30	0.61
1:C:337:ASN:HD22	1:C:356:LEU:HD13	1.66	0.61
1:B:474:ASP:HB3	1:B:477:VAL:HG23	1.83	0.61
1:B:484:ILE:HG23	1:B:488:LEU:HG	1.81	0.61
1:A:9:LEU:HB2	1:A:223:ALA:O	2.01	0.61
1:A:82:VAL:H	1:A:85:LEU:CD1	2.11	0.61
1:C:85:LEU:HD23	1:C:88:VAL:HG21	1.83	0.61
1:B:259:ILE:HD12	1:B:259:ILE:H	1.66	0.60
1:B:42:THR:HG21	1:B:50:LEU:HD21	1.84	0.60
1:C:145:ILE:HG22	1:C:146:PRO:HD2	1.81	0.60
1:B:290:ASP:HB2	1:B:296:ASN:ND2	2.16	0.60
1:B:222:GLY:HA2	1:B:318:HIS:HB2	1.83	0.60
1:B:320:THR:HG23	1:B:321:TYR:N	2.17	0.60
1:C:10:ARG:HA	1:C:13:LEU:HD12	1.81	0.60
1:C:85:LEU:HA	1:C:88:VAL:HG23	1.82	0.60
1:C:290:ASP:HB3	1:C:292:THR:H	1.66	0.60
1:C:474:ASP:OD1	1:C:476:ASP:HB2	2.02	0.60
1:B:226:ALA:HB3	1:B:249:ARG:HE	1.67	0.59
1:C:158:LEU:HD11	1:C:180:ARG:HB2	1.84	0.59
1:B:313:GLU:C	1:B:315:ALA:N	2.55	0.59
1:A:77:MET:HB2	1:A:79:GLN:OE1	2.03	0.59
1:C:12:PHE:CD2	1:C:225:PRO:HG3	2.38	0.59
1:B:131:GLN:HG2	1:B:259:ILE:HD11	1.85	0.59
1:C:337:ASN:ND2	1:C:356:LEU:HD13	2.18	0.59
1:A:82:VAL:N	1:A:85:LEU:HD12	2.12	0.58
1:C:272:VAL:HB	1:C:310:THR:HB	1.85	0.58
1:C:28:PRO:HA	1:C:54:ASN:O	2.03	0.58
1:A:463:THR:OG1	1:A:464:GLN:N	2.36	0.58
1:B:224:ASP:HB2	1:B:225:PRO:HD2	1.85	0.58
1:C:182:GLN:OE1	1:C:285:GLU:HG2	2.03	0.58
1:C:82:VAL:HG12	1:C:85:LEU:HD12	1.85	0.57
1:B:158:LEU:O	1:B:160:THR:HG23	2.05	0.57
1:A:212:GLY:H	1:A:279:GLN:HE22	1.52	0.57
1:C:199:GLY:O	1:C:200:ALA:CB	2.52	0.57
1:B:222:GLY:HA2	1:B:318:HIS:CB	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:ALA:O	1:C:382:MET:HG3	2.05	0.56
1:A:360:GLY:O	1:A:364:ARG:HB2	2.04	0.56
1:B:142:LEU:HD12	1:B:187:ASN:HA	1.86	0.56
1:B:486:ASP:O	1:B:488:LEU:N	2.38	0.56
1:C:369:THR:HA	1:C:401:CYS:O	2.05	0.56
1:C:85:LEU:HA	1:C:88:VAL:CG2	2.35	0.56
1:B:249:ARG:HH11	1:B:251:THR:HG23	1.71	0.56
1:A:165:VAL:HG21	1:A:265:VAL:HG12	1.87	0.56
1:C:31:PRO:HA	1:C:35:ILE:HD12	1.88	0.56
1:A:379:LYS:HD3	1:C:432:ASN:O	2.05	0.56
1:A:194:LEU:N	1:A:197:ARG:NH1	2.53	0.56
1:A:32:HIS:CE1	1:A:33:LEU:HD12	2.41	0.55
1:A:81:ASP:H	1:A:85:LEU:HD11	1.71	0.55
1:A:161:TRP:CD1	1:A:320:THR:HB	2.42	0.55
1:C:69:THR:CG2	1:C:71:LYS:HE2	2.36	0.55
1:A:193:TRP:HB2	1:A:200:ALA:HB2	1.89	0.55
1:A:25:ILE:O	1:A:25:ILE:HD13	2.07	0.55
1:C:153:GLU:HB2	1:C:295:TYR:CE1	2.42	0.55
1:B:65:ASN:HD22	1:B:72:ARG:HH12	1.53	0.55
1:B:30:ASP:HB3	1:B:34:GLU:HG3	1.89	0.55
1:B:386:TRP:NE1	1:B:450:LYS:HD3	2.23	0.54
1:B:459:TRP:O	1:B:462:GLU:HB2	2.07	0.54
1:C:66:LEU:HD23	1:C:318:HIS:CE1	2.42	0.54
1:B:81:ASP:C	1:B:83:SER:H	2.11	0.54
1:C:405:VAL:HG13	1:C:412:ASP:HB3	1.89	0.54
1:B:408:ARG:HG3	1:B:408:ARG:NH1	2.22	0.54
1:B:42:THR:O	1:B:46:GLY:N	2.32	0.54
1:C:304:PHE:C	1:C:304:PHE:CD1	2.81	0.54
1:A:79:GLN:CB	1:A:85:LEU:HD13	2.38	0.53
1:B:126:ARG:C	1:B:128:ALA:N	2.62	0.53
1:C:87:GLU:HA	1:C:90:LYS:HD2	1.91	0.53
1:B:61:PRO:HB2	1:B:316:ILE:HG23	1.90	0.53
1:A:79:GLN:HB2	1:A:85:LEU:HD13	1.90	0.53
1:A:325:PRO:HB2	1:A:359:GLU:HA	1.91	0.53
1:B:363:TYR:CE1	1:B:364:ARG:HG2	2.44	0.53
1:C:365:LEU:HD23	1:C:366:ALA:N	2.24	0.53
1:C:274:GLU:HB2	1:C:308:HIS:HB2	1.91	0.53
1:A:475:PRO:O	1:A:478:VAL:HB	2.09	0.52
1:B:390:ARG:O	1:B:393:MET:HG2	2.09	0.52
1:C:136:SER:HB3	1:C:308:HIS:CD2	2.43	0.52
1:C:93:ALA:HB3	1:C:346:LYS:HZ1	1.67	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:HG3	1:B:288:TYR:OH	2.08	0.52
1:B:291:HIS:O	1:B:325:PRO:HD3	2.08	0.52
1:B:313:GLU:O	1:B:315:ALA:N	2.38	0.52
1:A:128:ALA:HB3	1:A:131:GLN:HG3	1.92	0.52
1:A:212:GLY:H	1:A:279:GLN:NE2	2.07	0.52
1:A:429:LEU:HD22	1:B:424:ALA:HA	1.90	0.52
1:A:90:LYS:CG	1:A:93:ALA:HB3	2.38	0.52
1:C:54:ASN:OD1	1:C:54:ASN:N	2.42	0.52
1:B:65:ASN:ND2	1:B:72:ARG:HH12	2.07	0.52
1:B:193:TRP:HH2	1:B:215:PHE:HE2	1.57	0.52
1:A:193:TRP:HA	1:A:197:ARG:HH11	1.75	0.52
1:B:352:VAL:HG21	1:B:403:ASP:HB3	1.92	0.52
1:B:474:ASP:O	1:B:478:VAL:HG23	2.10	0.52
1:B:42:THR:HG22	1:B:47:GLY:HA3	1.91	0.51
1:C:130:CYS:CB	1:C:269:ALA:HB3	2.39	0.51
1:C:131:GLN:HA	1:C:310:THR:HG23	1.92	0.51
1:A:23:LYS:HD2	1:B:489:ALA:O	2.10	0.51
1:B:42:THR:CG2	1:B:47:GLY:HA3	2.40	0.51
1:B:75:MET:HA	1:B:79:GLN:O	2.11	0.51
1:C:130:CYS:O	1:C:310:THR:CG2	2.59	0.51
1:A:90:LYS:CD	1:A:339:VAL:HG13	2.19	0.51
1:B:417:ILE:O	1:B:421:MET:HG2	2.11	0.51
1:A:399:ILE:HD13	1:A:417:ILE:HD11	1.93	0.51
1:A:437:TYR:H	1:A:437:TYR:HD1	1.58	0.51
1:B:353:ASP:CG	1:B:408:ARG:HH12	2.13	0.51
1:B:42:THR:HG22	1:B:47:GLY:CA	2.41	0.51
1:C:339:VAL:O	1:C:342:PRO:HD2	2.10	0.51
1:C:341:VAL:HB	1:C:342:PRO:HD3	1.92	0.51
1:A:193:TRP:HE1	1:A:302:PRO:HG2	1.75	0.51
1:B:329:PRO:O	1:B:333:GLY:N	2.42	0.51
1:C:354:PHE:HE2	1:C:356:LEU:HD11	1.75	0.51
1:B:328:GLU:HB3	1:B:329:PRO:HD3	1.93	0.50
1:B:82:VAL:HG12	1:B:85:LEU:HD13	1.92	0.50
1:C:351:ILE:HA	1:C:370:ILE:HG22	1.94	0.50
1:A:153:GLU:HB2	1:A:295:TYR:CZ	2.46	0.50
1:C:25:ILE:HG21	1:C:52:PHE:CD1	2.46	0.50
1:A:21:GLU:HB3	1:A:72:ARG:HD3	1.94	0.50
1:B:55:PRO:HG3	1:B:60:MET:O	2.12	0.50
1:B:70:PRO:HD3	1:B:331:VAL:HG13	1.94	0.50
1:C:320:THR:HG23	1:C:321:TYR:N	2.27	0.50
1:C:145:ILE:CG2	1:C:146:PRO:HD2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:CG2	1:A:71:LYS:HB3	2.42	0.50
1:A:228:ILE:C	1:A:230:GLY:H	2.15	0.49
1:A:69:THR:HG22	1:A:71:LYS:HB3	1.94	0.49
1:B:320:THR:HG23	1:B:321:TYR:H	1.77	0.49
1:B:329:PRO:HA	1:B:332:LEU:HB2	1.94	0.49
1:C:233:THR:HB	1:C:234:PRO:HD2	1.94	0.49
1:C:373:GLN:O	1:C:459:TRP:CH2	2.65	0.49
1:B:258:CYS:HB3	1:B:274:GLU:CD	2.33	0.49
1:C:231:ALA:O	1:C:232:VAL:HG13	2.11	0.49
1:B:66:LEU:O	1:B:72:ARG:HD2	2.13	0.49
1:B:413:VAL:O	1:B:416:ALA:HB3	2.13	0.48
1:A:136:SER:HB3	1:A:308:HIS:CD2	2.48	0.48
1:B:459:TRP:N	1:B:459:TRP:CD1	2.80	0.48
1:C:10:ARG:HG3	1:C:312:ARG:HH22	1.78	0.48
1:C:484:ILE:HD12	1:C:488:LEU:HD11	1.95	0.48
1:C:194:LEU:O	1:C:196:HIS:N	2.46	0.48
1:B:32:HIS:CD2	1:B:33:LEU:HG	2.49	0.48
1:A:490:ILE:HG21	1:B:42:THR:HG23	1.95	0.48
1:A:374:TYR:HE1	1:A:377:HIS:HA	1.77	0.48
1:A:83:SER:O	1:A:87:GLU:HB2	2.14	0.48
1:B:365:LEU:HD23	1:B:366:ALA:N	2.28	0.48
1:C:132:GLN:HB3	1:C:313:GLU:HG3	1.94	0.48
1:A:390:ARG:O	1:A:393:MET:HG2	2.13	0.48
1:B:374:TYR:O	1:B:377:HIS:HB2	2.13	0.48
1:C:165:VAL:HA	1:C:175:ASN:O	2.14	0.48
1:A:141:ASP:OD1	1:A:186:LYS:HG3	2.13	0.48
1:A:55:PRO:HG2	1:A:58:TYR:HB2	1.96	0.48
1:B:257:LYS:NZ	1:B:262:ASP:OD1	2.36	0.48
1:C:233:THR:CB	1:C:234:PRO:HD2	2.44	0.48
1:C:456:THR:O	1:C:458:LYS:HD3	2.13	0.48
1:A:15:LEU:O	1:A:19:GLN:HG2	2.14	0.48
1:A:348:PHE:HB2	1:A:351:ILE:CD1	2.43	0.48
1:A:411:ASN:HA	1:B:359:GLU:HG2	1.95	0.48
1:B:409:ASP:OD1	1:B:411:ASN:N	2.43	0.47
1:A:32:HIS:O	1:A:33:LEU:HB2	2.13	0.47
1:B:194:LEU:O	1:B:196:HIS:N	2.48	0.47
1:B:123:LYS:O	1:B:254:GLU:HA	2.13	0.47
1:B:130:CYS:HB3	1:B:267:ALA:O	2.14	0.47
1:C:288:TYR:O	1:C:295:TYR:HA	2.14	0.47
1:A:125:LEU:HD11	1:A:254:GLU:OE1	2.14	0.47
1:A:221:LEU:HB2	1:A:271:ILE:HB	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HB2	1:B:22:LEU:HB2	1.95	0.47
1:C:130:CYS:HB3	1:C:269:ALA:HB3	1.96	0.47
1:A:34:GLU:O	1:A:38:ILE:HG13	2.15	0.47
1:A:469:ARG:NH2	1:B:297:GLU:OE2	2.48	0.47
1:B:226:ALA:CB	1:B:249:ARG:HE	2.28	0.47
1:C:91:LEU:O	1:C:94:PHE:HB2	2.14	0.47
1:A:135:VAL:HG13	1:A:139:ASP:HB3	1.97	0.47
1:B:29:VAL:HG21	1:B:52:PHE:HD1	1.78	0.47
1:B:386:TRP:CE2	1:B:450:LYS:HD3	2.50	0.47
1:A:272:VAL:N	1:A:310:THR:O	2.47	0.47
1:A:328:GLU:HB3	1:A:329:PRO:HD3	1.97	0.47
1:A:363:TYR:CZ	1:A:364:ARG:HG3	2.49	0.47
1:C:356:LEU:HD23	1:C:363:TYR:HA	1.96	0.47
1:A:194:LEU:N	1:A:197:ARG:HH11	2.12	0.47
1:A:488:LEU:HD21	1:B:25:ILE:HG23	1.96	0.46
1:B:79:GLN:HG3	1:B:84:ALA:HB3	1.97	0.46
1:C:183:LEU:HA	1:C:189:LEU:HD23	1.96	0.46
1:B:169:PRO:HB3	1:B:206:TRP:CE3	2.51	0.46
1:B:82:VAL:HA	1:B:85:LEU:HD12	1.97	0.46
1:C:334:VAL:CG2	1:C:358:PRO:HD3	2.45	0.46
1:B:65:ASN:ND2	1:B:68:GLY:HA3	2.30	0.46
1:C:232:VAL:O	1:C:336:LEU:HD13	2.15	0.46
1:B:425:ARG:HG2	1:B:426:ASP:OD1	2.15	0.46
1:B:444:VAL:CG2	1:B:447:LEU:HB3	2.45	0.46
1:C:328:GLU:HB3	1:C:329:PRO:HD3	1.96	0.46
1:A:130:CYS:O	1:A:310:THR:CG2	2.61	0.46
1:A:165:VAL:CG1	1:A:174:GLN:NE2	2.79	0.46
1:C:21:GLU:OE2	1:C:71:LYS:NZ	2.49	0.46
1:A:23:LYS:HE3	1:A:24:ARG:O	2.16	0.46
1:B:354:PHE:HD1	1:B:368:VAL:HG22	1.81	0.46
1:B:459:TRP:HB3	1:B:460:PRO:CD	2.45	0.46
1:C:133:LYS:HB2	1:C:311:GLN:HG3	1.98	0.46
1:A:357:PRO:HB3	1:A:359:GLU:OE1	2.16	0.46
1:B:402:ASP:OD2	1:B:456:THR:HA	2.16	0.46
1:A:130:CYS:CB	1:A:269:ALA:HB3	2.45	0.46
1:C:230:GLY:HA2	1:C:244:PHE:HD2	1.79	0.46
1:C:421:MET:HG2	1:C:454:ASP:O	2.16	0.46
1:B:242:TYR:CE1	1:B:266:PRO:HG3	2.44	0.45
1:A:153:GLU:OE1	1:B:472:LYS:NZ	2.49	0.45
1:C:170:HIS:C	1:C:171:LYS:HG2	2.37	0.45
1:C:372:LYS:HE2	1:C:459:TRP:CD1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HG3	1:A:252:LYS:H	1.57	0.45
1:A:90:LYS:HA	1:A:93:ALA:HB3	1.98	0.45
1:B:82:VAL:CG1	1:B:85:LEU:CD1	2.94	0.45
1:C:47:GLY:O	1:C:72:ARG:NH2	2.49	0.45
1:B:35:ILE:HG23	1:B:52:PHE:CE2	2.52	0.45
1:B:82:VAL:HG13	1:B:85:LEU:CD1	2.47	0.45
1:C:62:VAL:HG23	1:C:146:PRO:HG2	1.99	0.45
1:C:169:PRO:HG3	1:C:206:TRP:HA	1.98	0.45
1:A:490:ILE:HG13	1:B:23:LYS:HG3	1.99	0.45
1:C:337:ASN:O	1:C:339:VAL:N	2.50	0.45
1:A:228:ILE:O	1:A:230:GLY:N	2.46	0.44
1:A:457:ASN:OD1	1:A:467:TRP:NE1	2.49	0.44
1:B:136:SER:HA	1:B:307:THR:O	2.18	0.44
1:A:440:PHE:HA	1:B:465:ARG:NH2	2.31	0.44
1:C:388:PHE:CD2	1:C:389:LEU:HG	2.52	0.44
1:C:484:ILE:CD1	1:C:488:LEU:HD11	2.48	0.44
1:C:304:PHE:HD1	1:C:305:THR:N	2.16	0.44
1:A:31:PRO:HA	1:A:35:ILE:HD12	1.99	0.44
1:C:288:TYR:H	1:C:296:ASN:HB2	1.82	0.44
1:C:391:GLN:H	1:C:391:GLN:HE21	1.66	0.44
1:A:192:ARG:HD2	1:A:285:GLU:CD	2.38	0.44
1:A:123:LYS:O	1:A:254:GLU:HA	2.17	0.44
1:A:71:LYS:HE2	1:A:75:MET:HE3	2.00	0.44
1:C:199:GLY:O	1:C:200:ALA:HB3	2.17	0.44
1:C:422:ASP:O	1:C:423:PRO:C	2.56	0.44
1:B:324:ARG:O	1:B:324:ARG:HG3	2.18	0.43
1:A:90:LYS:HD3	1:A:343:ILE:CG1	2.49	0.43
1:B:330:ALA:O	1:B:334:VAL:HG23	2.18	0.43
1:B:65:ASN:HD22	1:B:72:ARG:NH1	2.17	0.43
1:C:184:ILE:HG21	1:C:190:ILE:HD11	1.99	0.43
1:C:68:GLY:H	1:C:72:ARG:HH12	1.65	0.43
1:A:215:PHE:HA	1:A:216:PRO:HD3	1.92	0.43
1:A:69:THR:HG22	1:A:71:LYS:H	1.84	0.43
1:C:297:GLU:OE2	1:C:297:GLU:HA	2.17	0.43
1:A:81:ASP:O	1:A:82:VAL:HB	2.17	0.43
1:B:191:MET:CE	1:B:217:VAL:HG11	2.48	0.43
1:C:474:ASP:O	1:C:478:VAL:HG23	2.18	0.43
1:A:481:ILE:HG13	1:B:37:GLU:HG2	1.99	0.43
1:A:43:LEU:HD23	1:A:43:LEU:O	2.19	0.43
1:B:60:MET:SD	1:B:271:ILE:HD11	2.59	0.43
1:A:147:ILE:HG23	1:A:317:TYR:OH	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HA	1:B:309:ILE:HD11	2.00	0.43
1:B:141:ASP:O	1:B:144:ARG:HB2	2.18	0.43
1:C:15:LEU:O	1:C:19:GLN:HG2	2.19	0.43
1:B:338:GLU:OE2	1:B:408:ARG:NH2	2.52	0.42
1:A:444:VAL:CG2	1:A:447:LEU:HB3	2.50	0.42
1:A:471:ILE:CG2	1:B:151:TRP:CE3	3.02	0.42
1:C:85:LEU:O	1:C:88:VAL:HB	2.19	0.42
1:B:175:ASN:ND2	1:B:199:GLY:HA2	2.34	0.42
1:C:70:PRO:HA	1:C:73:VAL:HG23	2.00	0.42
1:B:391:GLN:NE2	1:B:391:GLN:H	2.15	0.42
1:B:367:VAL:HG22	1:B:399:ILE:HB	2.02	0.42
1:B:409:ASP:OD1	1:B:409:ASP:C	2.57	0.42
1:B:125:LEU:HD21	1:B:254:GLU:HG2	2.00	0.42
1:A:69:THR:HG22	1:A:71:LYS:N	2.35	0.42
1:C:167:ARG:O	1:C:215:PHE:HE1	2.02	0.42
1:C:361:CYS:O	1:C:362:SER:HB2	2.19	0.42
1:A:359:GLU:HG2	1:B:411:ASN:HA	2.01	0.42
1:B:433:THR:HB	1:B:434:PRO:CD	2.49	0.42
1:B:256:VAL:HG22	1:B:257:LYS:O	2.19	0.42
1:C:163:LEU:H	1:C:163:LEU:HD12	1.84	0.42
1:C:207:CYS:HA	1:C:279:GLN:HE22	1.85	0.42
1:C:332:LEU:HA	1:C:332:LEU:HD23	1.92	0.42
1:C:337:ASN:C	1:C:339:VAL:N	2.72	0.42
1:B:125:LEU:CB	1:B:128:ALA:HB2	2.47	0.42
1:B:29:VAL:HG23	1:B:54:ASN:O	2.20	0.42
1:B:325:PRO:HB2	1:B:358:PRO:O	2.20	0.42
1:C:417:ILE:HG12	1:C:453:LEU:HD23	2.02	0.42
1:A:440:PHE:C	1:A:440:PHE:CD1	2.94	0.41
1:B:422:ASP:O	1:B:423:PRO:C	2.58	0.41
1:C:170:HIS:C	1:C:171:LYS:CG	2.88	0.41
1:C:252:LYS:HB2	1:C:252:LYS:HE2	1.85	0.41
1:A:423:PRO:HB3	1:B:451:MET:HB2	2.01	0.41
1:A:47:GLY:HA2	1:A:48:PRO:HD2	1.72	0.41
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.91	0.41
1:C:72:ARG:HA	1:C:75:MET:HB2	2.03	0.41
1:C:74:ALA:HB1	1:C:79:GLN:HB3	2.01	0.41
1:A:49:ALA:HB2	1:A:72:ARG:NH1	2.36	0.41
1:B:86:ARG:HH11	1:B:341:VAL:HG12	1.85	0.41
1:B:82:VAL:CG1	1:B:85:LEU:HD13	2.49	0.41
1:C:484:ILE:O	1:C:488:LEU:HG	2.21	0.41
1:B:83:SER:O	1:B:86:ARG:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:PHE:HB2	1:A:351:ILE:HD12	2.03	0.41
1:A:90:LYS:HD3	1:A:343:ILE:HG13	2.03	0.41
1:A:90:LYS:HG2	1:A:93:ALA:HB3	2.02	0.41
1:B:386:TRP:CD1	1:B:450:LYS:HD3	2.56	0.41
1:B:52:PHE:C	1:B:54:ASN:H	2.24	0.41
1:C:8:ASP:O	1:C:11:ASP:HB2	2.21	0.41
1:C:217:VAL:HG21	1:C:277:ILE:HD11	2.03	0.40
1:A:122:THR:HB	1:A:253:THR:O	2.20	0.40
1:B:235:VAL:HG12	1:B:236:PRO:O	2.21	0.40
1:C:442:SER:HB2	1:C:447:LEU:O	2.20	0.40
1:C:490:ILE:HG23	1:C:491:PHE:CD2	2.56	0.40
1:A:447:LEU:HD13	1:C:375:ALA:HB1	2.04	0.40
1:B:215:PHE:HD2	1:B:277:ILE:HD12	1.86	0.40
1:B:44:ARG:NH2	1:B:324:ARG:O	2.55	0.40
1:B:33:LEU:HD23	1:B:149:THR:O	2.21	0.40
1:B:316:ILE:HG22	1:B:317:TYR:H	1.86	0.40
1:A:48:PRO:CG	1:B:490:ILE:HG22	2.52	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	432/505 (86%)	381 (88%)	40 (9%)	11 (2%)	5 29
1	B	457/505 (90%)	397 (87%)	49 (11%)	11 (2%)	6 30
1	C	442/505 (88%)	401 (91%)	31 (7%)	10 (2%)	6 31
All	All	1331/1515 (88%)	1179 (89%)	120 (9%)	32 (2%)	6 30

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	232	VAL
1	A	489	ALA
1	B	195	SER
1	B	489	ALA
1	C	8	ASP
1	C	195	SER
1	C	200	ALA
1	C	489	ALA
1	B	155	ALA
1	B	314	ASP
1	A	155	ALA
1	A	229	LEU
1	A	484	ILE
1	B	152	PRO
1	B	487	GLU
1	A	248	LEU
1	A	363	TYR
1	B	171	LYS
1	C	81	ASP
1	A	195	SER
1	A	482	ASP
1	B	33	LEU
1	B	53	GLU
1	C	488	LEU
1	A	89	GLY
1	C	234	PRO
1	C	222	GLY
1	C	423	PRO
1	B	70	PRO
1	C	169	PRO
1	B	127	GLY

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	371/430 (86%)	341 (92%)	30 (8%)	11 39
1	B	390/430 (91%)	345 (88%)	45 (12%)	5 22
1	C	377/430 (88%)	344 (91%)	33 (9%)	10 34
All	All	1138/1290 (88%)	1030 (90%)	108 (10%)	8 30

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	14	THR
1	A	23	LYS
1	A	25	ILE
1	A	27	LEU
1	A	77	MET
1	A	81	ASP
1	A	82	VAL
1	A	150	CYS
1	A	176	LEU
1	A	193	TRP
1	A	194	LEU
1	A	248	LEU
1	A	252	LYS
1	A	268	SER
1	A	300	SER
1	A	332	LEU
1	A	334	VAL
1	A	336	LEU
1	A	339	VAL
1	A	359	GLU
1	A	374	TYR
1	A	379	LYS
1	A	402	ASP
1	A	408	ARG
1	A	431	GLU
1	A	463	THR
1	A	476	ASP
1	A	486	ASP
1	A	490	ILE
1	B	14	THR
1	B	16	LEU
1	B	23	LYS
1	B	29	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	33	LEU
1	B	36	THR
1	B	42	THR
1	B	43	LEU
1	B	50	LEU
1	B	65	ASN
1	B	79	GLN
1	B	81	ASP
1	B	85	LEU
1	B	86	ARG
1	B	92	LEU
1	B	95	LEU
1	B	133	LYS
1	B	153	GLU
1	B	161	TRP
1	B	173	ARG
1	B	175	ASN
1	B	178	ILE
1	B	183	LEU
1	B	184	ILE
1	B	192	ARG
1	B	193	TRP
1	B	213	GLU
1	B	233	THR
1	B	239	LEU
1	B	251	THR
1	B	279	GLN
1	B	285	GLU
1	B	309	ILE
1	B	314	ASP
1	B	324	ARG
1	B	328	GLU
1	B	332	LEU
1	B	336	LEU
1	B	380	ARG
1	B	390	ARG
1	B	391	GLN
1	B	405	VAL
1	B	436	ASP
1	B	472	LYS
1	B	484	ILE
1	C	14	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	23	LYS
1	C	25	ILE
1	C	54	ASN
1	C	56	LYS
1	C	71	LYS
1	C	82	VAL
1	C	92	LEU
1	C	94	PHE
1	C	161	TRP
1	C	163	LEU
1	C	165	VAL
1	C	171	LYS
1	C	193	TRP
1	C	213	GLU
1	C	224	ASP
1	C	232	VAL
1	C	233	THR
1	C	242	TYR
1	C	251	THR
1	C	255	VAL
1	C	256	VAL
1	C	257	LYS
1	C	263	LEU
1	C	298	VAL
1	C	304	PHE
1	C	322	THR
1	C	324	ARG
1	C	345	GLN
1	C	391	GLN
1	C	393	MET
1	C	472	LYS
1	C	473	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	132	GLN
1	A	174	GLN
1	A	279	GLN
1	B	19	GLN
1	B	65	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	170	HIS
1	B	196	HIS
1	B	296	ASN
1	B	318	HIS
1	B	432	ASN
1	C	204	GLN
1	C	337	ASN
1	C	347	GLN
1	C	391	GLN
1	C	411	ASN

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	440/505 (87%)	-0.37	12 (2%) 54 38	29, 75, 144, 182	0
1	B	461/505 (91%)	0.10	32 (6%) 16 9	26, 115, 166, 244	2 (0%)
1	C	448/505 (88%)	-0.38	8 (1%) 68 55	31, 76, 135, 174	0
All	All	1349/1515 (89%)	-0.21	52 (3%) 39 24	26, 84, 153, 244	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ALA	7.9
1	C	95	LEU	5.8
1	B	238	THR	4.9
1	C	491	PHE	4.0
1	B	26	THR	4.0
1	B	239	LEU	3.9
1	B	81	ASP	3.9
1	B	208	ALA	3.8
1	B	247	LEU	3.7
1	B	126	ARG	3.6
1	A	196	HIS	3.5
1	A	126	ARG	3.4
1	A	123	LYS	3.3
1	A	474	ASP	3.3
1	C	196	HIS	3.2
1	B	250	GLY	3.2
1	A	195	SER	3.2
1	B	251	THR	3.1
1	C	94	PHE	3.1
1	C	127	GLY	3.1
1	B	53	GLU	2.9
1	B	162	GLY	2.8
1	B	144	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	80	GLU	2.8
1	A	93	ALA	2.7
1	C	91	LEU	2.7
1	B	319	SER	2.7
1	B	170	HIS	2.7
1	B	172	GLU	2.7
1	B	302	PRO	2.7
1	B	124	ARG	2.5
1	B	246	GLY	2.5
1	A	83	SER	2.5
1	C	197	ARG	2.4
1	B	25	ILE	2.4
1	B	218	SER	2.3
1	B	204	GLN	2.3
1	C	251	THR	2.3
1	B	171	LYS	2.3
1	A	485	TRP	2.2
1	A	122	THR	2.2
1	B	93	ALA	2.2
1	B	301	PHE	2.2
1	B	244	PHE	2.1
1	B	169	PRO	2.1
1	B	205	GLU	2.1
1	A	481	ILE	2.1
1	A	124	ARG	2.1
1	A	489	ALA	2.0
1	B	196	HIS	2.0
1	B	299	ASP	2.0
1	B	228	ILE	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.