W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:51 AM GMT

PDB ID	:	2V2T
Title	:	X-RAY STRUCTURE OF A NF-KB P50-RELB-DNA COMPLEX
Authors	:	Moorthy, A.K.; Huang, D.B.; Wang, V.Y.; Vu, D.; Ghosh, G.
Deposited on	:	2007-06-07
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 (i)) were used in the production of this report:

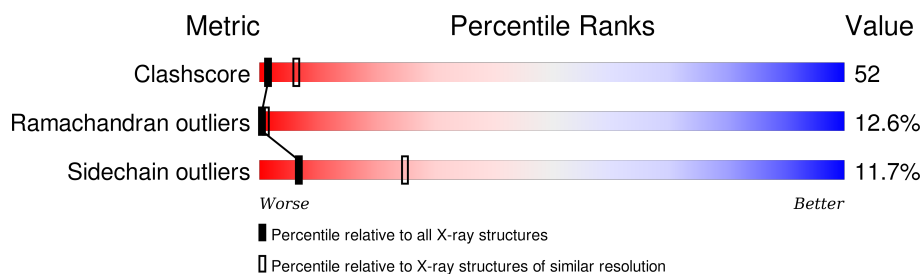|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	Percentile Ranks	Value
Clashscore		52
Ramachandran outliers		12.6%
Sidechain outliers		11.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	288	27% 48% 19% • •
2	B	326	38% 45% 13% • •
3	C	11	45% 55%
3	D	11	64% 36%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5134 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 TRANSCRIPTION FACTOR RELB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total 2200	C 1373	N 395	O 417	S 15	0	0	0

- Molecule 2 is a protein called NUCLEAR FACTOR NF-KAPPA-B P105 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	313	Total 2458	C 1557	N 429	O 460	S 12	0	0	0

- Molecule 3 is a DNA chain called 5'-D(*CP*GP*GP*GP*AP*AP*TP*TP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total 221	C 106	N 41	O 64	P 10	0	0	0
3	D	11	Total 221	C 106	N 41	O 64	P 10	0	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total 14	O 14	0	0
4	B	17	Total 17	O 17	0	0
4	C	1	Total 1	O 1	0	0
4	D	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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

Note EDS was not executed.

- Molecule 1: TRANSCRIPTION FACTOR RELB
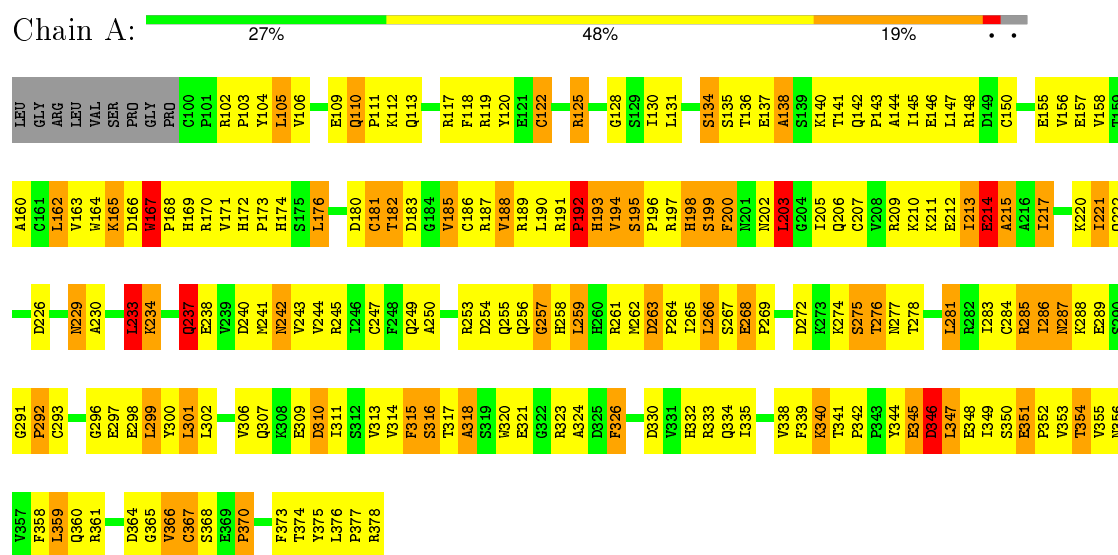
Chain A:

- Molecule 2: NUCLEAR FACTOR NF-KAPPA-B P105 SUBUNIT
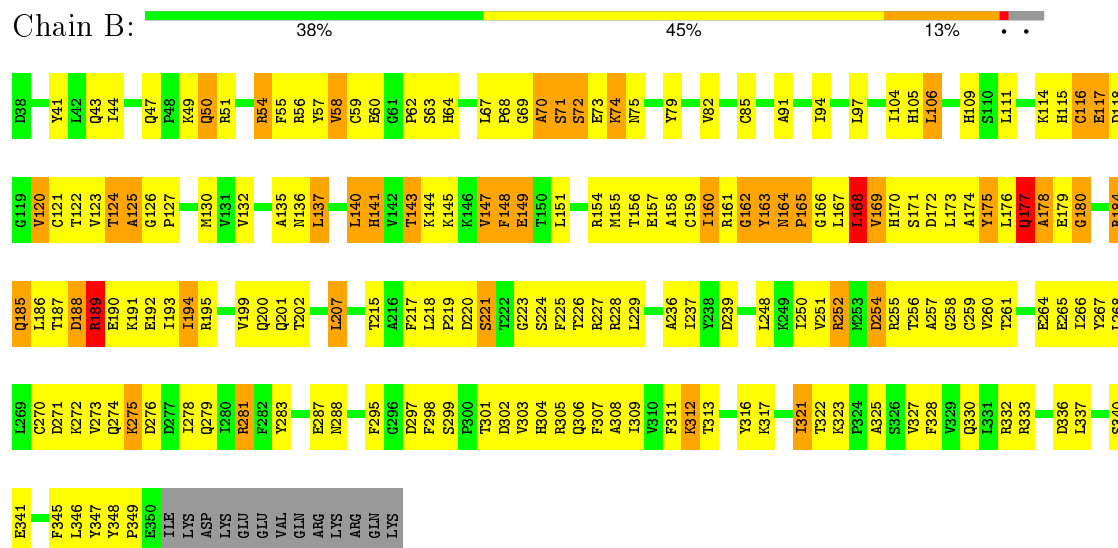
Chain B:
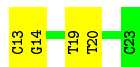
• Molecule 3: 5'-D(*CP*GP*GP*GP*AP*AP*TP*TP*CP*CP*CP)-3'

Chain C:

• Molecule 3: 5'-D(*CP*GP*GP*GP*AP*AP*TP*TP*CP*CP*CP)-3'

Chain D:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	91.44Å 91.44Å 419.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.05	Depositor
% Data completeness (in resolution range)	91.6 (19.90-3.05)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5134	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.38	0/2248	0.67	2/3047 (0.1%)
2	B	0.41	0/2510	0.65	0/3391
3	C	0.42	0/247	0.73	0/379
3	D	0.39	0/247	0.70	0/379
All	All	0.40	0/5252	0.67	2/7196 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	285	ARG	CB-CA-C	5.03	120.47	110.40
1	A	330	ASP	CB-CA-C	5.03	120.46	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2200	0	2154	267	0
2	B	2458	0	2451	248	0
3	C	221	0	125	14	0
3	D	221	0	125	9	0
4	A	14	0	0	4	0
4	B	17	0	0	1	0
4	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
All	All	5134	0	4855	518	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 52.

All (518) 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:285:ARG:HG2	2:B:267:TYR:OH	1.09	1.24
1:A:110:GLN:HG2	1:A:268:GLU:HB2	1.27	1.16
2:B:207:LEU:HD12	2:B:207:LEU:H	1.05	1.14
1:A:194:VAL:HG13	1:A:195:SER:H	0.96	1.07
1:A:314:VAL:HG12	1:A:323:ARG:HB3	1.33	1.07
1:A:285:ARG:CG	2:B:267:TYR:OH	2.05	1.05
2:B:325:ALA:HB3	2:B:347:TYR:HB2	1.31	1.05
1:A:194:VAL:HG13	1:A:195:SER:N	1.73	1.02
1:A:283:ILE:HG23	1:A:301:LEU:HD21	1.38	1.01
1:A:275:SER:HB3	1:A:278:THR:HG22	1.44	0.98
2:B:303:VAL:HG22	2:B:309:ILE:HG12	1.44	0.98
1:A:158:VAL:HG23	1:A:188:VAL:HG13	1.46	0.97
1:A:194:VAL:CG1	1:A:195:SER:H	1.77	0.97
1:A:317:THR:HG22	1:A:318:ALA:H	1.28	0.97
1:A:189:ARG:HB3	1:A:189:ARG:NH1	1.80	0.94
2:B:207:LEU:HD12	2:B:207:LEU:N	1.83	0.94
1:A:198:HIS:HD2	1:A:200:PHE:H	1.15	0.93
1:A:283:ILE:HD11	1:A:359:LEU:HD13	1.48	0.93
2:B:163:TYR:O	2:B:165:PRO:HD3	1.70	0.92
3:C:2:DC:H4'	3:C:3:DG:H5"	1.48	0.91
1:A:194:VAL:HG22	1:A:196:PRO:CD	2.01	0.91
2:B:207:LEU:CD1	2:B:207:LEU:H	1.84	0.90
1:A:221:ILE:HD13	1:A:222:GLN:N	1.86	0.90
1:A:276:THR:HG23	1:A:277:ASN:H	1.33	0.90
1:A:347:LEU:HD12	1:A:349:ILE:H	1.34	0.90
1:A:189:ARG:HH11	1:A:189:ARG:HB3	1.36	0.89
2:B:79:TYR:CD2	2:B:135:ALA:HA	2.06	0.89
2:B:155:MET:HB3	2:B:169:VAL:HG22	1.54	0.89
1:A:354:THR:HA	1:A:374:THR:HG22	1.53	0.89
2:B:147:VAL:HG13	2:B:148:PHE:H	1.39	0.88
1:A:293:CYS:HA	1:A:375:TYR:CD1	2.10	0.87
1:A:293:CYS:HA	1:A:375:TYR:HD1	1.39	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LEU:HB3	1:A:377:PRO:HD2	1.55	0.86
1:A:285:ARG:HG2	2:B:267:TYR:HH	1.39	0.86
2:B:73:GLU:HG3	2:B:74:LYS:HG2	1.57	0.85
2:B:321:ILE:HD13	2:B:322:THR:H	1.43	0.83
2:B:189:ARG:CZ	2:B:189:ARG:HA	2.09	0.83
2:B:194:ILE:HD13	2:B:195:ARG:H	1.44	0.81
2:B:67:LEU:HD11	2:B:237:ILE:HD13	1.60	0.81
1:A:144:ALA:HB2	1:A:199:SER:HB3	1.62	0.81
2:B:260:VAL:HG13	2:B:316:TYR:HB3	1.63	0.80
1:A:213:ILE:HD11	1:A:241:MET:HE3	1.63	0.80
2:B:160:ILE:HG13	2:B:161:ARG:HG3	1.63	0.79
2:B:257:ALA:HB2	2:B:346:LEU:HB3	1.64	0.79
2:B:327:VAL:HG23	2:B:345:PHE:HB3	1.65	0.79
2:B:265:GLU:C	2:B:266:ILE:HD12	2.03	0.79
2:B:106:LEU:HD22	2:B:106:LEU:H	1.46	0.79
2:B:147:VAL:HG22	2:B:202:THR:HG22	1.64	0.78
1:A:332:HIS:CE1	2:B:251:VAL:HG11	2.18	0.78
1:A:340:LYS:HE3	1:A:340:LYS:N	1.99	0.77
1:A:162:LEU:H	1:A:162:LEU:HD12	1.50	0.77
1:A:213:ILE:HG22	1:A:214:GLU:N	1.97	0.77
2:B:255:ARG:HH11	2:B:258:GLY:HA2	1.49	0.76
1:A:283:ILE:HG23	1:A:301:LEU:CD2	2.15	0.76
1:A:194:VAL:HG22	1:A:196:PRO:HD2	1.67	0.76
1:A:281:LEU:HD12	1:A:281:LEU:H	1.51	0.75
2:B:74:LYS:HG3	2:B:75:ASN:H	1.52	0.75
1:A:209:ARG:HE	1:A:211:LYS:NZ	1.85	0.75
1:A:283:ILE:CG2	1:A:301:LEU:HD21	2.14	0.75
2:B:163:TYR:C	2:B:165:PRO:HD3	2.06	0.75
1:A:275:SER:HB3	1:A:278:THR:CG2	2.16	0.75
2:B:255:ARG:NH1	2:B:258:GLY:HA2	2.02	0.75
2:B:148:PHE:CE1	2:B:199:VAL:HG23	2.22	0.74
1:A:176:LEU:HG	1:A:203:LEU:CD1	2.17	0.74
2:B:165:PRO:HB2	2:B:174:ALA:HA	1.70	0.73
1:A:361:ARG:HH21	1:A:366:VAL:HG21	1.51	0.73
1:A:288:LYS:HG2	1:A:299:LEU:HD11	1.69	0.73
1:A:297:GLU:O	1:A:341:THR:HG23	1.89	0.73
2:B:106:LEU:HD22	2:B:106:LEU:N	2.05	0.72
1:A:162:LEU:CG	1:A:176:LEU:HD13	2.19	0.72
1:A:162:LEU:HG	1:A:176:LEU:HD13	1.69	0.72
1:A:192:PRO:O	1:A:194:VAL:HG12	1.90	0.72
2:B:257:ALA:CB	2:B:346:LEU:HB3	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLN:CG	1:A:268:GLU:HB2	2.16	0.71
2:B:160:ILE:HD11	2:B:161:ARG:NE	2.06	0.71
2:B:264:GLU:HB2	2:B:313:THR:OG1	1.91	0.71
1:A:198:HIS:CD2	1:A:200:PHE:H	2.05	0.71
1:A:194:VAL:HG22	1:A:196:PRO:HD3	1.71	0.71
1:A:335:ILE:HD11	2:B:307:PHE:HB2	1.71	0.71
1:A:191:ARG:O	1:A:192:PRO:O	2.09	0.70
2:B:94:ILE:HG22	2:B:122:THR:HG23	1.72	0.70
2:B:57:TYR:OH	3:D:19:DT:OP1	2.08	0.70
2:B:169:VAL:HG12	2:B:170:HIS:N	2.06	0.70
2:B:140:LEU:O	2:B:141:HIS:HB2	1.92	0.70
1:A:162:LEU:HD11	1:A:176:LEU:N	2.05	0.69
1:A:181:CYS:HG	1:A:186:CYS:HG	1.29	0.69
1:A:348:GLU:HG2	1:A:378:ARG:NH2	2.07	0.68
2:B:256:THR:HG22	2:B:256:THR:O	1.93	0.68
2:B:184:ARG:O	2:B:186:LEU:N	2.25	0.68
2:B:124:THR:O	2:B:125:ALA:HB2	1.94	0.68
1:A:242:ASN:HD22	1:A:242:ASN:H	1.41	0.68
3:C:2:DC:C4'	3:C:3:DG:H5"	2.23	0.68
1:A:144:ALA:HB2	1:A:199:SER:CB	2.23	0.68
1:A:188:VAL:HG21	1:A:198:HIS:CE1	2.28	0.68
2:B:155:MET:HB3	2:B:169:VAL:CG2	2.23	0.68
1:A:254:ASP:O	1:A:256:GLN:N	2.27	0.67
1:A:376:LEU:HB3	1:A:377:PRO:CD	2.23	0.67
1:A:276:THR:HG23	1:A:277:ASN:N	2.07	0.67
1:A:194:VAL:C	1:A:196:PRO:HD3	2.15	0.67
2:B:194:ILE:HD13	2:B:195:ARG:N	2.09	0.66
2:B:220:ASP:HB2	2:B:227:ARG:HG3	1.77	0.66
2:B:316:TYR:CG	2:B:317:LYS:N	2.61	0.66
2:B:189:ARG:O	2:B:193:ILE:HG13	1.96	0.66
1:A:300:TYR:CD2	1:A:338:VAL:HG22	2.29	0.66
2:B:160:ILE:HD11	2:B:161:ARG:CZ	2.26	0.66
1:A:198:HIS:CD2	1:A:199:SER:H	2.14	0.66
2:B:188:ASP:O	2:B:190:GLU:N	2.28	0.66
1:A:213:ILE:HD11	1:A:241:MET:CE	2.25	0.66
2:B:158:ALA:HB1	2:B:164:ASN:HB2	1.76	0.66
1:A:306:VAL:O	1:A:334:GLN:HB3	1.96	0.66
1:A:128:GLY:N	3:D:13:DC:H5"	2.11	0.65
2:B:123:VAL:HG11	2:B:132:VAL:HG21	1.79	0.65
1:A:364:ASP:OD2	1:A:366:VAL:HG22	1.97	0.65
1:A:140:LYS:HD2	1:A:140:LYS:H	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ALA:HB2	1:A:342:PRO:HD3	1.78	0.65
2:B:56:ARG:HG3	2:B:64:HIS:HB2	1.77	0.65
3:C:2:DC:H4'	3:C:3:DG:C5'	2.25	0.65
1:A:240:ASP:HB3	1:A:242:ASN:ND2	2.12	0.65
1:A:118:PHE:HE1	1:A:205:ILE:HD13	1.62	0.65
1:A:281:LEU:N	1:A:281:LEU:HD12	2.10	0.65
1:A:162:LEU:HD23	1:A:244:VAL:HG21	1.78	0.64
3:D:20:DT:H5'	3:D:20:DT:H6	1.62	0.64
1:A:170:ARG:HH11	1:A:230:ALA:HB1	1.61	0.64
2:B:155:MET:HE1	2:B:201:GLN:HE22	1.62	0.64
2:B:106:LEU:H	2:B:106:LEU:CD2	2.10	0.64
2:B:250:ILE:HD11	2:B:330:GLN:HA	1.80	0.63
2:B:109:HIS:ND1	2:B:141:HIS:HA	2.12	0.63
2:B:148:PHE:HA	2:B:202:THR:HG21	1.80	0.63
2:B:185:GLN:O	2:B:186:LEU:HB3	1.97	0.63
1:A:317:THR:HB	1:A:320:TRP:HB3	1.81	0.63
1:A:170:ARG:NH1	1:A:230:ALA:HB1	2.13	0.63
1:A:193:HIS:ND1	1:A:193:HIS:N	2.47	0.63
1:A:355:VAL:HG11	1:A:375:TYR:CD2	2.34	0.63
1:A:176:LEU:HG	1:A:203:LEU:HD11	1.79	0.62
2:B:299:SER:C	2:B:301:THR:H	2.02	0.62
1:A:221:ILE:HD13	1:A:222:GLN:H	1.64	0.62
2:B:44:ILE:HA	2:B:82:VAL:HG12	1.81	0.62
3:D:19:DT:C6	3:D:20:DT:H72	2.33	0.62
2:B:123:VAL:HG22	2:B:124:THR:O	2.00	0.62
1:A:314:VAL:HG12	1:A:323:ARG:CB	2.21	0.62
2:B:162:GLY:HA2	2:B:177:GLN:HA	1.81	0.62
2:B:176:LEU:O	2:B:178:ALA:N	2.32	0.62
1:A:361:ARG:NH2	1:A:366:VAL:HG21	2.15	0.62
1:A:317:THR:HG22	1:A:318:ALA:N	2.08	0.61
1:A:355:VAL:O	1:A:355:VAL:HG13	2.00	0.61
1:A:333:ARG:HG3	2:B:307:PHE:CD2	2.34	0.61
1:A:288:LYS:HG2	1:A:299:LEU:CD1	2.30	0.61
1:A:339:PHE:C	1:A:340:LYS:HE3	2.21	0.61
1:A:262:MET:O	1:A:263:ASP:O	2.18	0.61
2:B:257:ALA:HB1	2:B:346:LEU:O	2.01	0.61
1:A:156:VAL:HG12	1:A:157:GLU:N	2.15	0.61
1:A:156:VAL:N	1:A:190:LEU:O	2.31	0.61
2:B:49:LYS:HD2	2:B:70:ALA:HA	1.83	0.61
2:B:215:THR:HG22	2:B:217:PHE:CE1	2.36	0.60
1:A:297:GLU:O	1:A:299:LEU:HD23	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LEU:HD21	2:B:333:ARG:NH1	2.15	0.60
1:A:355:VAL:HG11	1:A:375:TYR:CE2	2.36	0.60
2:B:49:LYS:O	2:B:50:GLN:CB	2.49	0.60
1:A:172:HIS:CG	1:A:173:PRO:HD2	2.36	0.60
2:B:140:LEU:O	2:B:141:HIS:CB	2.49	0.60
2:B:73:GLU:HG3	2:B:74:LYS:H	1.67	0.60
2:B:220:ASP:O	2:B:221:SER:O	2.19	0.60
2:B:156:THR:HG23	2:B:194:ILE:HG13	1.83	0.60
2:B:57:TYR:HB2	2:B:60:GLU:HG3	1.83	0.59
1:A:188:VAL:HG21	1:A:198:HIS:HE1	1.67	0.59
1:A:242:ASN:ND2	1:A:242:ASN:H	2.00	0.59
1:A:283:ILE:CD1	1:A:359:LEU:HD13	2.28	0.59
1:A:155:GLU:CG	1:A:189:ARG:HH22	2.15	0.59
2:B:174:ALA:C	2:B:176:LEU:H	2.05	0.59
2:B:322:THR:CA	2:B:349:PRO:HG2	2.32	0.59
1:A:162:LEU:HD11	1:A:176:LEU:H	1.67	0.59
1:A:217:ILE:HD13	1:A:217:ILE:C	2.23	0.59
1:A:313:VAL:HG12	1:A:326:PHE:HE2	1.68	0.59
2:B:162:GLY:O	2:B:164:ASN:N	2.35	0.58
1:A:289:GLU:HA	1:A:373:PHE:HD2	1.68	0.58
2:B:322:THR:HA	2:B:349:PRO:HG2	1.84	0.58
1:A:245:ARG:NE	1:A:266:LEU:HD12	2.19	0.58
2:B:160:ILE:HD11	2:B:161:ARG:NH2	2.19	0.58
2:B:104:ILE:O	2:B:104:ILE:HG12	2.02	0.58
2:B:165:PRO:HD2	2:B:167:LEU:H	1.69	0.58
2:B:312:LYS:N	2:B:312:LYS:HD2	2.18	0.58
1:A:245:ARG:HD2	1:A:267:SER:O	2.03	0.57
1:A:209:ARG:O	1:A:212:GLU:N	2.36	0.57
1:A:167:TRP:HB3	1:A:168:PRO:CD	2.34	0.57
2:B:187:THR:O	2:B:191:LYS:HB2	2.04	0.57
2:B:67:LEU:HD11	2:B:237:ILE:CD1	2.32	0.57
1:A:189:ARG:HH11	1:A:189:ARG:CB	2.15	0.57
2:B:148:PHE:HE1	2:B:199:VAL:HG23	1.67	0.57
1:A:355:VAL:HG21	1:A:375:TYR:HE2	1.69	0.57
2:B:322:THR:C	2:B:349:PRO:HG2	2.25	0.56
1:A:245:ARG:HH21	1:A:269:PRO:HG3	1.69	0.56
1:A:287:ASN:HB2	1:A:300:TYR:N	2.21	0.56
2:B:126:GLY:H	2:B:127:PRO:CD	2.17	0.56
1:A:250:ALA:HB3	1:A:262:MET:CG	2.35	0.56
2:B:251:VAL:HG12	2:B:270:CYS:HA	1.87	0.56
1:A:334:GLN:NE2	3:C:6:DA:H3'	2.21	0.56

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:LEU:C	2:B:268:LEU:HD23	2.26	0.56
1:A:117:ARG:NH2	1:A:119:ARG:HH22	2.03	0.56
2:B:109:HIS:CE1	2:B:141:HIS:HA	2.41	0.56
2:B:71:SER:O	2:B:72:SER:C	2.43	0.56
1:A:272:ASP:OD1	1:A:274:LYS:HE3	2.06	0.56
1:A:293:CYS:HB3	1:A:376:LEU:O	2.06	0.56
1:A:281:LEU:CD1	1:A:281:LEU:H	2.18	0.56
1:A:111:PRO:HA	1:A:143:PRO:HG3	1.86	0.56
1:A:277:ASN:HB3	1:A:307:GLN:NE2	2.20	0.56
2:B:148:PHE:CA	2:B:202:THR:HG21	2.35	0.56
1:A:287:ASN:HB2	1:A:300:TYR:H	1.70	0.56
2:B:126:GLY:N	2:B:127:PRO:CD	2.69	0.56
1:A:155:GLU:HA	1:A:190:LEU:O	2.05	0.55
2:B:174:ALA:C	2:B:176:LEU:N	2.60	0.55
1:A:315:PHE:HB3	1:A:355:VAL:HG22	1.86	0.55
2:B:189:ARG:HA	2:B:189:ARG:NE	2.21	0.55
2:B:304:HIS:HB3	2:B:308:ALA:HB3	1.87	0.55
2:B:106:LEU:HD21	2:B:168:LEU:HG	1.88	0.55
1:A:268:GLU:HA	1:A:268:GLU:OE1	2.05	0.55
2:B:260:VAL:CG1	2:B:316:TYR:HB3	2.35	0.55
1:A:253:ARG:NE	1:A:257:GLY:O	2.38	0.55
1:A:192:PRO:O	1:A:193:HIS:C	2.43	0.55
2:B:164:ASN:HA	2:B:168:LEU:CD2	2.34	0.55
2:B:97:LEU:HG	2:B:111:LEU:HG	1.89	0.55
1:A:174:HIS:NE2	1:A:241:MET:HG3	2.21	0.55
2:B:174:ALA:O	2:B:176:LEU:N	2.39	0.55
1:A:158:VAL:HA	1:A:249:GLN:O	2.06	0.55
2:B:71:SER:O	2:B:73:GLU:N	2.40	0.55
1:A:186:CYS:C	4:A:2004:HOH:O	2.45	0.54
2:B:123:VAL:CG1	2:B:132:VAL:HG21	2.37	0.54
2:B:163:TYR:HB3	2:B:228:ARG:HD2	1.89	0.54
2:B:305:ARG:CG	2:B:305:ARG:HH21	2.21	0.54
1:A:264:PRO:C	1:A:265:ILE:HD12	2.28	0.54
1:A:226:ASP:OD1	1:A:229:ASN:HA	2.08	0.54
1:A:259:LEU:O	1:A:259:LEU:HD23	2.08	0.54
2:B:266:ILE:N	2:B:266:ILE:HD12	2.22	0.54
2:B:218:LEU:HB2	2:B:227:ARG:HB2	1.88	0.54
1:A:172:HIS:ND1	1:A:173:PRO:HD2	2.22	0.54
2:B:155:MET:HE1	2:B:201:GLN:NE2	2.23	0.54
2:B:69:GLY:O	2:B:71:SER:N	2.41	0.54
2:B:147:VAL:HG13	2:B:148:PHE:N	2.16	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:VAL:HG13	2:B:316:TYR:CB	2.36	0.53
2:B:54:ARG:NE	2:B:56:ARG:NH2	2.56	0.53
2:B:164:ASN:OD1	2:B:164:ASN:N	2.38	0.53
2:B:259:CYS:SG	2:B:261:THR:HG22	2.47	0.53
1:A:213:ILE:HG22	1:A:214:GLU:H	1.70	0.53
1:A:298:GLU:O	1:A:299:LEU:HD22	2.09	0.53
2:B:126:GLY:N	2:B:127:PRO:HD3	2.23	0.53
2:B:219:PRO:HA	2:B:224:SER:O	2.07	0.53
2:B:299:SER:C	2:B:301:THR:N	2.60	0.53
1:A:135:SER:CA	1:A:141:THR:HG22	2.38	0.53
2:B:218:LEU:HG	2:B:229:LEU:HD21	1.91	0.53
1:A:135:SER:N	1:A:141:THR:HG22	2.24	0.53
2:B:166:GLY:HA2	2:B:170:HIS:O	2.09	0.53
1:A:209:ARG:H	1:A:212:GLU:CB	2.22	0.53
2:B:55:PHE:CE1	2:B:239:ASP:HB2	2.44	0.52
2:B:164:ASN:HA	2:B:168:LEU:HD23	1.90	0.52
1:A:240:ASP:HB3	1:A:242:ASN:HD21	1.73	0.52
2:B:117:GLU:O	2:B:118:ASP:HB2	2.09	0.52
1:A:181:CYS:HA	1:A:186:CYS:HA	1.90	0.52
1:A:166:ASP:O	1:A:167:TRP:C	2.47	0.52
1:A:233:LEU:O	1:A:234:LYS:HB2	2.10	0.52
1:A:276:THR:CG2	1:A:277:ASN:H	2.13	0.52
1:A:198:HIS:O	1:A:199:SER:CB	2.58	0.52
1:A:213:ILE:O	1:A:214:GLU:C	2.47	0.52
2:B:120:VAL:HG22	2:B:120:VAL:O	2.10	0.52
1:A:285:ARG:CG	1:A:286:ILE:H	2.23	0.52
2:B:221:SER:C	2:B:223:GLY:N	2.63	0.51
1:A:135:SER:H	1:A:141:THR:CG2	2.23	0.51
1:A:344:TYR:O	1:A:346:ASP:N	2.43	0.51
2:B:160:ILE:HD11	2:B:161:ARG:HE	1.73	0.51
1:A:250:ALA:HB3	1:A:262:MET:SD	2.50	0.51
2:B:321:ILE:HD13	2:B:322:THR:N	2.19	0.51
1:A:113:GLN:HG3	1:A:269:PRO:O	2.11	0.51
2:B:67:LEU:HD23	2:B:68:PRO:N	2.26	0.51
2:B:221:SER:C	2:B:223:GLY:H	2.13	0.51
2:B:55:PHE:CD1	2:B:239:ASP:HB2	2.46	0.51
1:A:275:SER:O	1:A:277:ASN:N	2.44	0.51
1:A:350:SER:O	1:A:352:PRO:HD3	2.10	0.51
2:B:298:PHE:HB2	2:B:302:ASP:HB2	1.92	0.51
2:B:163:TYR:HB3	2:B:228:ARG:CD	2.41	0.51
1:A:104:TYR:CE2	1:A:148:ARG:HB2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:C	1:A:276:THR:H	2.15	0.51
2:B:124:THR:O	2:B:125:ALA:CB	2.59	0.51
2:B:256:THR:CG2	2:B:256:THR:O	2.57	0.50
1:A:209:ARG:HE	1:A:211:LYS:HZ1	1.55	0.50
2:B:260:VAL:HG22	2:B:347:TYR:HB3	1.92	0.50
1:A:277:ASN:HB3	1:A:307:GLN:HE22	1.76	0.50
2:B:164:ASN:HB3	2:B:168:LEU:HD23	1.93	0.50
2:B:73:GLU:HG3	2:B:74:LYS:N	2.25	0.50
2:B:156:THR:CG2	2:B:194:ILE:HG13	2.41	0.50
1:A:131:LEU:O	1:A:143:PRO:HG3	2.11	0.50
1:A:156:VAL:HG12	1:A:157:GLU:H	1.77	0.50
1:A:181:CYS:O	1:A:182:THR:HG23	2.11	0.50
1:A:245:ARG:HE	1:A:266:LEU:HD12	1.76	0.50
1:A:171:VAL:HG21	1:A:220:LYS:HG2	1.94	0.50
1:A:315:PHE:N	1:A:315:PHE:CD1	2.80	0.50
2:B:109:HIS:CE1	2:B:207:LEU:HB3	2.47	0.49
2:B:164:ASN:CB	2:B:168:LEU:HD23	2.43	0.49
2:B:148:PHE:HA	2:B:202:THR:CG2	2.41	0.49
2:B:51:ARG:HH11	2:B:51:ARG:HG2	1.77	0.49
2:B:56:ARG:HH11	2:B:64:HIS:CE1	2.30	0.49
1:A:157:GLU:O	1:A:250:ALA:HA	2.12	0.49
1:A:257:GLY:O	1:A:258:HIS:C	2.51	0.49
2:B:91:ALA:HA	2:B:225:PHE:CE1	2.47	0.49
1:A:176:LEU:HG	1:A:203:LEU:HD13	1.94	0.49
3:C:2:DC:O2	3:C:2:DC:O4'	2.28	0.49
1:A:197:ARG:O	1:A:198:HIS:C	2.51	0.49
2:B:41:TYR:CE1	2:B:85:CYS:HB2	2.48	0.49
2:B:170:HIS:C	2:B:172:ASP:H	2.17	0.49
1:A:335:ILE:CD1	2:B:307:PHE:HB2	2.39	0.48
2:B:56:ARG:HG3	2:B:64:HIS:CB	2.43	0.48
1:A:209:ARG:H	1:A:212:GLU:HB3	1.78	0.48
1:A:156:VAL:O	1:A:190:LEU:N	2.41	0.48
2:B:162:GLY:HA2	2:B:177:GLN:C	2.33	0.48
1:A:162:LEU:HD12	1:A:162:LEU:N	2.25	0.48
1:A:213:ILE:O	1:A:215:ALA:N	2.45	0.48
2:B:94:ILE:C	2:B:94:ILE:HD12	2.33	0.48
3:C:8:DT:H2"	3:C:9:DT:C5'	2.43	0.48
1:A:186:CYS:SG	1:A:203:LEU:HD21	2.54	0.48
1:A:256:GLN:O	1:A:258:HIS:N	2.47	0.48
1:A:272:ASP:OD1	1:A:274:LYS:HG2	2.13	0.48
1:A:202:ASN:O	1:A:203:LEU:C	2.52	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HG13	1:A:197:ARG:CB	2.43	0.48
1:A:209:ARG:O	1:A:211:LYS:N	2.47	0.48
2:B:305:ARG:HG2	2:B:305:ARG:HH21	1.77	0.48
1:A:258:HIS:HA	4:A:2008:HOH:O	2.13	0.48
2:B:43:GLN:NE2	2:B:85:CYS:SG	2.87	0.48
2:B:173:LEU:C	2:B:175:TYR:H	2.16	0.48
2:B:177:GLN:HE21	2:B:177:GLN:CA	2.25	0.48
2:B:274:GLN:O	2:B:276:ASP:N	2.47	0.48
2:B:155:MET:O	2:B:158:ALA:HB3	2.14	0.48
1:A:353:VAL:HG22	1:A:354:THR:N	2.29	0.48
1:A:174:HIS:N	1:A:174:HIS:CD2	2.80	0.47
2:B:177:GLN:O	2:B:178:ALA:HB3	2.14	0.47
1:A:237:GLN:HB3	1:A:238:GLU:H	1.53	0.47
2:B:145:LYS:HD3	2:B:145:LYS:HA	1.70	0.47
2:B:54:ARG:HE	2:B:56:ARG:NH2	2.12	0.47
1:A:194:VAL:C	1:A:196:PRO:CD	2.82	0.47
1:A:197:ARG:O	1:A:199:SER:N	2.47	0.47
2:B:299:SER:O	2:B:301:THR:N	2.47	0.47
1:A:120:TYR:OH	3:C:9:DT:H5'	2.14	0.47
1:A:317:THR:HG1	1:A:320:TRP:HE3	1.60	0.47
1:A:118:PHE:CD1	1:A:205:ILE:HB	2.50	0.47
3:C:9:DT:H2"	3:C:10:DC:C6	2.50	0.47
1:A:195:SER:N	1:A:196:PRO:CD	2.78	0.47
1:A:199:SER:O	1:A:200:PHE:O	2.33	0.47
1:A:214:GLU:OE1	1:A:214:GLU:HA	2.15	0.47
1:A:242:ASN:ND2	1:A:242:ASN:N	2.62	0.47
2:B:260:VAL:HG12	2:B:260:VAL:O	2.13	0.47
1:A:128:GLY:H	3:D:13:DC:H5"	1.80	0.47
1:A:358:PHE:HB3	1:A:370:PRO:HA	1.96	0.47
2:B:189:ARG:HH21	2:B:192:GLU:HG2	1.80	0.46
2:B:265:GLU:HA	2:B:311:PHE:O	2.14	0.46
2:B:251:VAL:O	2:B:252:ARG:O	2.32	0.46
2:B:305:ARG:CG	2:B:305:ARG:NH2	2.77	0.46
2:B:44:ILE:HD12	2:B:47:GLN:HE22	1.80	0.46
1:A:111:PRO:O	1:A:112:LYS:C	2.52	0.46
2:B:173:LEU:O	2:B:174:ALA:HB3	2.15	0.46
2:B:67:LEU:C	2:B:67:LEU:HD23	2.36	0.46
2:B:186:LEU:HD11	2:B:190:GLU:OE2	2.15	0.46
2:B:118:ASP:O	2:B:120:VAL:HG12	2.15	0.46
1:A:243:VAL:HG13	1:A:243:VAL:O	2.16	0.46
2:B:74:LYS:HG3	2:B:75:ASN:N	2.27	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:O	1:A:136:THR:OG1	2.34	0.46
1:A:145:ILE:HD12	1:A:146:GLU:N	2.30	0.46
2:B:322:THR:O	2:B:349:PRO:HG2	2.16	0.46
2:B:165:PRO:HG2	2:B:166:GLY:H	1.82	0.45
1:A:292:PRO:HA	1:A:376:LEU:HB2	1.98	0.45
1:A:310:ASP:OD2	1:A:361:ARG:HG3	2.15	0.45
2:B:278:ILE:HG13	2:B:279:GLN:N	2.31	0.45
2:B:199:VAL:HG12	2:B:200:GLN:N	2.31	0.45
2:B:56:ARG:O	2:B:140:LEU:O	2.35	0.45
2:B:163:TYR:CB	2:B:228:ARG:CZ	2.94	0.45
1:A:209:ARG:HB2	1:A:212:GLU:HB2	1.99	0.45
2:B:144:LYS:N	3:D:19:DT:OP2	2.44	0.45
2:B:50:GLN:HG3	2:B:236:ALA:O	2.17	0.45
1:A:338:VAL:HG11	2:B:252:ARG:NH1	2.32	0.45
1:A:202:ASN:O	1:A:203:LEU:O	2.35	0.45
1:A:302:LEU:HD13	2:B:267:TYR:CD2	2.51	0.45
1:A:198:HIS:CG	1:A:199:SER:H	2.32	0.45
2:B:304:HIS:N	2:B:308:ALA:O	2.37	0.45
2:B:278:ILE:HD12	2:B:332:ARG:O	2.17	0.45
1:A:198:HIS:HD2	1:A:200:PHE:N	1.97	0.45
2:B:105:HIS:CD2	2:B:105:HIS:N	2.83	0.45
1:A:162:LEU:CD1	1:A:176:LEU:HD13	2.46	0.45
1:A:135:SER:HA	1:A:141:THR:HG22	1.97	0.45
2:B:137:LEU:HA	2:B:137:LEU:HD23	1.79	0.45
1:A:213:ILE:CG2	1:A:214:GLU:N	2.67	0.45
2:B:297:ASP:O	2:B:298:PHE:HB3	2.17	0.45
2:B:271:ASP:O	2:B:273:VAL:HG13	2.17	0.45
1:A:242:ASN:HD22	1:A:242:ASN:N	2.02	0.45
2:B:165:PRO:CG	2:B:166:GLY:H	2.30	0.44
2:B:57:TYR:CE1	3:D:19:DT:H2'	2.51	0.44
2:B:143:THR:C	2:B:145:LYS:N	2.71	0.44
1:A:102:ARG:HG3	1:A:103:PRO:HD2	1.99	0.44
1:A:105:LEU:C	1:A:105:LEU:HD12	2.37	0.44
2:B:194:ILE:CD1	2:B:195:ARG:N	2.77	0.44
2:B:97:LEU:HD21	2:B:111:LEU:HD21	1.99	0.44
1:A:155:GLU:CA	1:A:190:LEU:O	2.65	0.44
2:B:162:GLY:HA2	2:B:177:GLN:CA	2.46	0.44
2:B:221:SER:O	2:B:223:GLY:N	2.50	0.44
1:A:182:THR:O	1:A:183:ASP:HB2	2.17	0.44
1:A:128:GLY:HA3	3:D:13:DC:O5'	2.18	0.44
1:A:155:GLU:HG3	1:A:189:ARG:HH22	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:HD11	2:B:190:GLU:CD	2.38	0.44
2:B:156:THR:O	2:B:159:CYS:N	2.50	0.44
1:A:176:LEU:HB3	1:A:186:CYS:SG	2.57	0.44
2:B:163:TYR:HB2	2:B:228:ARG:CZ	2.47	0.44
1:A:378:ARG:O	1:A:378:ARG:HG2	2.18	0.44
1:A:117:ARG:CZ	1:A:119:ARG:NH2	2.81	0.44
1:A:180:ASP:HB3	1:A:187:ARG:O	2.18	0.44
1:A:194:VAL:CG1	1:A:195:SER:N	2.46	0.43
2:B:104:ILE:C	2:B:105:HIS:HD2	2.21	0.43
1:A:347:LEU:HD11	1:A:349:ILE:HG12	1.99	0.43
3:C:8:DT:H2''	3:C:9:DT:H5''	2.00	0.43
2:B:341:GLU:HA	2:B:341:GLU:OE1	2.17	0.43
1:A:245:ARG:HD3	1:A:269:PRO:HG3	1.99	0.43
3:C:9:DT:H2''	3:C:10:DC:H6	1.82	0.43
1:A:158:VAL:CG2	1:A:188:VAL:HG13	2.32	0.43
2:B:123:VAL:HG11	2:B:132:VAL:CG2	2.47	0.43
1:A:261:ARG:HH11	1:A:261:ARG:HG3	1.82	0.43
1:A:360:GLN:HG3	1:A:367:CYS:HB3	2.00	0.43
2:B:105:HIS:ND1	2:B:201:GLN:CD	2.72	0.43
2:B:106:LEU:N	2:B:106:LEU:CD2	2.73	0.43
2:B:176:LEU:O	2:B:177:GLN:C	2.57	0.43
1:A:117:ARG:NH2	1:A:119:ARG:NH2	2.66	0.43
1:A:281:LEU:N	1:A:281:LEU:CD1	2.80	0.43
2:B:151:LEU:O	2:B:154:ARG:N	2.52	0.43
2:B:62:PRO:O	2:B:64:HIS:N	2.49	0.43
1:A:143:PRO:O	1:A:199:SER:O	2.36	0.43
2:B:151:LEU:HA	2:B:151:LEU:HD23	1.72	0.43
2:B:44:ILE:HG21	2:B:47:GLN:NE2	2.34	0.43
3:C:8:DT:C2'	3:C:9:DT:H5''	2.49	0.43
1:A:189:ARG:CZ	1:A:189:ARG:HB3	2.46	0.43
1:A:316:SER:O	1:A:355:VAL:HG23	2.19	0.43
1:A:130:ILE:HD12	1:A:203:LEU:HD12	2.00	0.43
1:A:345:GLU:O	1:A:346:ASP:C	2.57	0.43
1:A:306:VAL:HG21	1:A:311:ILE:HD13	2.01	0.42
2:B:333:ARG:HE	2:B:336:ASP:CG	2.23	0.42
2:B:179:GLU:HB2	2:B:180:GLY:H	1.70	0.42
1:A:145:ILE:CD1	1:A:197:ARG:CB	2.97	0.42
1:A:375:TYR:O	1:A:376:LEU:HD23	2.19	0.42
1:A:185:VAL:HG22	4:A:2004:HOH:O	2.19	0.42
1:A:167:TRP:O	1:A:169:HIS:N	2.53	0.42
1:A:174:HIS:H	1:A:174:HIS:CD2	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:O	1:A:321:GLU:HG2	2.18	0.42
2:B:305:ARG:O	2:B:307:PHE:CD1	2.73	0.42
1:A:276:THR:CG2	1:A:277:ASN:N	2.77	0.42
1:A:105:LEU:HD12	1:A:106:VAL:N	2.33	0.42
1:A:262:MET:O	1:A:263:ASP:C	2.57	0.42
2:B:257:ALA:CB	2:B:346:LEU:O	2.67	0.42
2:B:91:ALA:HA	2:B:225:PHE:HE1	1.83	0.42
2:B:166:GLY:CA	2:B:171:SER:HA	2.50	0.42
2:B:189:ARG:NH2	2:B:192:GLU:HG2	2.35	0.42
2:B:126:GLY:HA2	2:B:130:MET:SD	2.60	0.42
2:B:116:CYS:HA	2:B:121:CYS:HA	2.02	0.42
2:B:114:LYS:HE3	2:B:115:HIS:CE1	2.55	0.42
1:A:183:ASP:O	1:A:185:VAL:N	2.52	0.42
1:A:296:GLY:N	1:A:341:THR:O	2.45	0.42
1:A:136:THR:O	1:A:138:ALA:N	2.53	0.42
1:A:194:VAL:O	1:A:196:PRO:HD3	2.19	0.42
1:A:278:THR:HG23	1:A:278:THR:O	2.18	0.42
2:B:251:VAL:O	2:B:252:ARG:C	2.58	0.42
1:A:339:PHE:CD1	1:A:339:PHE:N	2.86	0.42
2:B:321:ILE:HD12	2:B:323:LYS:H	1.85	0.42
2:B:164:ASN:HA	2:B:168:LEU:HD22	2.01	0.42
2:B:148:PHE:O	2:B:149:GLU:C	2.57	0.42
2:B:248:LEU:HB2	2:B:340:SER:HB3	2.02	0.42
2:B:162:GLY:C	2:B:164:ASN:N	2.74	0.41
1:A:355:VAL:HG12	1:A:373:PHE:O	2.19	0.41
2:B:186:LEU:HD21	2:B:190:GLU:OE1	2.19	0.41
1:A:185:VAL:CG2	4:A:2004:HOH:O	2.68	0.41
3:D:13:DC:H2"	3:D:14:DG:C8	2.54	0.41
2:B:147:VAL:O	2:B:148:PHE:C	2.59	0.41
1:A:311:ILE:HD12	1:A:311:ILE:HA	1.90	0.41
1:A:125:ARG:NH2	1:A:206:GLN:OE1	2.54	0.41
2:B:64:HIS:CD2	3:C:3:DG:N7	2.88	0.41
2:B:190:GLU:C	2:B:192:GLU:N	2.72	0.41
1:A:140:LYS:CD	1:A:140:LYS:H	2.30	0.41
2:B:143:THR:O	2:B:145:LYS:N	2.52	0.41
2:B:273:VAL:O	2:B:306:GLN:HG2	2.19	0.41
1:A:155:GLU:CD	1:A:189:ARG:HH22	2.24	0.41
2:B:259:CYS:HB3	2:B:261:THR:HG22	2.01	0.41
2:B:321:ILE:CD1	2:B:323:LYS:H	2.34	0.41
1:A:181:CYS:C	1:A:182:THR:HG23	2.41	0.41
2:B:165:PRO:CG	2:B:166:GLY:N	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:TYR:HA	2:B:349:PRO:HD3	1.92	0.41
2:B:49:LYS:O	2:B:50:GLN:HB3	2.17	0.41
1:A:165:LYS:O	1:A:245:ARG:NH1	2.53	0.41
1:A:147:LEU:HB3	1:A:150:CYS:SG	2.61	0.41
2:B:316:TYR:OH	2:B:317:LYS:HE2	2.20	0.41
1:A:198:HIS:O	1:A:199:SER:HB3	2.20	0.41
1:A:349:ILE:HG23	1:A:351:GLU:H	1.85	0.41
2:B:259:CYS:HA	2:B:348:TYR:O	2.20	0.41
2:B:266:ILE:N	2:B:266:ILE:CD1	2.83	0.41
2:B:283:TYR:CE2	2:B:328:PHE:HB3	2.56	0.41
2:B:58:VAL:HG13	2:B:59:CYS:H	1.86	0.41
1:A:277:ASN:CB	1:A:307:GLN:HE22	2.32	0.41
1:A:105:LEU:HD13	1:A:145:ILE:HB	2.03	0.41
2:B:190:GLU:C	2:B:192:GLU:H	2.24	0.41
2:B:194:ILE:CG1	2:B:195:ARG:N	2.84	0.41
1:A:162:LEU:HD11	1:A:176:LEU:HD13	2.02	0.41
2:B:51:ARG:HA	4:B:2011:HOH:O	2.20	0.41
1:A:356:ASN:O	1:A:356:ASN:OD1	2.39	0.41
2:B:169:VAL:CG1	2:B:170:HIS:N	2.75	0.41
1:A:174:HIS:CG	1:A:207:CYS:HA	2.55	0.41
1:A:162:LEU:H	1:A:162:LEU:CD1	2.20	0.41
2:B:268:LEU:O	2:B:308:ALA:HA	2.21	0.41
1:A:213:ILE:CG2	1:A:214:GLU:H	2.31	0.40
1:A:160:ALA:O	1:A:185:VAL:HA	2.20	0.40
1:A:212:GLU:OE2	1:A:212:GLU:HA	2.21	0.40
1:A:315:PHE:N	1:A:315:PHE:HD1	2.19	0.40
2:B:157:GLU:O	2:B:160:ILE:HG12	2.21	0.40
1:A:365:GLY:O	1:A:366:VAL:C	2.59	0.40
1:A:122:CYS:SG	3:C:10:DC:OP1	2.79	0.40
2:B:317:LYS:HB3	2:B:317:LYS:HE2	1.85	0.40
2:B:336:ASP:O	2:B:337:LEU:HB2	2.22	0.40
1:A:167:TRP:HB3	1:A:168:PRO:HD3	2.01	0.40
1:A:134:SER:HB2	1:A:141:THR:HG21	2.03	0.40
1:A:120:TYR:CZ	3:C:9:DT:H5'	2.56	0.40
2:B:281:ARG:HB2	2:B:295:PHE:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/288 (96%)	192 (69%)	43 (16%)	42 (15%)	0	0
2	B	311/326 (95%)	233 (75%)	46 (15%)	32 (10%)	1	3
All	All	588/614 (96%)	425 (72%)	89 (15%)	74 (13%)	0	1

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	SER
1	A	137	GLU
1	A	138	ALA
1	A	164	TRP
1	A	167	TRP
1	A	185	VAL
1	A	192	PRO
1	A	194	VAL
1	A	195	SER
1	A	199	SER
1	A	203	LEU
1	A	213	ILE
1	A	214	GLU
1	A	234	LYS
1	A	263	ASP
1	A	276	THR
1	A	292	PRO
1	A	345	GLU
2	B	50	GLN
2	B	71	SER
2	B	140	LEU
2	B	141	HIS
2	B	163	TYR
2	B	165	PRO
2	B	169	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	177	GLN
2	B	185	GLN
2	B	221	SER
2	B	252	ARG
2	B	254	ASP
2	B	275	LYS
2	B	288	ASN
1	A	165	LYS
1	A	181	CYS
1	A	198	HIS
1	A	200	PHE
1	A	210	LYS
1	A	215	ALA
1	A	233	LEU
1	A	257	GLY
1	A	284	CYS
1	A	291	GLY
1	A	346	ASP
2	B	70	ALA
2	B	72	SER
2	B	117	GLU
2	B	125	ALA
2	B	188	ASP
1	A	122	CYS
1	A	182	THR
1	A	255	GLN
1	A	366	VAL
2	B	63	SER
2	B	160	ILE
2	B	175	TYR
2	B	189	ARG
2	B	272	LYS
2	B	287	GLU
1	A	229	ASN
1	A	310	ASP
2	B	74	LYS
1	A	275	SER
1	A	368	SER
2	B	178	ALA
1	A	237	GLN
1	A	318	ALA
1	A	326	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	148	PHE
2	B	168	LEU
1	A	286	ILE
2	B	180	GLY
1	A	370	PRO
2	B	147	VAL
2	B	162	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	246/257 (96%)	209 (85%)	37 (15%)	3	14
2	B	268/282 (95%)	245 (91%)	23 (9%)	13	43
All	All	514/539 (95%)	454 (88%)	60 (12%)	7	25

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	109	GLU
1	A	110	GLN
1	A	125	ARG
1	A	142	GLN
1	A	162	LEU
1	A	163	VAL
1	A	167	TRP
1	A	176	LEU
1	A	188	VAL
1	A	192	PRO
1	A	193	HIS
1	A	203	LEU
1	A	214	GLU
1	A	217	ILE
1	A	221	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	233	LEU
1	A	237	GLN
1	A	242	ASN
1	A	247	CYS
1	A	259	LEU
1	A	266	LEU
1	A	268	GLU
1	A	281	LEU
1	A	287	ASN
1	A	299	LEU
1	A	301	LEU
1	A	309	GLU
1	A	315	PHE
1	A	316	SER
1	A	340	LYS
1	A	346	ASP
1	A	347	LEU
1	A	351	GLU
1	A	354	THR
1	A	359	LEU
1	A	367	CYS
2	B	54	ARG
2	B	58	VAL
2	B	106	LEU
2	B	116	CYS
2	B	120	VAL
2	B	124	THR
2	B	136	ASN
2	B	137	LEU
2	B	143	THR
2	B	149	GLU
2	B	164	ASN
2	B	168	LEU
2	B	177	GLN
2	B	184	ARG
2	B	189	ARG
2	B	194	ILE
2	B	207	LEU
2	B	226	THR
2	B	254	ASP
2	B	275	LYS
2	B	281	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	312	LYS
2	B	321	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	142	GLN
1	A	198	HIS
1	A	202	ASN
1	A	235	ASN
1	A	242	ASN
1	A	255	GLN
1	A	258	HIS
1	A	287	ASN
1	A	307	GLN
1	A	360	GLN
2	B	43	GLN
2	B	50	GLN
2	B	81	GLN
2	B	96	GLN
2	B	115	HIS
2	B	136	ASN
2	B	177	GLN
2	B	185	GLN
2	B	200	GLN
2	B	201	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.