



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:24 pm BST

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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

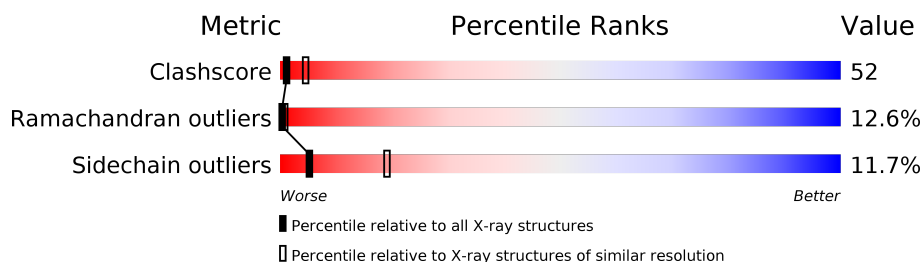
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	288	
2	B	326	
3	C	11	
3	D	11	

## 2 Entry composition

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	C	N	O	S	0	0	0
			2200	1373	395	417	15			

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

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

- 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	C	N	O	P	0	0	0
			221	106	41	64	10			
3	D	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			

- Molecule 4 is water.

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



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

Chain C:  45% 55%



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

Chain D:  64% 36%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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(°)	Ideal(°)
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

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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
1:A:221:ILE:HD13	1:A:222:GLN:N	1.86	0.90
2:B:207:LEU:CD1	2:B:207:LEU:H	1.84	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

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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:265:GLU:C	2:B:266:ILE:HD12	2.03	0.79
2:B:327:VAL:HG23	2:B:345:PHE:HB3	1.65	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:N	1:A:340:LYS:HE3	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
1:A:209:ARG:HE	1:A:211:LYS:NZ	1.85	0.75
2:B:74:LYS:HG3	2:B:75:ASN:H	1.52	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
1:A:162:LEU:CG	1:A:176:LEU:HD13	2.19	0.72
2:B:106:LEU:HD22	2:B:106:LEU:N	2.05	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

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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:OP2	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
1:A:242:ASN:HD22	1:A:242:ASN:H	1.41	0.68
2:B:124:THR:O	2:B:125:ALA:HB2	1.94	0.68
2:B:184:ARG:O	2:B:186:LEU:N	2.25	0.68
1:A:144:ALA:HB2	1:A:199:SER:CB	2.23	0.68
3:C:2:DC:C4'	3:C:3:DG:H5''	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
1:A:300:TYR:CD2	1:A:338:VAL:HG22	2.29	0.66
2:B:189:ARG:O	2:B:193:ILE:HG13	1.96	0.66
2:B:316:TYR:CG	2:B:317:LYS:N	2.61	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
1:A:213:ILE:HD11	1:A:241:MET:CE	2.25	0.66
2:B:188:ASP:O	2:B:190:GLU:N	2.28	0.66
1:A:306:VAL:O	1:A:334:GLN:HB3	1.96	0.66
2:B:158:ALA:HB1	2:B:164:ASN:HB2	1.76	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:140:LYS:H	1:A:140:LYS:HD2	1.61	0.65
1:A:364:ASP:OD2	1:A:366:VAL:HG22	1.97	0.65

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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
1:A:118:PHE:HE1	1:A:205:ILE:HD13	1.62	0.65
1:A:240:ASP:HB3	1:A:242:ASN:ND2	2.12	0.65
3:C:2:DC:H4'	3:C:3:DG:C5'	2.25	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
1:A:170:ARG:HH11	1:A:230:ALA:HB1	1.61	0.64
3:D:20:DT:H5'	3:D:20:DT:H6	1.62	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:185:GLN:O	2:B:186:LEU:HB3	1.97	0.63
2:B:148:PHE:HA	2:B:202:THR:HG21	1.80	0.63
1:A:170:ARG:NH1	1:A:230:ALA:HB1	2.13	0.63
1:A:317:THR:HB	1:A:320:TRP:HB3	1.81	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
2:B:123:VAL:HG22	2:B:124:THR:O	2.00	0.62
3:D:19:DT:C6	3:D:20:DT:H72	2.33	0.62
1:A:314:VAL:HG12	1:A:323:ARG:CB	2.21	0.62
1:A:361:ARG:NH2	1:A:366:VAL:HG21	2.15	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: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

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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:220:ASP:O	2:B:221:SER:O	2.19	0.60
2:B:73:GLU:HG3	2:B:74:LYS:H	1.67	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:155:GLU:CG	1:A:189:ARG:HH22	2.15	0.59
1:A:283:ILE:CD1	1:A:359:LEU:HD13	2.28	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:C	1:A:217:ILE:HD13	2.23	0.59
1:A:313:VAL:HG12	1:A:326:PHE:HE2	1.68	0.59
1:A:289:GLU:HA	1:A:373:PHE:HD2	1.68	0.58
2:B:162:GLY:O	2:B:164:ASN:N	2.35	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:167:TRP:HB3	1:A:168:PRO:CD	2.34	0.57
1:A:209:ARG:O	1:A:212:GLU:N	2.36	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
1:A:355:VAL:HG21	1:A:375:TYR:HE2	1.69	0.57
2:B:148:PHE:HE1	2:B:199:VAL:HG23	1.67	0.57
1:A:245:ARG:HH21	1:A:269:PRO:HG3	1.69	0.56
2:B:322:THR:C	2:B:349:PRO:HG2	2.25	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:117:ARG:NH2	1:A:119:ARG:HH22	2.03	0.56
1:A:250:ALA:HB3	1:A:262:MET:CG	2.35	0.56
1:A:334:GLN:NE2	3:C:6:DA:H3'	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:VAL:HG12	2:B:270:CYS:HA	1.87	0.56
2:B:268:LEU:C	2:B:268:LEU:HD23	2.26	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:281:LEU:CD1	1:A:281:LEU:H	2.18	0.56
1:A:293:CYS:HB3	1:A:376:LEU:O	2.06	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
1:A:315:PHE:HB3	1:A:355:VAL:HG22	1.86	0.55
2:B:174:ALA:C	2:B:176:LEU:N	2.60	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:253:ARG:NE	1:A:257:GLY:O	2.38	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:192:PRO:O	1:A:193:HIS:C	2.43	0.55
2:B:97:LEU:HG	2:B:111:LEU:HG	1.89	0.55
2:B:164:ASN:HA	2:B:168:LEU:CD2	2.34	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
1:A:264:PRO:C	1:A:265:ILE:HD12	2.28	0.54
2:B:305:ARG:CG	2:B:305:ARG:HH21	2.21	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
1:A:172:HIS:ND1	1:A:173:PRO:HD2	2.22	0.54
2:B:218:LEU:HB2	2:B:227:ARG:HB2	1.88	0.54
2:B:266:ILE:N	2:B:266:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:VAL:HG13	2:B:316:TYR:CB	2.36	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: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
2:B:54:ARG:NE	2:B:56:ARG:NH2	2.56	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
1:A:135:SER:N	1:A:141:THR:HG22	2.24	0.53
2:B:218:LEU:HG	2:B:229:LEU:HD21	1.91	0.53
1:A:209:ARG:H	1:A:212:GLU:CB	2.22	0.53
2:B:166:GLY:HA2	2:B:170:HIS:O	2.09	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:166:ASP:O	1:A:167:TRP:C	2.47	0.52
1:A:181:CYS:HA	1:A:186:CYS:HA	1.90	0.52
1:A:233:LEU:O	1:A:234:LYS:HB2	2.10	0.52
1:A:198:HIS:O	1:A:199:SER:CB	2.58	0.52
1:A:276:THR:CG2	1:A:277:ASN:H	2.13	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
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:221:SER:C	2:B:223:GLY:N	2.63	0.51
2:B:160:ILE:HD11	2:B:161:ARG:HE	1.73	0.51
1:A:113:GLN:HG3	1:A:269:PRO:O	2.11	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
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
1:A:104:TYR:CE2	1:A:148:ARG:HB2	2.45	0.51
2:B:163:TYR:HB3	2:B:228:ARG:CD	2.41	0.51

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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
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:156:THR:CG2	2:B:194:ILE:HG13	2.41	0.50
2:B:260:VAL:HG22	2:B:347:TYR:HB3	1.92	0.50
2:B:73:GLU:HG3	2:B:74:LYS:N	2.25	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: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:109:HIS:CE1	2:B:207:LEU:HB3	2.47	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
1:A:162:LEU:HD12	1:A:162:LEU:N	2.25	0.48
2:B:162:GLY:HA2	2:B:177:GLN:C	2.33	0.48
1:A:213:ILE:O	1:A:215:ALA:N	2.45	0.48
2:B:94:ILE:HD12	2:B:94:ILE:C	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:202:ASN:O	1:A:203:LEU:C	2.52	0.48
1:A:272:ASP:OD1	1:A:274:LYS:HG2	2.13	0.48

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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
1:A:258:HIS:HA	4:A:2008:HOH:O	2.13	0.48
2:B:305:ARG:HG2	2:B:305:ARG:HH21	1.77	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
1:A:353:VAL:HG22	1:A:354:THR:N	2.29	0.48
2:B:155:MET:O	2:B:158:ALA:HB3	2.14	0.48
1:A:174:HIS:N	1:A:174:HIS:CD2	2.80	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:177:GLN:O	2:B:178:ALA:HB3	2.14	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
2:B:54:ARG:HE	2:B:56:ARG:NH2	2.12	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
1:A:358:PHE:HB3	1:A:370:PRO:HA	1.96	0.47
2:B:260:VAL:O	2:B:260:VAL:HG12	2.13	0.47
1:A:128:GLY:H	3:D:13:DC:H5''	1.80	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:HD23	2:B:67:LEU:C	2.36	0.46
2:B:118:ASP:O	2:B:120:VAL:HG12	2.15	0.46
2:B:186:LEU:HD11	2:B:190:GLU:OE2	2.15	0.46
1:A:243:VAL:HG13	1:A:243:VAL:O	2.16	0.46
1:A:135:SER:O	1:A:136:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LYS:HG3	2:B:75:ASN:N	2.27	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
1:A:310:ASP:OD2	1:A:361:ARG:HG3	2.15	0.45
1:A:292:PRO:HA	1:A:376:LEU:HB2	1.98	0.45
2:B:165:PRO:HG2	2:B:166:GLY:H	1.82	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
1:A:209:ARG:HB2	1:A:212:GLU:HB2	1.99	0.45
2:B:163:TYR:CB	2:B:228:ARG:CZ	2.94	0.45
2:B:50:GLN:HG3	2:B:236:ALA:O	2.17	0.45
2:B:56:ARG:O	2:B:140:LEU:O	2.35	0.45
2:B:144:LYS:N	3:D:19:DT:OP1	2.44	0.45
1:A:202:ASN:O	1:A:203:LEU:O	2.35	0.45
1:A:338:VAL:HG11	2:B:252:ARG:NH1	2.32	0.45
1:A:198:HIS:CG	1:A:199:SER:H	2.32	0.45
1:A:302:LEU:HD13	2:B:267:TYR:CD2	2.51	0.45
2:B:278:ILE:HD12	2:B:332:ARG:O	2.17	0.45
2:B:304:HIS:N	2:B:308:ALA:O	2.37	0.45
1:A:135:SER:HA	1:A:141:THR:HG22	1.97	0.45
1:A:162:LEU:CD1	1:A:176:LEU:HD13	2.46	0.45
1:A:198:HIS:HD2	1:A:200:PHE:N	1.97	0.45
2:B:105:HIS:N	2:B:105:HIS:CD2	2.83	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:271:ASP:O	2:B:273:VAL:HG13	2.17	0.45
2:B:297:ASP:O	2:B:298:PHE:HB3	2.17	0.45
1:A:242:ASN:HD22	1:A:242:ASN:N	2.02	0.45
1:A:102:ARG:HG3	1:A:103:PRO:HD2	1.99	0.44
2:B:143:THR:C	2:B:145:LYS:N	2.71	0.44
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
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:128:GLY:HA3	3:D:13:DC:O5'	2.18	0.44
1:A:182:THR:O	1:A:183:ASP:HB2	2.17	0.44
1:A:155:GLU:HG3	1:A:189:ARG:HH22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:HD11	2:B:190:GLU:CD	2.38	0.44
1:A:176:LEU:HB3	1:A:186:CYS:SG	2.57	0.44
2:B:156:THR:O	2:B:159:CYS:N	2.50	0.44
1:A:378:ARG:HG2	1:A:378:ARG:O	2.18	0.44
2:B:163:TYR:HB2	2:B:228:ARG:CZ	2.47	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
1:A:347:LEU:HD11	1:A:349:ILE:HG12	1.99	0.43
2:B:104:ILE:C	2:B:105:HIS:HD2	2.21	0.43
2:B:341:GLU:HA	2:B:341:GLU:OE1	2.17	0.43
3:C:8:DT:H2"	3:C:9:DT:H5"	2.00	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
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:123:VAL:HG11	2:B:132:VAL:CG2	2.47	0.43
2:B:105:HIS:ND1	2:B:201:GLN:CD	2.72	0.43
1:A:117:ARG:NH2	1:A:119:ARG:NH2	2.66	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: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
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:62:PRO:O	2:B:64:HIS:N	2.49	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:130:ILE:HD12	1:A:203:LEU:HD12	2.00	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: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:179:GLU:HB2	2:B:180:GLY:H	1.70	0.42
2:B:333:ARG:HE	2:B:336:ASP:CG	2.23	0.42
1:A:167:TRP:O	1:A:169:HIS:N	2.53	0.42
1:A:185:VAL:HG22	4:A:2004:HOH:O	2.19	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:174:HIS:CD2	1:A:174:HIS:H	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:HG2	1:A:321:GLU:O	2.18	0.42
2:B:305:ARG:O	2:B:307:PHE:CD1	2.73	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
1:A:276:THR:CG2	1:A:277:ASN:N	2.77	0.42
2:B:91:ALA:HA	2:B:225:PHE:HE1	1.83	0.42
2:B:257:ALA:CB	2:B:346:LEU:O	2.67	0.42
2:B:114:LYS:HE3	2:B:115:HIS:CE1	2.55	0.42
2:B:116:CYS:HA	2:B:121:CYS:HA	2.02	0.42
2:B:126:GLY:HA2	2:B:130:MET:SD	2.60	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
1:A:136:THR:O	1:A:138:ALA:N	2.53	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: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
1:A:339:PHE:CD1	1:A:339:PHE:N	2.86	0.42
2:B:251:VAL:O	2:B:252:ARG:C	2.58	0.42
2:B:321:ILE:HD12	2:B:323:LYS:H	1.85	0.42
2:B:148:PHE:O	2:B:149:GLU:C	2.57	0.42
2:B:164:ASN:HA	2:B:168:LEU:HD22	2.01	0.42
2:B:248:LEU:HB2	2:B:340:SER:HB3	2.02	0.42
1:A:185:VAL:CG2	4:A:2004:HOH:O	2.68	0.41
1:A:355:VAL:HG12	1:A:373:PHE:O	2.19	0.41
2:B:162:GLY:C	2:B:164:ASN:N	2.74	0.41
2:B:186:LEU:HD21	2:B:190:GLU:OE1	2.19	0.41
3:D:13:DC:H2"	3:D:14:DG:C8	2.54	0.41
1:A:125:ARG:NH2	1:A:206:GLN:OE1	2.54	0.41
1:A:311:ILE:HD12	1:A:311:ILE:HA	1.90	0.41
2:B:147:VAL:O	2:B:148:PHE:C	2.59	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:190:GLU:C	2:B:192:GLU:N	2.72	0.41
2:B:273:VAL:O	2:B:306:GLN:HG2	2.19	0.41
2:B:64:HIS:CD2	3:C:3:DG:N7	2.88	0.41
1:A:155:GLU:CD	1:A:189:ARG:HH22	2.24	0.41
1:A:181:CYS:C	1:A:182:THR:HG23	2.41	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:147:LEU:HB3	1:A:150:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:O	1:A:245:ARG:NH1	2.53	0.41
2:B:165:PRO:CG	2:B:166:GLY:N	2.83	0.41
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: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:316:TYR:OH	2:B:317:LYS:HE2	2.20	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:105:LEU:HD13	1:A:145:ILE:HB	2.03	0.41
1:A:162:LEU:HD11	1:A:176:LEU:HD13	2.02	0.41
1:A:356:ASN:O	1:A:356:ASN:OD1	2.39	0.41
2:B:194:ILE:CG1	2:B:195:ARG:N	2.84	0.41
2:B:51:ARG:HA	4:B:2011:HOH:O	2.20	0.41
1:A:277:ASN:CB	1:A:307:GLN:HE22	2.32	0.41
2:B:190:GLU:C	2:B:192:GLU:H	2.24	0.41
1:A:162:LEU:H	1:A:162:LEU:CD1	2.20	0.41
1:A:174:HIS:CG	1:A:207:CYS:HA	2.55	0.41
2:B:169:VAL:CG1	2:B:170:HIS:N	2.75	0.41
2:B:268:LEU:O	2:B:308:ALA:HA	2.21	0.41
1:A:160:ALA:O	1:A:185:VAL:HA	2.20	0.40
1:A:213:ILE:CG2	1:A:214:GLU:H	2.31	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
1:A:365:GLY:O	1:A:366:VAL:C	2.59	0.40
2:B:157:GLU:O	2:B:160:ILE:HG12	2.21	0.40
1:A:122:CYS:SG	3:C:10:DC:OP2	2.79	0.40
1:A:120:TYR:CZ	3:C:9:DT:H5'	2.56	0.40
1:A:134:SER:HB2	1:A:141:THR:HG21	2.03	0.40
1:A:167:TRP:HB3	1:A:168:PRO:HD3	2.01	0.40
2:B:281:ARG:HB2	2:B:295:PHE:HE1	1.87	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

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	0	2
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

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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

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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 ⓘ

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	11
2	B	268/282 (95%)	245 (91%)	23 (9%)	10	33
All	All	514/539 (95%)	454 (88%)	60 (12%)	5	19

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

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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

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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 ⓘ

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.