Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:22 AM GMT

PDB ID	:	2GUW
Title	:	Crystal structure of AMP Nucleosidase from Salmonella typhimurium LT2
Authors	:	Rao, K.N.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-05-01
Resolution	:	2.64 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:

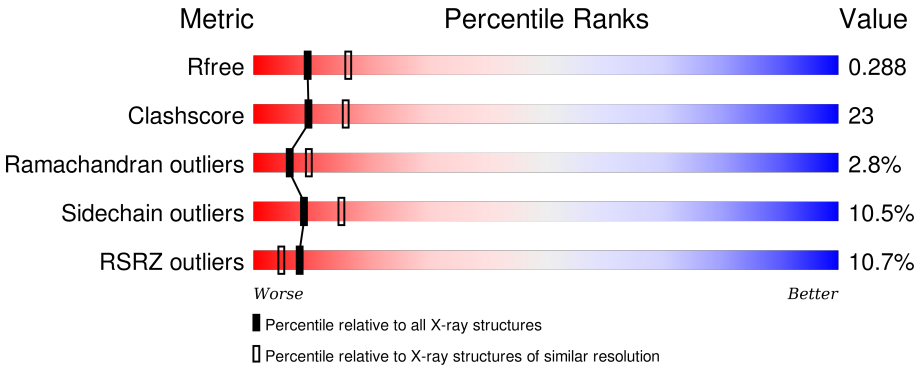
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	484	12% 49% 30% 6% 15%
1	B	484	4% 57% 25% · 14%
1	C	484	11% 45% 31% 5% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9415 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3182	2018	562	593	9			
1	B	418	Total	C	N	O	S	0	0	0
			3240	2060	561	609	10			
1	C	394	Total	C	N	O	S	0	0	0
			2964	1883	519	554	8			

- Molecule 2 is water.

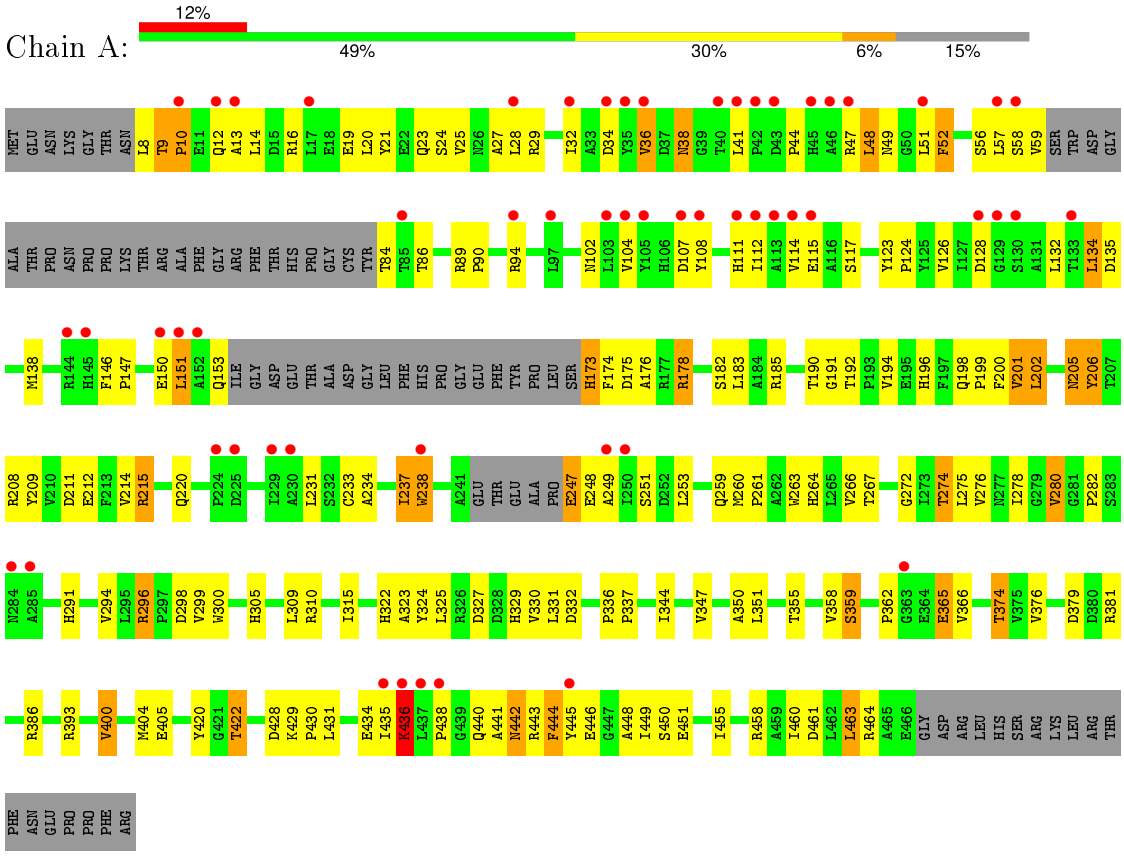
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	13	Total	O	0	0
			13	13		
2	C	3	Total	O	0	0
			3	3		

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.

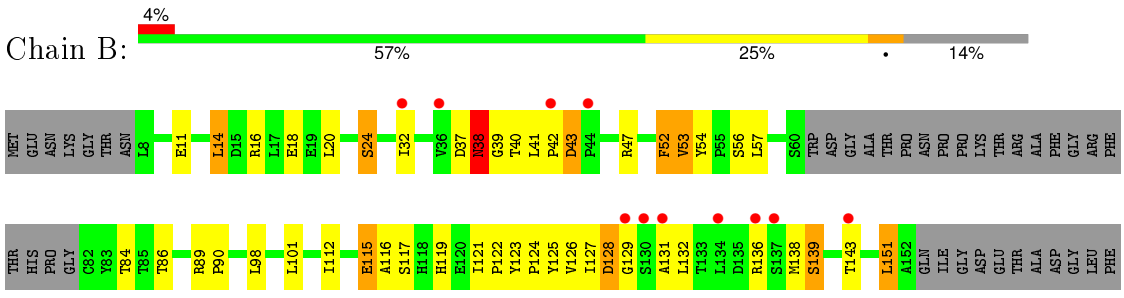
- Molecule 1: AMP nucleosidase

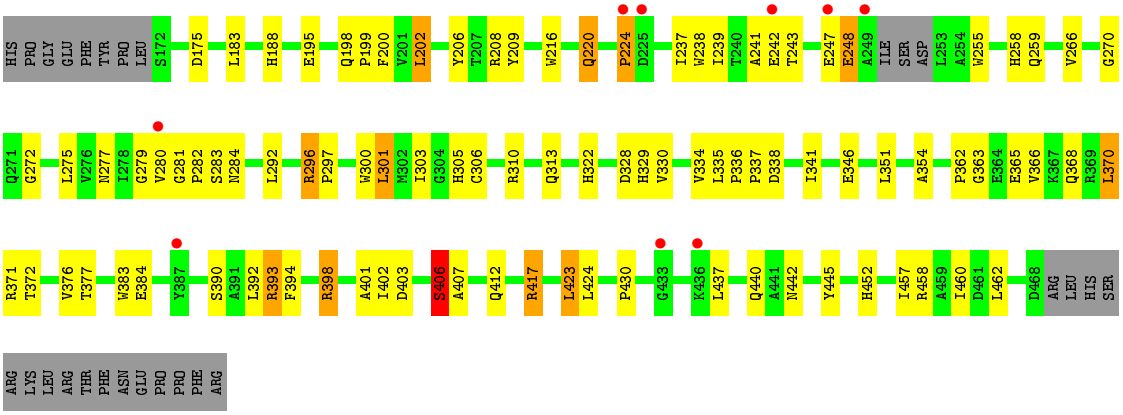
Chain A:



- Molecule 1: AMP nucleosidase

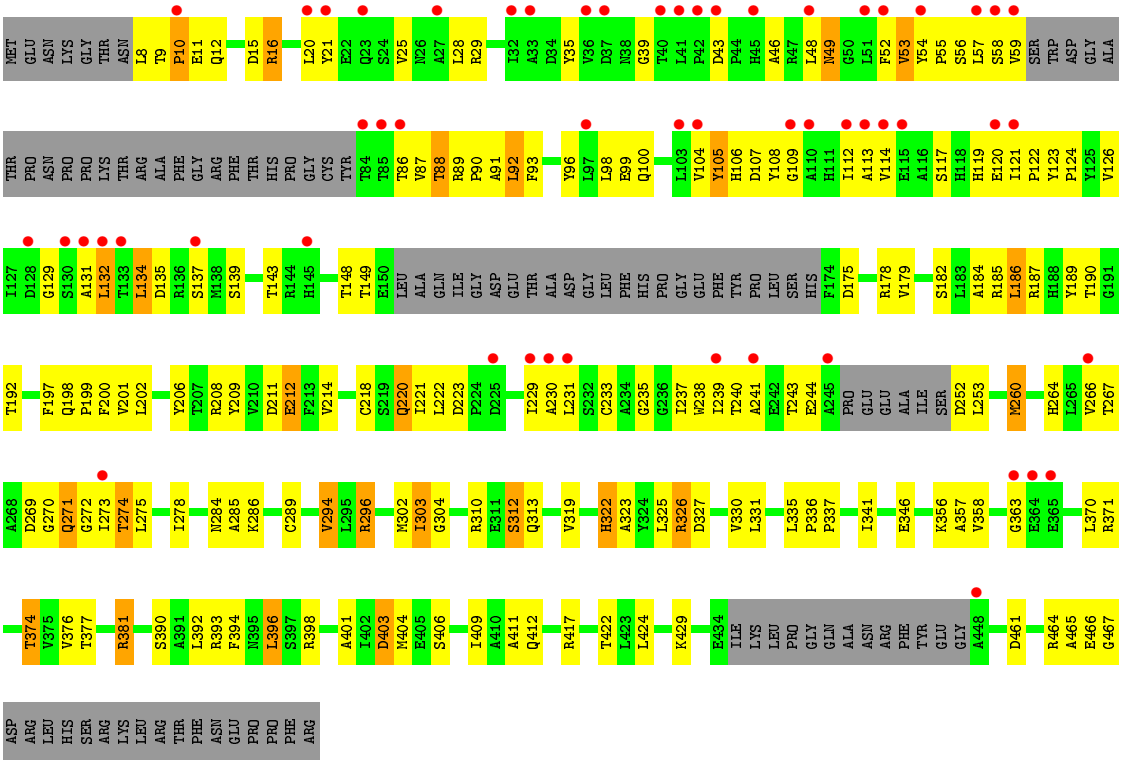
Chain B:





- Molecule 1: AMP nucleosidase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	116.49Å 170.28Å 204.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.07 – 2.64 48.36 – 2.64	Depositor EDS
% Data completeness (in resolution range)	93.0 (45.07-2.64) 92.8 (48.36-2.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.282 0.241 , 0.288	Depositor DCC
R_{free} test set	1381 reflections (2.48%)	DCC
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 59111 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9415	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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	0.40	0/3261	0.62	0/4453
1	B	0.41	0/3320	0.65	0/4537
1	C	0.37	0/3034	0.61	0/4154
All	All	0.39	0/9615	0.63	0/13144

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	3182	0	3052	163	0
1	B	3240	0	3122	120	0
1	C	2964	0	2812	150	0
2	A	13	0	0	0	0
2	B	13	0	0	1	0
2	C	3	0	0	0	0
All	All	9415	0	8986	417	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 23.

All (417) 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:377:THR:HG21	1:B:407:ALA:H	1.05	1.09
1:B:393:ARG:HG3	1:B:393:ARG:HH11	1.18	1.07
1:B:151:LEU:HD12	1:B:151:LEU:H	1.20	1.03
1:B:198:GLN:HE21	1:B:272:GLY:H	1.12	0.96
1:A:151:LEU:H	1:A:151:LEU:HD22	1.34	0.92
1:C:29:ARG:HH12	1:C:129:GLY:HA3	1.32	0.92
1:B:14:LEU:HD13	1:B:98:LEU:HG	1.55	0.88
1:A:381:ARG:HH22	1:B:259:GLN:HE22	1.21	0.88
1:C:356:LYS:HD2	1:C:363:GLY:HA2	1.57	0.87
1:B:377:THR:HG21	1:B:407:ALA:N	1.90	0.87
1:C:330:VAL:HG13	1:C:331:LEU:HD22	1.59	0.84
1:A:202:LEU:HD13	1:A:460:ILE:HD11	1.59	0.84
1:A:8:LEU:HG	1:A:111:HIS:HB3	1.57	0.84
1:A:355:THR:O	1:A:359:SER:HB3	1.79	0.83
1:B:237:ILE:HD12	1:B:237:ILE:H	1.43	0.82
1:C:58:SER:HB3	1:C:113:ALA:HB3	1.61	0.82
1:C:123:TYR:O	1:C:126:VAL:HG12	1.81	0.80
1:C:240:THR:O	1:C:243:THR:HG22	1.82	0.79
1:B:198:GLN:HE22	1:B:270:GLY:HA2	1.47	0.79
1:A:205:ASN:HD22	1:A:205:ASN:H	1.30	0.79
1:C:202:LEU:HG	1:C:273:ILE:HD11	1.63	0.79
1:A:381:ARG:HH22	1:B:259:GLN:NE2	1.80	0.79
1:C:143:THR:HG23	1:C:148:THR:HG21	1.63	0.79
1:C:289:CYS:HB2	1:C:412:GLN:HG2	1.65	0.77
1:C:222:LEU:HD12	1:C:223:ASP:N	1.99	0.77
1:C:322:HIS:HE1	1:C:374:THR:HG22	1.50	0.77
1:A:296:ARG:HH11	1:A:296:ARG:HB3	1.50	0.77
1:B:398:ARG:HE	1:C:417:ARG:NH1	1.82	0.76
1:A:381:ARG:NH2	1:B:259:GLN:HE22	1.82	0.75
1:B:393:ARG:HH11	1:B:393:ARG:CG	1.96	0.75
1:B:237:ILE:N	1:B:237:ILE:HD12	2.02	0.75
1:B:209:TYR:OH	1:B:452:HIS:HD2	1.69	0.74
1:B:41:LEU:HB2	1:B:42:PRO:HD2	1.69	0.74
1:C:218:CYS:O	1:C:221:ILE:HG22	1.86	0.74
1:A:198:GLN:NE2	1:A:272:GLY:H	1.86	0.74
1:A:178:ARG:O	1:A:178:ARG:HD3	1.90	0.72
1:A:332:ASP:OD1	1:A:337:PRO:HG3	1.91	0.71
1:A:47:ARG:HA	1:A:51:LEU:HB2	1.71	0.70
1:A:205:ASN:ND2	1:A:205:ASN:H	1.89	0.70
1:A:134:LEU:HD12	1:A:134:LEU:N	2.07	0.69
1:C:390:SER:HB3	1:C:394:PHE:CE1	2.27	0.69
1:B:296:ARG:HA	1:B:296:ARG:HE	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASP:OD1	1:A:393:ARG:NH2	2.22	0.69
1:A:34:ASP:O	1:A:38:ASN:HB3	1.94	0.68
1:A:28:LEU:HD23	1:A:126:VAL:HG11	1.75	0.68
1:A:198:GLN:HE21	1:A:272:GLY:H	1.39	0.67
1:C:132:LEU:HD21	1:C:134:LEU:HG	1.76	0.67
1:C:29:ARG:NH1	1:C:129:GLY:HA3	2.07	0.67
1:C:56:SER:HA	1:C:86:THR:HA	1.77	0.66
1:A:178:ARG:HH11	1:A:178:ARG:HG3	1.60	0.66
1:B:127:ILE:CG2	1:B:131:ALA:HB2	2.26	0.66
1:C:132:LEU:CD2	1:C:134:LEU:HG	2.26	0.66
1:C:197:PHE:HA	1:C:264:HIS:CD2	2.30	0.66
1:B:351:LEU:HB3	1:B:423:LEU:HD23	1.77	0.66
1:C:325:LEU:HB3	1:C:376:VAL:HG22	1.77	0.66
1:A:198:GLN:HE21	1:A:272:GLY:N	1.94	0.66
1:B:86:THR:HG21	1:B:119:HIS:HD2	1.60	0.66
1:C:89:ARG:N	1:C:90:PRO:HD3	2.11	0.65
1:C:275:LEU:C	1:C:275:LEU:HD23	2.16	0.65
1:C:198:GLN:HB3	1:C:272:GLY:O	1.96	0.65
1:B:255:TRP:HE1	1:B:277:ASN:ND2	1.94	0.65
1:A:296:ARG:NH1	1:A:296:ARG:HB3	2.11	0.65
1:C:370:LEU:HD12	1:C:371:ARG:H	1.62	0.64
1:A:89:ARG:HB3	1:A:89:ARG:HH11	1.62	0.64
1:C:285:ALA:HB1	1:C:409:ILE:HD12	1.79	0.64
1:A:123:TYR:O	1:A:126:VAL:HG22	1.98	0.64
1:C:132:LEU:HD22	1:C:134:LEU:H	1.62	0.64
1:C:8:LEU:HA	1:C:112:ILE:HB	1.80	0.64
1:B:377:THR:CG2	1:B:407:ALA:H	1.97	0.64
1:A:178:ARG:HD3	1:A:178:ARG:C	2.18	0.64
1:A:275:LEU:HD23	1:A:275:LEU:C	2.17	0.64
1:B:248:GLU:CD	1:B:248:GLU:H	2.02	0.64
1:C:381:ARG:HD2	1:C:404:MET:SD	2.38	0.64
1:C:237:ILE:HD12	1:C:237:ILE:H	1.63	0.64
1:B:393:ARG:HG3	1:B:393:ARG:NH1	1.99	0.63
1:B:237:ILE:CD1	1:B:237:ILE:H	2.11	0.63
1:B:198:GLN:NE2	1:B:272:GLY:H	1.92	0.63
1:C:179:VAL:HA	1:C:294:VAL:HG21	1.80	0.62
1:B:362:PRO:HD2	1:B:365:GLU:OE2	2.00	0.62
1:C:392:LEU:HG	1:C:396:LEU:HD22	1.82	0.62
1:B:362:PRO:O	1:B:366:VAL:HG23	2.00	0.62
1:B:14:LEU:CD1	1:B:98:LEU:HG	2.28	0.62
1:C:231:LEU:HD12	1:C:264:HIS:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:CE1	1:A:449:ILE:HG23	2.34	0.62
1:A:325:LEU:HB3	1:A:376:VAL:HG22	1.82	0.62
1:A:199:PRO:HG2	1:A:200:PHE:CD1	2.34	0.62
1:A:146:PHE:HB3	1:A:147:PRO:HD2	1.82	0.62
1:C:260:MET:HE1	1:C:284:ASN:HB3	1.82	0.61
1:C:202:LEU:HD22	1:C:303:ILE:HD13	1.83	0.61
1:C:289:CYS:CB	1:C:412:GLN:HG2	2.30	0.61
1:C:175:ASP:O	1:C:179:VAL:HG12	2.00	0.61
1:A:185:ARG:HD3	1:A:291:HIS:CE1	2.35	0.60
1:B:377:THR:HG22	1:B:403:ASP:OD2	2.00	0.60
1:A:151:LEU:CD2	1:A:151:LEU:H	2.13	0.60
1:A:344:ILE:HB	1:A:347:VAL:HG22	1.83	0.60
1:B:101:LEU:HG	1:B:112:ILE:HD13	1.83	0.60
1:B:53:VAL:HG11	1:B:117:SER:O	2.01	0.60
1:C:206:TYR:HB3	1:C:209:TYR:HD2	1.67	0.60
1:A:362:PRO:O	1:A:365:GLU:HB2	2.02	0.60
1:C:92:LEU:HD12	1:C:93:PHE:H	1.67	0.60
1:A:56:SER:HB2	1:A:117:SER:HB3	1.83	0.60
1:B:151:LEU:HD12	1:B:151:LEU:N	2.05	0.60
1:B:14:LEU:O	1:B:18:GLU:HG3	2.02	0.59
1:C:21:TYR:O	1:C:25:VAL:HG23	2.01	0.59
1:B:412:GLN:HA	1:B:412:GLN:HE21	1.67	0.59
1:B:335:LEU:HD21	1:B:341:ILE:HD11	1.83	0.59
1:A:206:TYR:HB3	1:A:209:TYR:CD1	2.38	0.59
1:A:324:TYR:OH	1:A:422:THR:HG23	2.02	0.59
1:A:59:VAL:HG12	1:A:112:ILE:HG22	1.84	0.59
1:A:16:ARG:HH11	1:A:16:ARG:HG3	1.69	0.58
1:A:183:LEU:HD22	1:A:194:VAL:HG11	1.85	0.58
1:A:291:HIS:O	1:A:294:VAL:HG22	2.03	0.58
1:A:347:VAL:HG21	1:A:420:TYR:O	2.04	0.58
1:C:370:LEU:HD12	1:C:371:ARG:N	2.17	0.58
1:C:296:ARG:HH11	1:C:296:ARG:HG3	1.69	0.58
1:C:187:ARG:HG3	1:C:192:THR:O	2.04	0.57
1:A:198:GLN:HE21	1:A:272:GLY:CA	2.17	0.57
1:C:206:TYR:HB3	1:C:209:TYR:CD2	2.38	0.57
1:B:202:LEU:HB3	1:B:275:LEU:HD23	1.84	0.57
1:B:127:ILE:O	1:B:128:ASP:HB2	2.05	0.57
1:A:436:LYS:HD3	1:A:442:ASN:OD1	2.04	0.57
1:B:199:PRO:HG2	1:B:200:PHE:CD1	2.40	0.57
1:A:275:LEU:HD23	1:A:276:VAL:N	2.20	0.57
1:B:151:LEU:CD1	1:B:151:LEU:H	1.99	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:HIS:O	1:B:258:HIS:HD2	1.88	0.56
1:B:121:ILE:N	1:B:121:ILE:HD12	2.21	0.56
1:A:430:PRO:O	1:B:151:LEU:HD11	2.06	0.56
1:B:398:ARG:NE	1:C:417:ARG:CZ	2.69	0.56
1:B:398:ARG:NE	1:C:417:ARG:NH1	2.53	0.56
1:C:240:THR:HG22	1:C:241:ALA:N	2.21	0.56
1:A:282:PRO:HG3	1:A:379:ASP:HB3	1.87	0.56
1:A:198:GLN:HE21	1:A:272:GLY:HA3	1.71	0.56
1:C:202:LEU:HB3	1:C:303:ILE:HD11	1.87	0.56
1:C:229:ILE:HG13	1:C:230:ALA:N	2.20	0.55
1:B:305:HIS:HB3	1:B:445:TYR:OH	2.07	0.55
1:B:412:GLN:HA	1:B:412:GLN:NE2	2.22	0.55
1:A:266:VAL:HG12	1:A:267:THR:N	2.22	0.55
1:A:151:LEU:HD12	1:B:384:GLU:HB3	1.90	0.55
1:B:437:LEU:O	1:B:440:GLN:HG3	2.08	0.54
1:C:286:LYS:HG3	1:C:412:GLN:NE2	2.21	0.54
1:C:92:LEU:HD12	1:C:93:PHE:N	2.22	0.54
1:A:200:PHE:HB3	1:A:460:ILE:HD13	1.89	0.54
1:B:376:VAL:HG12	1:B:401:ALA:O	2.06	0.54
1:A:444:PHE:CD1	1:A:444:PHE:N	2.74	0.54
1:B:198:GLN:HE21	1:B:272:GLY:N	1.93	0.54
1:A:209:TYR:CZ	1:A:449:ILE:HG23	2.42	0.54
1:C:20:LEU:CB	1:C:55:PRO:HB3	2.38	0.54
1:C:235:GLY:O	1:C:237:ILE:HD12	2.08	0.54
1:C:25:VAL:O	1:C:29:ARG:HG3	2.07	0.54
1:B:38:ASN:HB2	1:B:40:THR:HG23	1.90	0.54
1:C:59:VAL:HG11	1:C:104:VAL:HG11	1.89	0.54
1:C:310:ARG:NH1	1:C:371:ARG:HH21	2.06	0.54
1:C:266:VAL:HG12	1:C:267:THR:N	2.23	0.54
1:A:151:LEU:N	1:A:151:LEU:HD22	2.15	0.53
1:B:123:TYR:O	1:B:126:VAL:HG22	2.08	0.53
1:B:282:PRO:HB3	1:B:328:ASP:HB2	1.90	0.53
1:C:92:LEU:HD13	1:C:93:PHE:CD2	2.43	0.53
1:C:48:LEU:HD23	1:C:48:LEU:O	2.08	0.53
1:B:206:TYR:CE2	1:B:208:ARG:HB2	2.42	0.53
1:B:32:ILE:HD11	1:B:123:TYR:HB2	1.91	0.53
1:A:215:ARG:HG2	1:A:215:ARG:HH11	1.73	0.53
1:A:25:VAL:HG12	1:A:29:ARG:HH12	1.74	0.53
1:C:10:PRO:HG2	1:C:105:TYR:CG	2.44	0.53
1:C:20:LEU:HB2	1:C:55:PRO:HB3	1.91	0.53
1:C:322:HIS:CE1	1:C:374:THR:HG22	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:CG1	1:B:117:SER:H	2.22	0.53
1:A:57:LEU:C	1:A:57:LEU:HD23	2.29	0.53
1:A:21:TYR:OH	1:A:89:ARG:HD3	2.09	0.52
1:C:465:ALA:C	1:C:467:GLY:H	2.13	0.52
1:A:86:THR:HG23	1:A:176:ALA:H	1.73	0.52
1:B:127:ILE:HG23	1:B:131:ALA:HB2	1.91	0.52
1:A:259:GLN:HE22	1:B:280:VAL:HG11	1.73	0.52
1:C:220:GLN:HE21	1:C:220:GLN:N	2.07	0.52
1:C:237:ILE:HD12	1:C:237:ILE:N	2.25	0.52
1:A:102:ASN:C	1:A:104:VAL:H	2.13	0.52
1:C:211:ASP:O	1:C:214:VAL:HG12	2.10	0.52
1:A:199:PRO:HG2	1:A:200:PHE:CE1	2.44	0.52
1:B:216:TRP:CZ3	1:B:457:ILE:HD13	2.45	0.51
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.76	0.51
1:A:323:ALA:HB3	1:A:374:THR:HG22	1.92	0.51
1:C:221:ILE:HD11	1:C:239:ILE:O	2.10	0.51
1:C:53:VAL:HA	1:C:119:HIS:O	2.11	0.51
1:B:123:TYR:CG	1:B:124:PRO:HD3	2.46	0.51
1:A:310:ARG:O	1:A:429:LYS:NZ	2.43	0.51
1:A:9:THR:OG1	1:A:12:GLN:HB3	2.11	0.50
1:A:8:LEU:O	1:A:12:GLN:HB3	2.10	0.50
1:C:218:CYS:HA	1:C:221:ILE:HG22	1.93	0.50
1:C:310:ARG:HH11	1:C:310:ARG:HG3	1.76	0.50
1:A:231:LEU:HD12	1:A:264:HIS:O	2.11	0.50
1:A:350:ALA:HB2	1:A:463:LEU:HD13	1.92	0.50
1:B:417:ARG:HH11	1:C:398:ARG:NH1	2.10	0.50
1:A:173:HIS:O	1:A:174:PHE:HB2	2.11	0.50
1:C:56:SER:HB3	1:C:117:SER:HB3	1.93	0.50
1:A:435:ILE:O	1:A:436:LYS:HG3	2.11	0.50
1:A:444:PHE:H	1:A:444:PHE:HD1	1.60	0.50
1:C:98:LEU:C	1:C:100:GLN:H	2.15	0.50
1:A:192:THR:HG22	1:A:234:ALA:HA	1.93	0.50
1:A:428:ASP:OD2	1:A:430:PRO:HG3	2.12	0.50
1:C:313:GLN:HG3	1:C:429:LYS:HZ3	1.77	0.49
1:B:16:ARG:O	1:B:20:LEU:HB2	2.11	0.49
1:B:122:PRO:HD2	1:B:125:TYR:HD2	1.77	0.49
1:C:123:TYR:N	1:C:124:PRO:HD2	2.27	0.49
1:A:209:TYR:CE1	1:A:449:ILE:HD12	2.47	0.49
1:C:206:TYR:CD2	1:C:208:ARG:HB2	2.47	0.49
1:B:354:ALA:HB1	1:B:458:ARG:HB3	1.94	0.49
1:A:458:ARG:O	1:A:461:ASP:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:TRP:O	1:B:220:GLN:HB2	2.12	0.49
1:B:390:SER:HB3	1:B:394:PHE:CE1	2.47	0.49
1:C:253:LEU:O	1:C:253:LEU:HG	2.13	0.49
1:A:212:GLU:O	1:A:215:ARG:HB3	2.13	0.49
1:A:151:LEU:HD21	1:B:430:PRO:O	2.13	0.49
1:A:310:ARG:NH1	1:A:400:VAL:HG23	2.27	0.49
1:A:205:ASN:N	1:A:205:ASN:ND2	2.50	0.48
1:C:89:ARG:O	1:C:92:LEU:HD12	2.13	0.48
1:C:390:SER:HB3	1:C:394:PHE:CZ	2.47	0.48
1:A:435:ILE:C	1:A:436:LYS:HG3	2.34	0.48
1:A:20:LEU:HD13	1:A:115:GLU:O	2.13	0.48
1:C:233:CYS:HB2	1:C:237:ILE:HB	1.96	0.48
1:A:12:GLN:C	1:A:14:LEU:H	2.17	0.48
1:A:325:LEU:HD23	1:A:376:VAL:HG22	1.95	0.48
1:B:127:ILE:O	1:B:128:ASP:CB	2.62	0.48
1:C:198:GLN:HB2	1:C:274:THR:HG22	1.95	0.48
1:C:235:GLY:C	1:C:237:ILE:HD12	2.33	0.48
1:C:12:GLN:O	1:C:15:ASP:N	2.47	0.48
1:B:127:ILE:HG21	1:B:131:ALA:HB2	1.94	0.48
1:B:11:GLU:HB2	2:B:487:HOH:O	2.14	0.48
1:A:151:LEU:O	1:A:153:GLN:HG2	2.14	0.48
1:C:221:ILE:HD13	1:C:239:ILE:HG22	1.96	0.47
1:A:386:ARG:HD2	1:B:334:VAL:CG1	2.43	0.47
1:C:182:SER:O	1:C:186:LEU:HB2	2.14	0.47
1:C:86:THR:HG21	1:C:119:HIS:HD2	1.78	0.47
1:C:285:ALA:HB1	1:C:409:ILE:CD1	2.43	0.47
1:B:437:LEU:HB2	1:B:440:GLN:OE1	2.15	0.47
1:A:27:ALA:HB1	1:A:51:LEU:CD2	2.44	0.47
1:B:383:TRP:CE2	1:B:402:ILE:HD13	2.49	0.47
1:C:28:LEU:HA	1:C:52:PHE:CE2	2.49	0.47
1:C:187:ARG:O	1:C:190:THR:O	2.33	0.47
1:A:16:ARG:HB2	1:A:114:VAL:HG11	1.96	0.47
1:C:412:GLN:HA	1:C:412:GLN:OE1	2.15	0.47
1:A:446:GLU:C	1:A:448:ALA:H	2.17	0.47
1:A:315:ILE:HG13	1:A:436:LYS:HE3	1.97	0.47
1:A:358:VAL:CG2	1:A:458:ARG:HG3	2.44	0.47
1:A:19:GLU:O	1:A:23:GLN:HB2	2.14	0.47
1:A:214:VAL:HG11	1:A:249:ALA:HB3	1.96	0.47
1:A:41:LEU:HD22	1:A:41:LEU:N	2.29	0.47
1:C:218:CYS:HA	1:C:221:ILE:CG2	2.45	0.47
1:A:32:ILE:O	1:A:36:VAL:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ILE:HG22	1:C:238:TRP:N	2.29	0.47
1:A:20:LEU:O	1:A:23:GLN:HB3	2.14	0.47
1:C:273:ILE:HG13	1:C:274:THR:N	2.29	0.47
1:C:43:ASP:HB3	1:C:46:ALA:HB2	1.97	0.47
1:A:305:HIS:HB3	1:A:445:TYR:OH	2.14	0.47
1:A:13:ALA:HA	1:A:114:VAL:HG11	1.96	0.47
1:A:206:TYR:HB3	1:A:209:TYR:HD1	1.79	0.47
1:C:461:ASP:HA	1:C:464:ARG:NH1	2.30	0.47
1:B:338:ASP:OD2	1:C:393:ARG:NH2	2.47	0.47
1:A:434:GLU:CA	1:B:143:THR:HG21	2.44	0.47
1:A:261:PRO:HB2	1:A:263:TRP:CH2	2.50	0.47
1:B:202:LEU:HB3	1:B:275:LEU:CD2	2.45	0.46
1:C:43:ASP:HB3	1:C:46:ALA:CB	2.45	0.46
1:A:84:THR:HG23	1:A:84:THR:O	2.16	0.46
1:B:241:ALA:C	1:B:243:THR:H	2.18	0.46
1:A:198:GLN:HB2	1:A:274:THR:HG22	1.96	0.46
1:A:94:ARG:HH11	1:A:94:ARG:HG3	1.81	0.46
1:A:332:ASP:OD1	1:A:337:PRO:CG	2.61	0.46
1:A:58:SER:OG	1:A:84:THR:HB	2.15	0.46
1:C:270:GLY:O	1:C:271:GLN:NE2	2.49	0.46
1:B:198:GLN:HE22	1:B:270:GLY:CA	2.24	0.46
1:A:89:ARG:HB3	1:A:89:ARG:NH1	2.27	0.46
1:B:310:ARG:HB2	1:B:313:GLN:HG3	1.97	0.46
1:B:393:ARG:NH1	1:B:393:ARG:CG	2.65	0.45
1:A:386:ARG:HG2	1:A:386:ARG:HH11	1.80	0.45
1:B:47:ARG:HG2	1:B:52:PHE:CE1	2.52	0.45
1:A:24:SER:CB	1:A:52:PHE:HA	2.46	0.45
1:C:16:ARG:HD2	1:C:114:VAL:HG12	1.98	0.45
1:A:12:GLN:O	1:A:13:ALA:HB3	2.16	0.45
1:C:53:VAL:HG11	1:C:117:SER:O	2.16	0.45
1:A:192:THR:CG2	1:A:234:ALA:HA	2.46	0.45
1:A:451:GLU:O	1:A:455:ILE:HG13	2.17	0.45
1:A:57:LEU:O	1:A:57:LEU:HD23	2.16	0.45
1:A:259:GLN:O	1:A:260:MET:HG3	2.16	0.45
1:A:14:LEU:HG	1:A:94:ARG:NH1	2.31	0.45
1:B:202:LEU:HD13	1:B:460:ILE:CD1	2.47	0.45
1:C:199:PRO:HG2	1:C:200:PHE:CD1	2.52	0.45
1:C:313:GLN:HG3	1:C:429:LYS:NZ	2.32	0.45
1:B:43:ASP:N	1:B:43:ASP:OD1	2.48	0.45
1:C:175:ASP:OD1	1:C:175:ASP:C	2.56	0.45
1:C:260:MET:HE2	1:C:278:ILE:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:HIS:CD2	1:A:438:PRO:HG2	2.52	0.45
1:A:443:ARG:HG2	1:A:443:ARG:HH11	1.83	0.45
1:A:381:ARG:HB2	1:A:404:MET:SD	2.57	0.44
1:C:325:LEU:HA	1:C:325:LEU:HD12	1.84	0.44
1:C:319:VAL:HG21	1:C:401:ALA:HB2	1.99	0.44
1:C:346:GLU:H	1:C:346:GLU:CD	2.20	0.44
1:A:21:TYR:CD2	1:A:90:PRO:HD2	2.53	0.44
1:A:104:VAL:O	1:A:108:TYR:HB2	2.18	0.44
1:C:35:TYR:O	1:C:39:GLY:HA2	2.16	0.44
1:C:201:VAL:HG22	1:C:274:THR:HG23	1.99	0.44
1:A:123:TYR:CG	1:A:124:PRO:HD3	2.53	0.44
1:A:190:THR:HA	1:A:260:MET:O	2.17	0.44
1:C:304:GLY:O	1:C:424:LEU:HA	2.18	0.44
1:B:247:GLU:CD	1:B:247:GLU:H	2.21	0.44
1:A:201:VAL:HA	1:A:274:THR:HG23	2.00	0.44
1:B:54:TYR:CE2	1:B:121:ILE:HG13	2.53	0.44
1:B:241:ALA:O	1:B:243:THR:N	2.46	0.44
1:C:137:SER:C	1:C:139:SER:H	2.20	0.44
1:C:394:PHE:N	1:C:394:PHE:CD1	2.85	0.44
1:A:436:LYS:NZ	1:A:442:ASN:ND2	2.66	0.44
1:A:259:GLN:NE2	1:B:280:VAL:HG11	2.33	0.44
1:C:336:PRO:HA	1:C:337:PRO:HD3	1.88	0.43
1:B:175:ASP:C	1:B:175:ASP:OD2	2.56	0.43
1:C:89:ARG:N	1:C:90:PRO:CD	2.80	0.43
1:B:121:ILE:H	1:B:121:ILE:HD12	1.82	0.43
1:A:44:PRO:O	1:A:48:LEU:HB2	2.18	0.43
1:A:251:SER:C	1:A:253:LEU:H	2.22	0.43
1:B:124:PRO:HA	1:B:127:ILE:HD12	1.99	0.43
1:C:394:PHE:HD1	1:C:394:PHE:N	2.17	0.43
1:C:296:ARG:HH11	1:C:296:ARG:CG	2.31	0.43
1:C:16:ARG:CZ	1:C:20:LEU:HD21	2.48	0.43
1:C:358:VAL:HG12	1:C:358:VAL:O	2.18	0.43
1:C:465:ALA:C	1:C:467:GLY:N	2.72	0.43
1:C:326:ARG:HD3	1:C:341:ILE:HD12	2.01	0.43
1:A:16:ARG:HG3	1:A:16:ARG:NH1	2.34	0.43
1:A:9:THR:OG1	1:A:12:GLN:CB	2.67	0.43
1:C:200:PHE:O	1:C:273:ILE:HD12	2.19	0.43
1:C:9:THR:HB	1:C:12:GLN:OE1	2.19	0.43
1:A:233:CYS:HB2	1:A:237:ILE:HG12	2.00	0.43
1:C:202:LEU:HD22	1:C:303:ILE:CD1	2.47	0.43
1:A:329:HIS:HA	1:A:332:ASP:OD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ASP:O	1:B:330:VAL:N	2.50	0.43
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.89	0.43
1:A:330:VAL:HG13	1:A:331:LEU:HG	2.01	0.43
1:C:55:PRO:HG2	1:C:87:VAL:HG22	2.00	0.42
1:B:437:LEU:HD23	1:B:440:GLN:OE1	2.19	0.42
1:C:122:PRO:C	1:C:124:PRO:HD2	2.40	0.42
1:C:322:HIS:C	1:C:322:HIS:ND1	2.72	0.42
1:A:191:GLY:O	1:A:234:ALA:O	2.36	0.42
1:C:54:TYR:CE2	1:C:88:THR:HB	2.54	0.42
1:A:296:ARG:HH11	1:A:296:ARG:CB	2.28	0.42
1:A:208:ARG:O	1:A:211:ASP:HB2	2.20	0.42
1:A:200:PHE:CZ	1:A:464:ARG:HG3	2.54	0.42
1:C:189:TYR:HB3	1:C:260:MET:HG3	2.01	0.42
1:C:20:LEU:HB3	1:C:55:PRO:HB3	2.02	0.42
1:A:107:ASP:O	1:A:108:TYR:CD1	2.72	0.42
1:C:49:ASN:HA	1:C:49:ASN:HD22	1.66	0.42
1:B:306:CYS:HB3	1:B:424:LEU:HD13	2.01	0.42
1:B:403:ASP:OD1	1:B:406:SER:HB2	2.20	0.42
1:B:56:SER:HB2	1:B:117:SER:HB3	2.01	0.42
1:B:238:TRP:O	1:B:239:ILE:HD13	2.19	0.42
1:A:440:GLN:O	1:A:441:ALA:HB3	2.20	0.42
1:A:325:LEU:CB	1:A:376:VAL:HG22	2.47	0.42
1:C:187:ARG:HG2	1:C:187:ARG:HH11	1.85	0.42
1:B:301:LEU:HB3	1:B:303:ILE:CD1	2.50	0.42
1:C:327:ASP:CG	1:C:393:ARG:HH12	2.22	0.42
1:B:89:ARG:N	1:B:90:PRO:HD3	2.34	0.42
1:A:112:ILE:HG13	1:A:112:ILE:O	2.20	0.42
1:B:132:LEU:HD12	1:B:132:LEU:N	2.35	0.42
1:A:443:ARG:NH1	1:A:443:ARG:HG2	2.35	0.41
1:A:132:LEU:O	1:A:132:LEU:HD23	2.20	0.41
1:C:201:VAL:HG22	1:C:274:THR:CG2	2.50	0.41
1:B:41:LEU:CB	1:B:42:PRO:HD2	2.46	0.41
1:B:417:ARG:NH1	1:C:398:ARG:NH1	2.68	0.41
1:A:132:LEU:HD23	1:A:132:LEU:C	2.40	0.41
1:A:247:GLU:N	1:A:247:GLU:OE1	2.53	0.41
1:B:377:THR:HA	1:B:403:ASP:O	2.20	0.41
1:C:302:MET:HB3	1:C:422:THR:HG22	2.02	0.41
1:C:323:ALA:HB3	1:C:374:THR:HB	2.02	0.41
1:C:221:ILE:HD11	1:C:230:ALA:HA	2.02	0.41
1:B:296:ARG:N	1:B:297:PRO:HD3	2.35	0.41
1:A:182:SER:OG	1:A:291:HIS:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:C	1:B:138:MET:H	2.22	0.41
1:A:134:LEU:N	1:A:134:LEU:CD1	2.79	0.41
1:C:178:ARG:NH1	1:C:182:SER:OG	2.54	0.41
1:B:195:GLU:CD	1:B:195:GLU:H	2.22	0.41
1:A:205:ASN:HD22	1:A:205:ASN:N	1.96	0.41
1:B:255:TRP:HE1	1:B:277:ASN:HD22	1.64	0.41
1:A:89:ARG:N	1:A:90:PRO:CD	2.83	0.41
1:A:446:GLU:HA	1:A:449:ILE:HG12	2.02	0.41
1:C:132:LEU:HD22	1:C:134:LEU:HG	2.02	0.41
1:C:266:VAL:HG12	1:C:267:THR:H	1.85	0.41
1:C:54:TYR:CE1	1:C:121:ILE:HA	2.55	0.41
1:A:202:LEU:CD1	1:A:460:ILE:HD11	2.40	0.41
1:C:240:THR:HG22	1:C:241:ALA:H	1.86	0.41
1:A:336:PRO:HA	1:A:337:PRO:HD3	1.82	0.41
1:C:341:ILE:CD1	1:C:411:ALA:HB2	2.51	0.41
1:A:280:VAL:HA	1:A:405:GLU:OE2	2.21	0.41
1:A:135:ASP:OD1	1:A:138:MET:HG2	2.21	0.41
1:A:10:PRO:O	1:A:12:GLN:O	2.39	0.41
1:A:8:LEU:HD12	1:A:8:LEU:N	2.35	0.41
1:C:53:VAL:HA	1:C:120:GLU:HA	2.02	0.41
1:A:185:ARG:HD3	1:A:291:HIS:NE2	2.36	0.41
1:C:208:ARG:O	1:C:212:GLU:HB2	2.21	0.41
1:B:202:LEU:HG	1:B:303:ILE:HD13	2.03	0.41
1:A:260:MET:HG2	1:A:278:ILE:HA	2.03	0.41
1:C:96:TYR:O	1:C:100:GLN:HB2	2.20	0.41
1:B:281:GLY:HA2	1:B:282:PRO:HD3	1.86	0.41
1:B:138:MET:O	1:B:139:SER:C	2.59	0.41
1:A:196:HIS:CD2	1:A:238:TRP:HE1	2.39	0.41
1:B:259:GLN:NE2	1:B:284:ASN:OD1	2.52	0.40
1:C:12:GLN:O	1:C:16:ARG:N	2.48	0.40
1:B:115:GLU:OE2	1:B:116:ALA:O	2.39	0.40
1:A:206:TYR:HD1	1:A:209:TYR:HE1	1.69	0.40
1:B:24:SER:OG	1:B:53:VAL:N	2.55	0.40
1:B:394:PHE:N	1:B:394:PHE:CD1	2.89	0.40
1:C:269:ASP:OD2	1:C:271:GLN:HB2	2.21	0.40
1:B:37:ASP:C	1:B:39:GLY:H	2.23	0.40
1:A:201:VAL:HG23	1:A:202:LEU:N	2.36	0.40
1:A:47:ARG:CA	1:A:51:LEU:HB2	2.48	0.40
1:B:370:LEU:HD13	1:B:370:LEU:O	2.19	0.40
1:B:336:PRO:HA	1:B:337:PRO:HD3	1.79	0.40
1:C:325:LEU:CB	1:C:376:VAL:HG22	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PRO:C	1:A:12:GLN:N	2.75	0.40
1:A:32:ILE:CD1	1:A:123:TYR:HB2	2.50	0.40
1:B:200:PHE:HB3	1:B:460:ILE:HD13	2.04	0.40
1:C:98:LEU:O	1:C:100:GLN:N	2.55	0.40
1:B:346:GLU:CD	1:B:346:GLU:H	2.24	0.40
1:C:377:THR:HA	1:C:403:ASP:O	2.20	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	403/484 (83%)	348 (86%)	47 (12%)	8 (2%)	9 16
1	B	410/484 (85%)	375 (92%)	25 (6%)	10 (2%)	7 12
1	C	384/484 (79%)	331 (86%)	38 (10%)	15 (4%)	4 5
All	All	1197/1452 (82%)	1054 (88%)	110 (9%)	33 (3%)	6 9

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	B	128	ASP
1	B	224	PRO
1	C	11	GLU
1	C	108	TYR
1	C	134	LEU
1	A	38	ASN
1	C	91	ALA
1	C	99	GLU
1	C	107	ASP
1	C	109	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	10	PRO
1	A	215	ARG
1	B	242	GLU
1	B	363	GLY
1	B	406	SER
1	A	248	GLU
1	A	436	LYS
1	B	38	ASN
1	B	139	SER
1	B	279	GLY
1	C	131	ALA
1	C	184	ALA
1	C	312	SER
1	C	357	ALA
1	C	10	PRO
1	C	53	VAL
1	C	466	GLU
1	B	329	HIS
1	C	406	SER
1	A	9	THR
1	B	129	GLY
1	A	299	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	327/403 (81%)	289 (88%)	38 (12%)	7 11
1	B	337/403 (84%)	304 (90%)	33 (10%)	10 18
1	C	297/403 (74%)	267 (90%)	30 (10%)	9 16
All	All	961/1209 (80%)	860 (90%)	101 (10%)	8 15

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	49	ASN
1	A	52	PHE
1	A	128	ASP
1	A	134	LEU
1	A	150	GLU
1	A	151	LEU
1	A	173	HIS
1	A	175	ASP
1	A	178	ARG
1	A	201	VAL
1	A	202	LEU
1	A	205	ASN
1	A	206	TYR
1	A	220	GLN
1	A	237	ILE
1	A	238	TRP
1	A	247	GLU
1	A	274	THR
1	A	280	VAL
1	A	296	ARG
1	A	298	ASP
1	A	300	TRP
1	A	309	LEU
1	A	322	HIS
1	A	351	LEU
1	A	359	SER
1	A	365	GLU
1	A	366	VAL
1	A	374	THR
1	A	400	VAL
1	A	422	THR
1	A	431	LEU
1	A	436	LYS
1	A	442	ASN
1	A	444	PHE
1	A	450	SER
1	A	463	LEU
1	B	14	LEU
1	B	24	SER
1	B	38	ASN
1	B	43	ASP
1	B	52	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	53	VAL
1	B	57	LEU
1	B	84	THR
1	B	115	GLU
1	B	151	LEU
1	B	202	LEU
1	B	220	GLN
1	B	224	PRO
1	B	248	GLU
1	B	266	VAL
1	B	283	SER
1	B	292	LEU
1	B	296	ARG
1	B	300	TRP
1	B	301	LEU
1	B	322	HIS
1	B	368	GLN
1	B	370	LEU
1	B	371	ARG
1	B	372	THR
1	B	392	LEU
1	B	393	ARG
1	B	398	ARG
1	B	406	SER
1	B	417	ARG
1	B	423	LEU
1	B	442	ASN
1	B	462	LEU
1	C	16	ARG
1	C	49	ASN
1	C	57	LEU
1	C	88	THR
1	C	92	LEU
1	C	105	TYR
1	C	106	HIS
1	C	132	LEU
1	C	135	ASP
1	C	149	THR
1	C	185	ARG
1	C	186	LEU
1	C	212	GLU
1	C	220	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	244	GLU
1	C	252	ASP
1	C	260	MET
1	C	271	GLN
1	C	274	THR
1	C	294	VAL
1	C	296	ARG
1	C	303	ILE
1	C	312	SER
1	C	322	HIS
1	C	326	ARG
1	C	335	LEU
1	C	374	THR
1	C	381	ARG
1	C	396	LEU
1	C	403	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	49	ASN
1	A	173	HIS
1	A	198	GLN
1	A	205	ASN
1	A	220	GLN
1	A	259	GLN
1	A	271	GLN
1	A	291	HIS
1	A	348	GLN
1	A	382	ASN
1	A	442	ASN
1	B	26	ASN
1	B	49	ASN
1	B	119	HIS
1	B	198	GLN
1	B	220	GLN
1	B	258	HIS
1	B	259	GLN
1	B	277	ASN
1	B	284	ASN
1	B	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	382	ASN
1	B	412	GLN
1	B	442	ASN
1	B	452	HIS
1	C	26	ASN
1	C	49	ASN
1	C	119	HIS
1	C	220	GLN
1	C	264	HIS
1	C	271	GLN
1	C	395	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	411/484 (84%)	0.81	56 (13%) 4 2	37, 72, 118, 129	0
1	B	418/484 (86%)	0.42	20 (4%) 34 28	38, 60, 103, 115	0
1	C	394/484 (81%)	0.74	55 (13%) 4 2	43, 82, 119, 124	0
All	All	1223/1452 (84%)	0.65	131 (10%) 8 5	37, 69, 116, 129	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	THR	9.0
1	C	42	PRO	8.6
1	B	130	SER	8.1
1	A	112	ILE	8.0
1	C	41	LEU	6.9
1	A	437	LEU	6.5
1	C	131	ALA	6.4
1	C	113	ALA	6.1
1	C	132	LEU	6.0
1	B	249	ALA	5.6
1	C	57	LEU	5.6
1	A	113	ALA	5.5
1	C	112	ILE	5.3
1	A	249	ALA	5.1
1	A	363	GLY	5.1
1	A	17	LEU	5.1
1	A	435	ILE	5.1
1	C	32	ILE	4.9
1	A	114	VAL	4.8
1	A	45	HIS	4.6
1	C	21	TYR	4.6
1	B	137	SER	4.5
1	A	32	ILE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	137	SER	4.4
1	A	46	ALA	4.4
1	A	250	ILE	4.3
1	A	108	TYR	4.3
1	B	131	ALA	4.2
1	A	129	GLY	4.2
1	A	133	THR	4.1
1	C	114	VAL	4.1
1	A	151	LEU	4.1
1	A	13	ALA	4.0
1	C	10	PRO	4.0
1	A	152	ALA	4.0
1	C	104	VAL	4.0
1	B	134	LEU	3.9
1	A	35	TYR	3.9
1	A	436	LYS	3.7
1	C	245	ALA	3.7
1	C	52	PHE	3.7
1	C	130	SER	3.6
1	A	57	LEU	3.6
1	A	105	TYR	3.5
1	A	128	ASP	3.5
1	C	48	LEU	3.5
1	C	23	GLN	3.5
1	A	225	ASP	3.5
1	A	224	PRO	3.4
1	C	363	GLY	3.4
1	B	42	PRO	3.4
1	A	104	VAL	3.4
1	A	36	VAL	3.4
1	C	37	ASP	3.4
1	C	45	HIS	3.3
1	C	103	LEU	3.3
1	C	231	LEU	3.3
1	A	40	THR	3.3
1	A	58	SER	3.2
1	A	97	LEU	3.1
1	A	10	PRO	3.1
1	A	438	PRO	3.1
1	A	12	GLN	3.1
1	A	47	ARG	3.1
1	C	109	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	58	SER	3.0
1	C	97	LEU	3.0
1	C	239	ILE	3.0
1	A	42	PRO	2.9
1	B	129	GLY	2.9
1	B	32	ILE	2.9
1	A	51	LEU	2.9
1	A	41	LEU	2.9
1	A	43	ASP	2.9
1	C	364	GLU	2.9
1	B	433	GLY	2.8
1	C	40	THR	2.8
1	A	144	ARG	2.7
1	B	387	TYR	2.7
1	A	115	GLU	2.7
1	A	230	ALA	2.7
1	C	110	ALA	2.7
1	C	448	ALA	2.7
1	A	229	ILE	2.6
1	C	51	LEU	2.6
1	B	242	GLU	2.6
1	C	365	GLU	2.5
1	C	128	ASP	2.5
1	C	27	ALA	2.5
1	A	28	LEU	2.5
1	C	54	TYR	2.5
1	C	225	ASP	2.5
1	B	143	THR	2.4
1	C	20	LEU	2.4
1	B	436	LYS	2.4
1	C	241	ALA	2.3
1	C	33	ALA	2.3
1	B	225	ASP	2.3
1	A	284	ASN	2.3
1	C	115	GLU	2.3
1	A	130	SER	2.3
1	B	136	ARG	2.3
1	A	103	LEU	2.3
1	A	238	TRP	2.3
1	A	445	TYR	2.3
1	C	86	THR	2.3
1	C	121	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	229	ILE	2.3
1	C	36	VAL	2.2
1	C	85	THR	2.2
1	A	145	HIS	2.2
1	C	59	VAL	2.2
1	C	273	ILE	2.2
1	A	85	THR	2.2
1	A	94	ARG	2.2
1	C	43	ASP	2.2
1	A	34	ASP	2.2
1	C	120	GLU	2.1
1	C	230	ALA	2.1
1	A	107	ASP	2.1
1	C	266	VAL	2.1
1	B	247	GLU	2.1
1	B	280	VAL	2.1
1	C	84	THR	2.1
1	C	145	HIS	2.1
1	A	150	GLU	2.1
1	B	44	PRO	2.1
1	A	285	ALA	2.1
1	A	111	HIS	2.0
1	B	224	PRO	2.0
1	B	36	VAL	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.