



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:11 AM GMT

PDB ID : 3DO7
Title : X-ray structure of a NF-kB p52/RelB/DNA complex
Authors : Fusco, A.; Huang, D.B.; Miller, D.; Vu, D.; Ghosh, G.
Deposited on : 2008-07-03
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

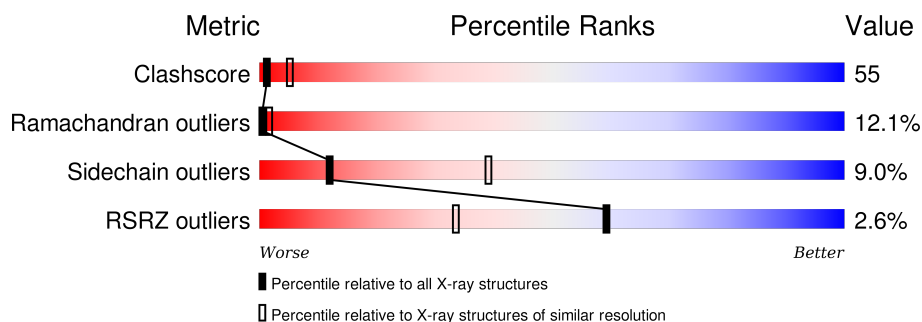
1 Overall quality at a glance

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	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	C	11	
1	D	11	
1	E	11	
2	A	296	
3	B	293	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5288 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 DNA chain called 5'-D(*DCP*DGP*DGP*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			
1	D	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			
1	E	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			

- Molecule 2 is a protein called Avian reticuloendotheliosis viral (V-rel) oncogene related B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	296	Total	C	N	O	S	0	0	0
			2327	1449	420	442	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	GLN	LEU	CONFLICT	UNP Q8VE46

- Molecule 3 is a protein called Nuclear factor NF-kappa-B p100 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	293	Total	C	N	O	S	0	0	0
			2268	1424	406	426	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	200	ASP	ALA	CONFLICT	UNP Q00653

- Molecule 4 is water.

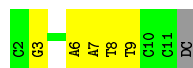
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	23	Total 23	O 23	0	0
4	C	1	Total 1	O 1	0	0
4	D	3	Total 3	O 3	0	0
4	E	4	Total 4	O 4	0	0

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.

- Molecule 1: 5'-D(*DCP*DGP*DGP*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DC)-3'

Chain C: 



- Molecule 1: 5'-D(*DCP*DGP*DGP*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DC)-3'

Chain D: 



- Molecule 1: 5'-D(*DCP*DGP*DGP*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DC)-3'

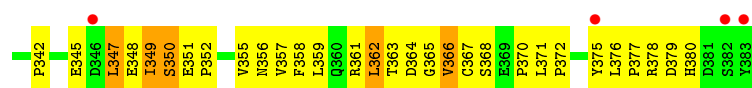
Chain E: 



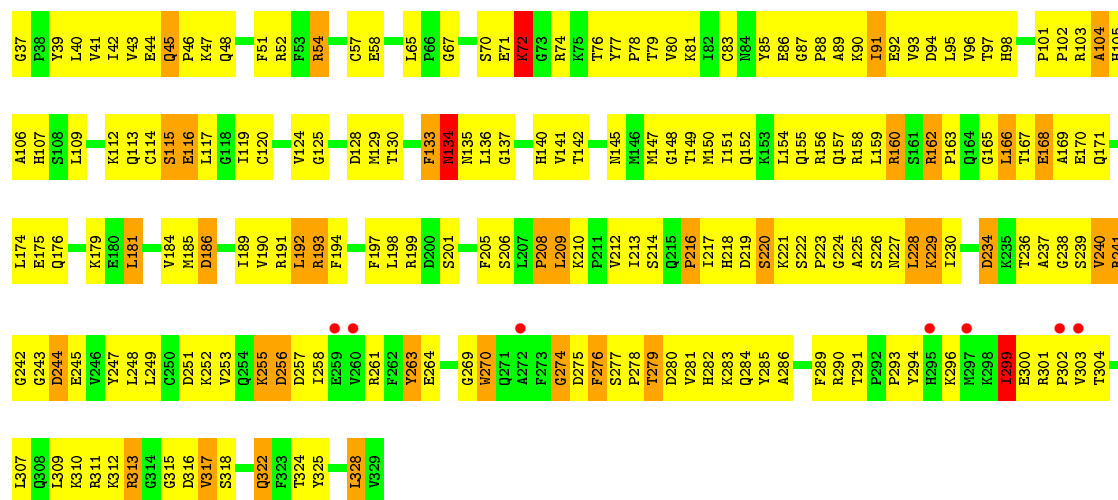
- Molecule 2: Avian reticuloendotheliosis viral (V-rel) oncogene related B

Chain A: 





● Molecule 3: Nuclear factor NF-kappa-B p100 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	77.64Å 124.13Å 189.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.19 – 3.05 34.07 – 3.05	Depositor EDS
% Data completeness (in resolution range)	81.4 (29.19-3.05) 87.7 (34.07-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 3.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.273 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	80.9	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 68.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 16342 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5288	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	C	0.43	0/226	0.78	0/347
1	D	0.44	0/247	0.72	0/379
1	E	0.51	0/247	1.02	1/379 (0.3%)
2	A	0.30	0/2378	0.55	0/3224
3	B	0.31	0/2315	0.58	0/3124
All	All	0.33	0/5413	0.61	1/7453 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3	DG	O4'-C1'-N9	5.13	111.59	108.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	DC	Sidechain
1	E	3	DG	Sidechain
1	E	7	DA	Sidechain
1	E	8	DT	Sidechain
1	E	9	DT	Sidechain

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	C	202	0	114	12	0
1	D	221	0	125	13	0
1	E	221	0	125	15	0
2	A	2327	0	2282	292	0
3	B	2268	0	2248	245	0
4	A	18	0	0	2	0
4	B	23	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	2	0
4	E	4	0	0	0	0
All	All	5288	0	4894	561	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 55.

All (561) 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)
2:A:127:ALA:HB1	2:A:202:ASN:HB3	1.41	1.01
2:A:361:ARG:HG2	2:A:363:THR:HG22	1.40	1.00
3:B:93:VAL:HG12	3:B:194:PHE:HA	1.42	0.99
2:A:292:PRO:HB2	2:A:294:THR:HG22	1.45	0.97
3:B:299:ILE:H	3:B:299:ILE:HD13	1.27	0.96
2:A:378:ARG:HG3	2:A:379:ASP:H	1.30	0.96
3:B:88:PRO:HB2	3:B:199:ARG:HH12	1.33	0.92
3:B:72:LYS:H	3:B:72:LYS:HD2	1.37	0.90
2:A:272:ASP:OD1	2:A:274:LYS:HG2	1.72	0.89
2:A:135:SER:HA	2:A:141:THR:HG22	1.54	0.88
3:B:109:LEU:HD21	3:B:136:LEU:HD11	1.53	0.88
3:B:328:LEU:H	3:B:328:LEU:HD13	1.37	0.88
3:B:317:VAL:HG22	3:B:318:SER:H	1.38	0.87
2:A:361:ARG:HH21	2:A:366:VAL:HG21	1.41	0.86
2:A:361:ARG:NH2	2:A:366:VAL:HG21	1.91	0.85
3:B:156:ARG:HA	3:B:160:ARG:HB2	1.57	0.85
3:B:70:SER:HB2	3:B:76:THR:HB	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:311:ILE:HD13	2:A:312:SER:N	1.93	0.83
3:B:218:HIS:HB3	3:B:225:ALA:HB1	1.58	0.83
3:B:44:GLU:HB3	3:B:79:THR:HG22	1.59	0.83
3:B:40:LEU:HD23	3:B:41:VAL:N	1.94	0.82
3:B:252:LYS:HB2	3:B:285:TYR:HE2	1.43	0.81
2:A:114:ARG:HB3	2:A:271:TYR:HB2	1.63	0.81
2:A:306:VAL:HG21	2:A:311:ILE:HG13	1.62	0.80
2:A:105:LEU:HD23	2:A:105:LEU:H	1.47	0.80
2:A:172:HIS:HD2	2:A:174:HIS:H	1.29	0.80
2:A:259:LEU:HD23	2:A:259:LEU:H	1.48	0.78
3:B:317:VAL:HG22	3:B:318:SER:N	1.97	0.78
2:A:314:VAL:HG12	2:A:323:ARG:HB3	1.64	0.78
2:A:320:TRP:HB2	2:A:345:GLU:OE2	1.84	0.78
3:B:240:VAL:HG13	3:B:241:ARG:H	1.48	0.78
1:E:11:DC:H2''	1:E:12:DC:O5'	1.84	0.77
2:A:347:LEU:HD11	2:A:349:ILE:HB	1.67	0.77
2:A:146:GLU:HG2	2:A:197:ARG:HB3	1.68	0.76
3:B:199:ARG:HA	3:B:205:PHE:HA	1.68	0.76
3:B:240:VAL:HG21	3:B:328:LEU:HD12	1.68	0.76
2:A:90:THR:HG23	2:A:91:LEU:H	1.51	0.75
2:A:253:ARG:CZ	2:A:259:LEU:HB3	2.18	0.74
2:A:170:ARG:HH21	2:A:232:SER:HB3	1.52	0.74
3:B:113:GLN:NE2	3:B:113:GLN:H	1.87	0.73
2:A:228:TYR:OH	2:A:266:LEU:HD21	1.88	0.73
3:B:94:ASP:HB3	3:B:119:ILE:HG12	1.71	0.73
2:A:347:LEU:HD13	2:A:348:GLU:N	2.04	0.73
2:A:130:ILE:HD12	2:A:203:LEU:HD12	1.71	0.72
3:B:328:LEU:HD13	3:B:328:LEU:N	2.04	0.72
2:A:110:GLN:NE2	2:A:268:GLU:H	1.87	0.72
1:D:20:DT:H1'	1:D:21:DC:H5''	1.70	0.72
3:B:150:MET:O	3:B:154:LEU:HD23	1.89	0.71
3:B:72:LYS:N	3:B:72:LYS:HD2	2.03	0.71
1:C:9:DT:H2'	2:A:122:CYS:SG	2.31	0.70
2:A:281:LEU:HB2	2:A:368:SER:HB3	1.72	0.70
3:B:85:TYR:HD2	3:B:87:GLY:H	1.39	0.70
2:A:352:PRO:HB3	2:A:375:TYR:O	1.91	0.70
2:A:148:ARG:O	2:A:149:ASP:HB2	1.91	0.70
3:B:109:LEU:HD12	3:B:137:GLY:O	1.91	0.69
2:A:316:SER:HA	2:A:321:GLU:HA	1.74	0.69
2:A:176:LEU:H	2:A:184:GLY:HA2	1.57	0.69
2:A:217:ILE:O	2:A:221:ILE:HG13	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:328:LEU:H	3:B:328:LEU:CD1	2.05	0.69
3:B:81:LYS:CB	3:B:130:THR:HG22	2.23	0.68
3:B:113:GLN:CD	3:B:113:GLN:H	1.97	0.68
2:A:205:ILE:HG22	2:A:206:GLN:N	2.07	0.68
2:A:210:LYS:HA	2:A:213:ILE:HG13	1.76	0.68
3:B:107:HIS:CD2	3:B:141:VAL:HG12	2.29	0.67
2:A:316:SER:O	2:A:317:THR:HG23	1.94	0.67
3:B:299:ILE:CD1	3:B:299:ILE:H	2.03	0.67
2:A:317:THR:CG2	2:A:355:VAL:HG23	2.25	0.67
2:A:102:ARG:HD2	2:A:102:ARG:N	2.10	0.67
2:A:172:HIS:CD2	2:A:174:HIS:H	2.10	0.67
3:B:107:HIS:CD2	3:B:141:VAL:H	2.12	0.67
2:A:103:PRO:HB3	2:A:149:ASP:O	1.94	0.67
3:B:162:ARG:CB	3:B:163:PRO:HD2	2.24	0.67
2:A:176:LEU:HD11	2:A:203:LEU:CD1	2.24	0.67
3:B:190:VAL:O	3:B:217:ILE:HG12	1.94	0.66
3:B:154:LEU:O	3:B:157:GLN:HG3	1.94	0.66
2:A:301:LEU:HD23	2:A:302:LEU:N	2.10	0.66
3:B:301:ARG:HB3	3:B:302:PRO:HD2	1.77	0.66
2:A:364:ASP:OD1	2:A:366:VAL:HG22	1.96	0.66
3:B:45:GLN:HG3	3:B:46:PRO:HD2	1.78	0.66
3:B:277:SER:OG	3:B:279:THR:HG22	1.96	0.66
3:B:47:LYS:O	3:B:217:ILE:HG22	1.95	0.65
3:B:317:VAL:CG2	3:B:318:SER:H	2.10	0.65
2:A:324:ALA:HA	2:A:342:PRO:HD3	1.78	0.65
3:B:96:VAL:HG22	3:B:191:ARG:O	1.97	0.65
2:A:318:ALA:O	2:A:319:SER:HB3	1.96	0.65
2:A:110:GLN:NE2	2:A:268:GLU:HB2	2.12	0.65
2:A:101:PRO:HG2	2:A:102:ARG:CD	2.26	0.65
3:B:310:LYS:HE2	3:B:317:VAL:HG23	1.79	0.65
2:A:165:LYS:HA	2:A:245:ARG:HD2	1.78	0.65
3:B:74:ARG:O	3:B:74:ARG:HG3	1.95	0.65
2:A:176:LEU:HD11	2:A:203:LEU:HD13	1.78	0.65
3:B:96:VAL:HG13	3:B:193:ARG:HG2	1.79	0.65
2:A:150:CYS:HA	2:A:153:LEU:HD12	1.78	0.65
2:A:110:GLN:NE2	2:A:268:GLU:N	2.45	0.65
3:B:97:THR:HG21	3:B:103:ARG:HB2	1.79	0.65
2:A:245:ARG:NH1	2:A:269:PRO:HD3	2.12	0.65
3:B:255:LYS:NZ	3:B:281:VAL:HB	2.12	0.64
3:B:104:ALA:HB3	3:B:150:MET:HE1	1.79	0.64
3:B:278:PRO:O	3:B:280:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:39:TYR:HD2	3:B:83:CYS:HB2	1.62	0.64
2:A:347:LEU:HD13	2:A:348:GLU:H	1.62	0.64
2:A:112:LYS:HA	2:A:133:GLU:HA	1.80	0.64
3:B:253:VAL:HG21	3:B:258:ILE:HD13	1.79	0.64
3:B:258:ILE:HD11	3:B:309:LEU:HD11	1.79	0.64
3:B:209:LEU:CD1	3:B:210:LYS:H	2.10	0.64
2:A:107:ILE:HD13	2:A:110:GLN:OE1	1.97	0.64
3:B:313:ARG:HE	3:B:313:ARG:HA	1.62	0.64
3:B:160:ARG:HA	3:B:160:ARG:NE	2.11	0.63
2:A:264:PRO:O	2:A:265:ILE:HD12	1.98	0.63
2:A:210:LYS:HA	2:A:213:ILE:CD1	2.28	0.63
1:D:13:DC:H2''	1:D:14:DG:C8	2.33	0.63
2:A:126:SER:O	2:A:178:GLY:HA2	1.98	0.63
3:B:157:GLN:HE22	3:B:158:ARG:NH2	1.97	0.63
2:A:311:ILE:H	2:A:362:LEU:HD12	1.64	0.63
2:A:243:VAL:HA	2:A:270:VAL:O	1.98	0.63
3:B:248:LEU:HD23	3:B:248:LEU:C	2.18	0.63
3:B:48:GLN:O	3:B:217:ILE:HA	1.97	0.62
3:B:181:LEU:HD13	3:B:181:LEU:O	1.99	0.62
2:A:292:PRO:HA	2:A:376:LEU:HB2	1.81	0.62
3:B:97:THR:CG2	3:B:103:ARG:HB2	2.30	0.62
2:A:243:VAL:HG23	2:A:270:VAL:O	2.00	0.61
1:D:23:DC:C6	1:E:3:DG:H1'	2.35	0.61
2:A:378:ARG:HG3	2:A:379:ASP:N	2.10	0.61
3:B:186:ASP:HB3	3:B:189:ILE:HG22	1.81	0.61
2:A:305:LYS:HA	2:A:334:GLN:O	2.01	0.61
3:B:261:ARG:O	3:B:307:LEU:HD12	2.00	0.61
2:A:131:LEU:HD11	2:A:140:LYS:HE3	1.83	0.61
2:A:259:LEU:CD2	2:A:259:LEU:H	2.14	0.61
3:B:309:LEU:O	3:B:310:LYS:HD3	2.00	0.60
3:B:190:VAL:HG23	3:B:217:ILE:HD11	1.84	0.60
3:B:96:VAL:CG1	3:B:193:ARG:HG2	2.30	0.60
2:A:162:LEU:HD13	2:A:176:LEU:HB2	1.83	0.60
2:A:233:LEU:HD22	2:A:233:LEU:N	2.17	0.60
2:A:242:ASN:HB3	2:A:278:THR:HG21	1.84	0.60
2:A:317:THR:HG23	2:A:355:VAL:HG23	1.84	0.60
3:B:240:VAL:HG13	3:B:241:ARG:N	2.17	0.60
3:B:274:GLY:HA3	3:B:289:PHE:HD2	1.65	0.60
3:B:94:ASP:OD2	3:B:193:ARG:HD2	2.02	0.60
2:A:103:PRO:HA	2:A:149:ASP:HB2	1.82	0.60
1:D:18:DA:H3'	3:B:223:PRO:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:213:ILE:O	2:A:217:ILE:HG13	2.02	0.59
3:B:40:LEU:HD21	3:B:80:VAL:HG21	1.84	0.59
3:B:92:GLU:HB3	3:B:119:ILE:HG21	1.83	0.59
2:A:347:LEU:HD13	2:A:349:ILE:H	1.67	0.59
2:A:170:ARG:NH2	2:A:232:SER:HB3	2.18	0.59
2:A:246:ILE:HD13	2:A:246:ILE:C	2.23	0.59
3:B:155:GLN:HG2	3:B:174:LEU:HD13	1.84	0.59
3:B:95:LEU:HG	3:B:109:LEU:HB2	1.83	0.59
3:B:40:LEU:HD21	3:B:80:VAL:CG2	2.33	0.59
2:A:98:GLY:O	2:A:100:CYS:N	2.35	0.59
2:A:304:ASP:HA	3:B:283:LYS:NZ	2.17	0.59
3:B:105:HIS:CD2	3:B:190:VAL:HG12	2.38	0.59
1:E:7:DA:H2'	1:E:8:DT:C6	2.38	0.59
2:A:241:MET:CE	2:A:241:MET:HA	2.32	0.59
3:B:181:LEU:HD22	3:B:184:VAL:CG1	2.33	0.58
2:A:160:ALA:HB1	2:A:246:ILE:HD11	1.85	0.58
2:A:94:LEU:C	2:A:96:SER:H	2.06	0.58
3:B:107:HIS:HD2	3:B:141:VAL:HG12	1.67	0.58
2:A:160:ALA:O	2:A:185:VAL:HA	2.03	0.58
3:B:184:VAL:O	3:B:184:VAL:HG22	2.01	0.58
3:B:114:CYS:HA	3:B:120:CYS:HA	1.86	0.58
2:A:218:GLU:O	2:A:222:GLN:HG3	2.03	0.58
1:D:21:DC:H5'	1:D:21:DC:H6	1.69	0.58
3:B:230:ILE:HD11	3:B:309:LEU:H	1.69	0.58
2:A:210:LYS:HA	2:A:213:ILE:CG1	2.34	0.58
3:B:44:GLU:HG2	3:B:76:THR:HG22	1.86	0.57
2:A:119:ARG:HD3	2:A:125:ARG:HG3	1.86	0.57
3:B:147:MET:HG3	3:B:148:GLY:N	2.19	0.57
2:A:135:SER:CA	2:A:141:THR:HG22	2.32	0.57
3:B:242:GLY:HA3	3:B:293:PRO:HD3	1.86	0.57
1:E:11:DC:C2'	1:E:12:DC:O5'	2.51	0.57
2:A:101:PRO:HG2	2:A:102:ARG:HD2	1.87	0.57
2:A:198:HIS:HA	4:A:431:HOH:O	2.04	0.57
2:A:160:ALA:CB	2:A:246:ILE:HD11	2.34	0.57
3:B:159:LEU:HG	3:B:166:LEU:HD12	1.85	0.57
1:D:13:DC:H2'	2:A:125:ARG:HE	1.70	0.57
3:B:299:ILE:N	3:B:299:ILE:HD13	2.09	0.56
2:A:110:GLN:HE22	2:A:268:GLU:N	2.02	0.56
2:A:210:LYS:HA	2:A:213:ILE:HD11	1.88	0.56
2:A:189:ARG:HG3	2:A:189:ARG:HH11	1.69	0.56
2:A:176:LEU:N	2:A:184:GLY:HA2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:67:GLY:O	3:B:70:SER:HB3	2.06	0.56
3:B:252:LYS:CB	3:B:285:TYR:HE2	2.17	0.56
2:A:210:LYS:C	2:A:212:GLU:H	2.08	0.56
3:B:244:ASP:O	3:B:291:THR:HG23	2.05	0.56
3:B:167:THR:HB	3:B:170:GLU:OE1	2.06	0.56
3:B:269:GLY:O	3:B:270:TRP:HB2	2.05	0.56
1:C:8:DT:H2''	1:C:9:DT:H5'	1.86	0.56
2:A:165:LYS:HA	2:A:245:ARG:CD	2.36	0.56
2:A:117:ARG:HG3	2:A:117:ARG:O	2.01	0.56
2:A:103:PRO:HA	2:A:149:ASP:CB	2.36	0.55
3:B:156:ARG:CA	3:B:160:ARG:HB2	2.32	0.55
2:A:105:LEU:N	2:A:105:LEU:HD23	2.18	0.55
3:B:145:ASN:C	3:B:147:MET:H	2.08	0.55
3:B:107:HIS:CD2	3:B:140:HIS:HA	2.42	0.55
3:B:72:LYS:H	3:B:72:LYS:CD	2.02	0.55
3:B:44:GLU:CB	3:B:79:THR:HG22	2.31	0.55
3:B:175:GLU:O	3:B:179:LYS:HG2	2.06	0.55
3:B:230:ILE:HD11	3:B:309:LEU:HB2	1.87	0.55
2:A:172:HIS:HD2	2:A:174:HIS:N	2.02	0.55
2:A:222:GLN:C	2:A:224:GLY:H	2.09	0.55
2:A:119:ARG:O	2:A:206:GLN:HA	2.07	0.55
2:A:379:ASP:CG	2:A:380:HIS:H	2.09	0.55
1:C:6:DA:P	2:A:276:THR:HG21	2.47	0.55
2:A:291:GLY:O	2:A:375:TYR:HA	2.07	0.54
2:A:100:CYS:HB3	2:A:101:PRO:CD	2.37	0.54
1:D:23:DC:H2'	1:E:3:DG:H2''	1.89	0.54
3:B:115:SER:O	3:B:117:LEU:N	2.41	0.54
3:B:274:GLY:HA3	3:B:289:PHE:CD2	2.41	0.54
3:B:313:ARG:HE	3:B:313:ARG:CA	2.21	0.54
3:B:89:ALA:O	3:B:124:VAL:HG22	2.07	0.54
3:B:44:GLU:OE2	3:B:44:GLU:HA	2.07	0.54
2:A:248:PHE:O	2:A:264:PRO:HA	2.07	0.54
3:B:278:PRO:O	3:B:281:VAL:N	2.33	0.54
2:A:90:THR:HG23	2:A:91:LEU:N	2.21	0.54
2:A:304:ASP:HB2	4:A:440:HOH:O	2.07	0.54
2:A:359:LEU:N	2:A:359:LEU:HD12	2.23	0.54
2:A:226:ASP:OD1	2:A:229:ASN:HA	2.08	0.54
2:A:246:ILE:HG23	2:A:246:ILE:O	2.07	0.54
2:A:205:ILE:CG2	2:A:206:GLN:N	2.70	0.54
1:C:8:DT:H1'	1:C:9:DT:H5''	1.89	0.54
2:A:352:PRO:HG3	2:A:377:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:ARG:O	2:A:335:ILE:HG13	2.08	0.54
2:A:254:ASP:OD2	2:A:256:GLN:HB2	2.07	0.54
2:A:301:LEU:HD23	2:A:301:LEU:C	2.28	0.54
2:A:243:VAL:HB	2:A:271:TYR:CD2	2.42	0.53
3:B:275:ASP:OD1	3:B:277:SER:HB3	2.08	0.53
3:B:249:LEU:N	3:B:249:LEU:HD12	2.22	0.53
2:A:253:ARG:HE	2:A:254:ASP:N	2.06	0.53
2:A:292:PRO:HB2	2:A:294:THR:CG2	2.31	0.53
2:A:132:GLY:O	2:A:134:SER:N	2.41	0.53
2:A:352:PRO:HG3	2:A:377:PRO:CD	2.39	0.53
2:A:105:LEU:HD13	2:A:250:ALA:HB2	1.91	0.53
2:A:320:TRP:CZ2	2:A:322:GLY:HA3	2.43	0.53
2:A:170:ARG:HE	2:A:232:SER:H	1.54	0.53
2:A:100:CYS:HB3	2:A:101:PRO:HD3	1.90	0.53
2:A:160:ALA:HA	2:A:246:ILE:HD11	1.91	0.53
2:A:142:GLN:NE2	2:A:200:PHE:O	2.42	0.53
3:B:241:ARG:O	3:B:293:PRO:HA	2.09	0.53
3:B:252:LYS:HB2	3:B:285:TYR:CE2	2.34	0.53
3:B:159:LEU:C	3:B:159:LEU:HD13	2.29	0.53
3:B:88:PRO:HB2	3:B:199:ARG:NH1	2.14	0.53
3:B:80:VAL:HG22	3:B:81:LYS:H	1.73	0.53
2:A:248:PHE:HB2	2:A:265:ILE:HB	1.90	0.53
2:A:94:LEU:O	2:A:97:PRO:HD2	2.09	0.53
3:B:43:VAL:HB	3:B:79:THR:HG23	1.91	0.53
2:A:234:LYS:O	2:A:235:ASN:HB2	2.08	0.53
3:B:151:ILE:HG23	3:B:152:GLN:N	2.24	0.53
3:B:105:HIS:NE2	3:B:190:VAL:HG12	2.24	0.52
2:A:259:LEU:HD23	2:A:259:LEU:N	2.20	0.52
3:B:125:GLY:O	3:B:129:MET:HE2	2.08	0.52
3:B:191:ARG:HD3	3:B:216:PRO:HG3	1.91	0.52
3:B:176:GLN:HA	3:B:176:GLN:NE2	2.25	0.52
2:A:326:PHE:CD1	2:A:326:PHE:N	2.78	0.52
3:B:197:PHE:CD1	3:B:208:PRO:HA	2.45	0.52
2:A:309:GLU:HA	2:A:328:GLN:NE2	2.24	0.52
2:A:311:ILE:HD13	2:A:312:SER:H	1.72	0.52
3:B:166:LEU:CD1	3:B:166:LEU:H	2.22	0.52
1:E:9:DT:H2''	1:E:10:DC:O5'	2.10	0.52
1:D:15:DG:H2''	1:D:16:DG:OP2	2.09	0.52
3:B:234:ASP:HB2	3:B:247:TYR:HB2	1.92	0.52
2:A:116:MET:SD	2:A:130:ILE:HA	2.50	0.51
3:B:103:ARG:O	3:B:104:ALA:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:308:LYS:HG3	2:A:309:GLU:H	1.75	0.51
2:A:320:TRP:CD1	2:A:345:GLU:HB3	2.45	0.51
3:B:145:ASN:C	3:B:147:MET:N	2.64	0.51
1:D:14:DG:N7	2:A:125:ARG:NH2	2.55	0.51
3:B:255:LYS:O	3:B:255:LYS:HG3	2.11	0.51
3:B:159:LEU:HB2	3:B:166:LEU:HB3	1.91	0.51
3:B:328:LEU:HD22	3:B:328:LEU:O	2.10	0.51
2:A:308:LYS:HG3	2:A:309:GLU:N	2.25	0.51
2:A:120:TYR:C	2:A:122:CYS:H	2.14	0.51
3:B:40:LEU:C	3:B:40:LEU:HD23	2.30	0.51
3:B:193:ARG:HD3	3:B:193:ARG:O	2.11	0.51
2:A:210:LYS:HG2	2:A:213:ILE:HD11	1.93	0.51
3:B:133:PHE:N	3:B:133:PHE:CD1	2.78	0.51
3:B:224:GLY:C	3:B:311:ARG:HH22	2.14	0.51
1:E:4:DG:H2'	1:E:5:DG:O4'	2.11	0.51
3:B:242:GLY:HA3	3:B:293:PRO:CD	2.40	0.51
2:A:164:TRP:CZ2	2:A:239:VAL:HG12	2.46	0.51
2:A:181:CYS:HA	2:A:185:VAL:O	2.11	0.50
2:A:127:ALA:CB	2:A:202:ASN:HB3	2.26	0.50
3:B:116:GLU:HB3	3:B:117:LEU:HD22	1.94	0.50
3:B:117:LEU:N	3:B:117:LEU:HD22	2.27	0.50
3:B:171:GLN:HE21	3:B:175:GLU:CD	2.14	0.50
3:B:167:THR:O	3:B:170:GLU:OE1	2.29	0.50
3:B:244:ASP:O	3:B:290:ARG:HA	2.11	0.50
2:A:131:LEU:HD22	2:A:131:LEU:N	2.26	0.50
2:A:308:LYS:HB3	2:A:331:VAL:HG11	1.93	0.50
2:A:167:TRP:HB3	2:A:168:PRO:HD3	1.94	0.50
3:B:209:LEU:HD12	3:B:210:LYS:H	1.76	0.50
2:A:155:GLU:HA	2:A:192:PRO:HD3	1.93	0.50
2:A:155:GLU:HB2	2:A:189:ARG:NH1	2.26	0.50
3:B:42:ILE:HD11	3:B:212:VAL:HG13	1.93	0.50
2:A:156:VAL:HG23	2:A:192:PRO:HG3	1.92	0.50
2:A:363:THR:HG23	2:A:364:ASP:N	2.27	0.49
2:A:314:VAL:HG12	2:A:323:ARG:CB	2.37	0.49
2:A:192:PRO:O	2:A:196:PRO:HB3	2.12	0.49
2:A:240:ASP:HB3	2:A:243:VAL:HG12	1.93	0.49
2:A:347:LEU:HD13	2:A:349:ILE:N	2.28	0.49
3:B:213:ILE:N	3:B:213:ILE:HD12	2.28	0.49
2:A:293:CYS:HA	2:A:375:TYR:CD2	2.46	0.49
3:B:192:LEU:HD23	3:B:194:PHE:CZ	2.47	0.49
2:A:292:PRO:CB	2:A:294:THR:HG22	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:213:ILE:HG21	2:A:239:VAL:HG21	1.94	0.49
3:B:192:LEU:HB2	3:B:214:SER:OG	2.12	0.49
3:B:71:GLU:HB3	3:B:72:LYS:HD2	1.94	0.49
3:B:171:GLN:O	3:B:175:GLU:HG3	2.13	0.49
1:C:3:DG:O6	3:B:54:ARG:NH1	2.45	0.49
3:B:46:PRO:HG3	3:B:192:LEU:HD22	1.94	0.49
2:A:176:LEU:HD12	2:A:204:GLY:O	2.13	0.49
2:A:194:VAL:O	2:A:194:VAL:HG23	2.13	0.49
3:B:228:LEU:HD13	3:B:316:ASP:OD1	2.12	0.49
1:C:7:DA:H2''	1:C:8:DT:H5'	1.95	0.49
2:A:160:ALA:CA	2:A:246:ILE:HD11	2.43	0.49
2:A:286:ILE:HG22	2:A:287:ASN:N	2.28	0.49
2:A:176:LEU:HD11	2:A:203:LEU:HD11	1.93	0.49
2:A:114:ARG:CB	2:A:271:TYR:HB2	2.40	0.49
3:B:248:LEU:C	3:B:249:LEU:HD12	2.33	0.49
3:B:109:LEU:CD2	3:B:136:LEU:HD11	2.34	0.48
3:B:294:TYR:C	3:B:296:LYS:H	2.16	0.48
1:C:7:DA:H2''	1:C:8:DT:C5'	2.43	0.48
3:B:219:ASP:C	3:B:221:LYS:H	2.16	0.48
2:A:311:ILE:N	2:A:362:LEU:HD12	2.27	0.48
1:E:9:DT:H2''	1:E:10:DC:C5'	2.44	0.48
2:A:332:HIS:HB3	2:A:336:ALA:HB3	1.96	0.48
2:A:131:LEU:HB3	2:A:135:SER:OG	2.12	0.48
2:A:315:PHE:HE2	2:A:324:ALA:HB2	1.78	0.48
3:B:42:ILE:HG13	3:B:212:VAL:HG11	1.95	0.48
3:B:253:VAL:HG21	3:B:258:ILE:CD1	2.44	0.48
2:A:306:VAL:O	2:A:334:GLN:HG2	2.13	0.48
3:B:80:VAL:HG22	3:B:81:LYS:N	2.28	0.48
2:A:318:ALA:O	2:A:319:SER:CB	2.61	0.48
2:A:253:ARG:HA	2:A:253:ARG:HE	1.79	0.48
3:B:98:HIS:HB2	3:B:189:ILE:HG23	1.94	0.48
3:B:219:ASP:O	3:B:221:LYS:N	2.47	0.48
3:B:322:GLN:HE21	3:B:322:GLN:CA	2.27	0.48
2:A:167:TRP:HB3	2:A:168:PRO:CD	2.43	0.47
2:A:148:ARG:HG3	2:A:148:ARG:HH11	1.79	0.47
2:A:303:CYS:O	3:B:282:HIS:NE2	2.45	0.47
1:E:6:DA:H2'	1:E:7:DA:C8	2.49	0.47
3:B:253:VAL:HG21	3:B:258:ILE:CG1	2.44	0.47
3:B:156:ARG:HG2	3:B:156:ARG:HH11	1.78	0.47
2:A:246:ILE:HD12	2:A:248:PHE:CZ	2.48	0.47
1:E:9:DT:H2''	1:E:10:DC:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:GLN:HE22	3:B:158:ARG:CZ	2.27	0.47
3:B:255:LYS:CE	3:B:281:VAL:HB	2.44	0.47
2:A:156:VAL:HG13	2:A:251:SER:O	2.14	0.47
3:B:48:GLN:O	3:B:218:HIS:N	2.43	0.47
3:B:113:GLN:CD	3:B:113:GLN:N	2.66	0.47
3:B:255:LYS:HD3	3:B:278:PRO:HB2	1.97	0.47
2:A:356:ASN:HB2	2:A:370:PRO:HB2	1.96	0.47
2:A:205:ILE:HG22	2:A:206:GLN:H	1.76	0.47
3:B:162:ARG:CB	3:B:163:PRO:CD	2.92	0.47
3:B:176:GLN:HA	3:B:176:GLN:HE21	1.79	0.47
3:B:44:GLU:H	3:B:79:THR:HG23	1.80	0.47
2:A:302:LEU:HD23	3:B:282:HIS:HB2	1.96	0.47
3:B:179:LYS:C	3:B:181:LEU:H	2.18	0.47
2:A:190:LEU:H	2:A:190:LEU:HD23	1.78	0.47
3:B:114:CYS:O	3:B:116:GLU:N	2.42	0.47
2:A:107:ILE:HA	2:A:145:ILE:HG22	1.97	0.47
2:A:97:PRO:HG2	2:A:98:GLY:H	1.79	0.47
3:B:322:GLN:HA	3:B:322:GLN:HE21	1.79	0.47
3:B:107:HIS:HD2	3:B:141:VAL:H	1.61	0.47
2:A:266:LEU:N	2:A:266:LEU:HD22	2.30	0.47
3:B:249:LEU:N	3:B:249:LEU:CD1	2.78	0.47
1:C:8:DT:H2''	1:C:9:DT:C5'	2.45	0.46
2:A:170:ARG:HE	2:A:232:SER:HB3	1.80	0.46
2:A:132:GLY:O	2:A:133:GLU:C	2.54	0.46
3:B:304:THR:HA	3:B:324:THR:HA	1.97	0.46
3:B:105:HIS:ND1	3:B:106:ALA:N	2.64	0.46
2:A:264:PRO:C	2:A:265:ILE:HD12	2.35	0.46
2:A:281:LEU:CB	2:A:368:SER:HB3	2.42	0.46
2:A:126:SER:O	2:A:178:GLY:CA	2.62	0.46
2:A:326:PHE:HD1	2:A:326:PHE:N	2.13	0.46
3:B:311:ARG:O	3:B:315:GLY:HA2	2.14	0.46
2:A:129:SER:O	2:A:130:ILE:C	2.53	0.46
1:C:9:DT:H5'	1:C:9:DT:H6	1.80	0.46
2:A:165:LYS:HG3	2:A:269:PRO:HG3	1.96	0.46
3:B:309:LEU:O	3:B:317:VAL:HA	2.15	0.46
2:A:333:ARG:HB3	3:B:285:TYR:CD1	2.50	0.46
2:A:205:ILE:CG2	2:A:206:GLN:H	2.27	0.46
2:A:302:LEU:HD23	3:B:282:HIS:CG	2.51	0.46
2:A:150:CYS:CA	2:A:153:LEU:HD12	2.43	0.46
2:A:155:GLU:HA	2:A:192:PRO:CD	2.45	0.46
2:A:227:PRO:HG3	2:A:249:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:268:GLU:HA	2:A:268:GLU:OE1	2.15	0.46
2:A:173:PRO:HG3	2:A:213:ILE:HG23	1.98	0.46
2:A:241:MET:HE2	2:A:241:MET:HA	1.98	0.46
1:E:7:DA:H2'	1:E:8:DT:H6	1.77	0.46
3:B:77:TYR:CG	3:B:134:ASN:HA	2.51	0.46
3:B:310:LYS:CE	3:B:317:VAL:HG23	2.45	0.46
2:A:317:THR:HG21	2:A:355:VAL:HG23	1.97	0.46
2:A:189:ARG:HG3	2:A:189:ARG:NH1	2.30	0.46
3:B:253:VAL:O	3:B:284:GLN:OE1	2.34	0.45
3:B:93:VAL:HG11	3:B:194:PHE:CD1	2.51	0.45
2:A:295:GLY:C	2:A:297:GLU:H	2.18	0.45
1:C:7:DA:H1'	1:C:8:DT:H5''	1.98	0.45
2:A:212:GLU:O	2:A:213:ILE:C	2.55	0.45
2:A:314:VAL:O	2:A:357:VAL:HG23	2.17	0.45
2:A:221:ILE:O	2:A:224:GLY:N	2.49	0.45
3:B:311:ARG:HB3	3:B:316:ASP:H	1.82	0.45
2:A:104:TYR:HA	2:A:262:MET:SD	2.57	0.45
3:B:245:GLU:HA	3:B:289:PHE:O	2.16	0.45
2:A:358:PHE:N	2:A:358:PHE:CD1	2.85	0.45
3:B:253:VAL:HG12	3:B:284:GLN:O	2.17	0.45
2:A:253:ARG:HE	2:A:254:ASP:H	1.64	0.45
2:A:111:PRO:O	2:A:112:LYS:C	2.55	0.45
2:A:156:VAL:HG23	2:A:192:PRO:CG	2.47	0.45
3:B:167:THR:O	3:B:169:ALA:N	2.49	0.45
2:A:292:PRO:HG3	2:A:376:LEU:HD12	1.97	0.45
3:B:95:LEU:HD12	3:B:107:HIS:O	2.16	0.45
2:A:306:VAL:HG22	2:A:307:GLN:N	2.31	0.45
2:A:206:GLN:HE21	2:A:206:GLN:HB3	1.49	0.45
2:A:151:GLY:HA2	2:A:193:HIS:HE1	1.82	0.45
3:B:93:VAL:HG23	3:B:93:VAL:O	2.17	0.45
2:A:315:PHE:HB2	2:A:322:GLY:O	2.16	0.45
2:A:330:ASP:HB3	2:A:338:VAL:HB	1.97	0.45
3:B:116:GLU:N	3:B:116:GLU:OE1	2.50	0.45
3:B:285:TYR:O	3:B:286:ALA:HB2	2.17	0.45
2:A:266:LEU:N	2:A:266:LEU:CD2	2.80	0.45
1:E:7:DA:H2''	1:E:8:DT:O5'	2.17	0.45
1:D:16:DG:H4'	4:D:435:HOH:O	2.17	0.45
3:B:219:ASP:OD1	3:B:219:ASP:C	2.55	0.45
3:B:212:VAL:C	3:B:213:ILE:HD12	2.38	0.44
2:A:94:LEU:O	2:A:96:SER:N	2.48	0.44
2:A:154:ARG:O	2:A:192:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:322:GLN:HA	3:B:322:GLN:NE2	2.32	0.44
2:A:243:VAL:HG22	2:A:244:VAL:N	2.33	0.44
2:A:150:CYS:O	2:A:153:LEU:HB2	2.17	0.44
2:A:283:ILE:HG22	2:A:284:CYS:N	2.31	0.44
2:A:168:PRO:O	2:A:170:ARG:N	2.43	0.44
2:A:110:GLN:O	2:A:133:GLU:N	2.48	0.44
2:A:190:LEU:N	2:A:190:LEU:HD23	2.32	0.44
3:B:86:GLU:OE1	3:B:198:LEU:HD23	2.18	0.44
2:A:361:ARG:C	2:A:363:THR:H	2.21	0.44
3:B:256:ASP:O	3:B:257:ASP:C	2.55	0.44
2:A:174:HIS:ND1	2:A:207:CYS:HA	2.32	0.44
2:A:355:VAL:HG22	2:A:356:ASN:N	2.33	0.44
2:A:287:ASN:OD1	2:A:300:TYR:HB2	2.17	0.44
3:B:255:LYS:HA	3:B:255:LYS:HE3	1.99	0.44
2:A:136:THR:O	2:A:140:LYS:HB3	2.17	0.44
2:A:253:ARG:CA	2:A:253:ARG:HE	2.31	0.44
2:A:101:PRO:O	2:A:102:ARG:HB2	2.17	0.44
3:B:278:PRO:O	3:B:279:THR:C	2.55	0.44
3:B:37:GLY:O	3:B:39:TYR:N	2.47	0.44
2:A:308:LYS:C	2:A:310:ASP:H	2.21	0.44
3:B:256:ASP:C	3:B:258:ILE:N	2.71	0.44
3:B:98:HIS:CB	3:B:189:ILE:HG23	2.48	0.44
2:A:109:GLU:OE2	2:A:132:GLY:HA3	2.18	0.44
2:A:98:GLY:O	2:A:99:PRO:C	2.56	0.43
3:B:209:LEU:HD13	3:B:210:LYS:H	1.83	0.43
2:A:193:HIS:O	2:A:195:SER:N	2.51	0.43
3:B:236:THR:HG23	3:B:237:ALA:N	2.33	0.43
2:A:163:VAL:O	2:A:164:TRP:O	2.36	0.43
3:B:113:GLN:HE22	3:B:135:ASN:HD22	1.67	0.43
3:B:191:ARG:HB3	3:B:213:ILE:CG2	2.48	0.43
2:A:246:ILE:HG22	2:A:267:SER:OG	2.19	0.43
2:A:275:SER:HB3	2:A:278:THR:HG22	1.99	0.43
2:A:359:LEU:O	2:A:367:CYS:HA	2.18	0.43
3:B:176:GLN:CA	3:B:176:GLN:HE21	2.30	0.43
2:A:253:ARG:NH1	2:A:259:LEU:N	2.66	0.43
3:B:263:TYR:HA	3:B:270:TRP:CZ3	2.54	0.43
3:B:192:LEU:HD23	3:B:194:PHE:HZ	1.84	0.43
2:A:146:GLU:HG2	2:A:197:ARG:CB	2.44	0.43
3:B:101:PRO:O	3:B:103:ARG:HG2	2.18	0.43
3:B:151:ILE:HG23	3:B:152:GLN:H	1.82	0.43
3:B:86:GLU:HG2	3:B:86:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:85:TYR:CD2	3:B:87:GLY:N	2.83	0.43
3:B:276:PHE:CD2	3:B:276:PHE:N	2.86	0.43
2:A:128:GLY:HA3	2:A:203:LEU:O	2.19	0.42
2:A:92:GLY:O	2:A:94:LEU:N	2.45	0.42
3:B:159:LEU:HD23	3:B:166:LEU:N	2.34	0.42
2:A:190:LEU:CD2	2:A:190:LEU:H	2.32	0.42
2:A:364:ASP:OD1	2:A:366:VAL:HG13	2.19	0.42
2:A:347:LEU:CD2	2:A:349:ILE:HD13	2.49	0.42
3:B:102:PRO:O	3:B:103:ARG:HD2	2.19	0.42
1:E:7:DA:H2''	1:E:8:DT:C5'	2.48	0.42
2:A:379:ASP:CG	2:A:380:HIS:N	2.71	0.42
3:B:156:ARG:HG2	3:B:156:ARG:NH1	2.35	0.42
2:A:226:ASP:O	2:A:228:TYR:N	2.53	0.42
3:B:186:ASP:CB	3:B:189:ILE:HG22	2.46	0.42
2:A:133:GLU:HG3	2:A:134:SER:N	2.34	0.42
3:B:181:LEU:HA	3:B:184:VAL:HG12	2.02	0.42
3:B:221:LYS:O	3:B:222:SER:C	2.56	0.42
2:A:371:LEU:HA	2:A:372:PRO:HD3	1.83	0.42
3:B:199:ARG:HG3	3:B:199:ARG:O	2.19	0.42
2:A:265:ILE:C	2:A:266:LEU:HD22	2.39	0.42
1:D:16:DG:H5''	4:D:405:HOH:O	2.19	0.42
2:A:298:GLU:C	2:A:299:LEU:HD22	2.40	0.42
2:A:116:MET:HE3	2:A:131:LEU:HD23	2.01	0.42
2:A:263:ASP:HA	2:A:264:PRO:HD3	1.91	0.42
2:A:301:LEU:HD23	2:A:302:LEU:C	2.40	0.42
2:A:126:SER:O	2:A:178:GLY:N	2.52	0.42
3:B:248:LEU:HD23	3:B:249:LEU:N	2.35	0.42
3:B:168:GLU:O	3:B:171:GLN:HB3	2.19	0.42
2:A:292:PRO:HD2	2:A:297:GLU:OE1	2.20	0.42
2:A:170:ARG:HE	2:A:232:SER:N	2.17	0.42
2:A:188:VAL:HG21	2:A:198:HIS:NE2	2.35	0.42
2:A:129:SER:O	2:A:131:LEU:HD13	2.20	0.42
3:B:310:LYS:HE2	3:B:317:VAL:CG2	2.49	0.42
2:A:335:ILE:HD12	2:A:335:ILE:C	2.40	0.42
3:B:189:ILE:O	3:B:189:ILE:HG23	2.20	0.42
2:A:351:GLU:HA	2:A:352:PRO:HD3	1.83	0.42
3:B:93:VAL:HG22	3:B:120:CYS:O	2.20	0.42
2:A:170:ARG:NE	2:A:232:SER:H	2.17	0.42
2:A:210:LYS:O	2:A:212:GLU:N	2.51	0.42
2:A:105:LEU:N	2:A:105:LEU:CD2	2.82	0.42
2:A:166:ASP:O	2:A:167:TRP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:147:MET:O	3:B:149:THR:N	2.53	0.42
3:B:149:THR:HG22	3:B:150:MET:N	2.35	0.42
2:A:94:LEU:C	2:A:96:SER:N	2.73	0.42
2:A:120:TYR:CE2	2:A:274:LYS:HE3	2.54	0.41
3:B:94:ASP:CG	3:B:193:ARG:HD2	2.39	0.41
2:A:365:GLY:O	2:A:366:VAL:C	2.59	0.41
2:A:267:SER:O	2:A:269:PRO:HD3	2.20	0.41
3:B:145:ASN:O	3:B:147:MET:N	2.54	0.41
2:A:124:GLY:O	2:A:125:ARG:HD3	2.20	0.41
2:A:96:SER:N	2:A:97:PRO:HD2	2.35	0.41
2:A:272:ASP:OD2	2:A:273:LYS:N	2.53	0.41
3:B:160:ARG:HE	3:B:160:ARG:HA	1.83	0.41
1:D:21:DC:H2'	3:B:57:CYS:SG	2.61	0.41
2:A:218:GLU:O	2:A:221:ILE:HB	2.21	0.41
3:B:269:GLY:O	3:B:270:TRP:CB	2.68	0.41
1:E:9:DT:H2'	1:E:10:DC:C6	2.55	0.41
3:B:228:LEU:HD13	3:B:316:ASP:CB	2.50	0.41
3:B:90:LYS:C	3:B:91:ILE:HG13	2.41	0.41
2:A:335:ILE:HD11	3:B:285:TYR:HB2	2.03	0.41
2:A:226:ASP:C	2:A:228:TYR:H	2.23	0.41
3:B:74:ARG:O	3:B:74:ARG:CG	2.67	0.41
2:A:337:ILE:HG22	2:A:339:PHE:HD1	1.84	0.41
3:B:181:LEU:CD1	3:B:185:MET:HB2	2.50	0.41
2:A:200:PHE:CD1	2:A:200:PHE:N	2.88	0.41
1:E:4:DG:C2'	1:E:5:DG:O5'	2.68	0.41
3:B:227:ASN:O	3:B:229:LYS:N	2.53	0.41
2:A:282:ARG:NH1	2:A:284:CYS:SG	2.94	0.41
2:A:171:VAL:HG13	2:A:171:VAL:O	2.21	0.41
2:A:118:PHE:CD2	2:A:118:PHE:N	2.88	0.41
2:A:272:ASP:CG	2:A:274:LYS:HG2	2.40	0.41
3:B:256:ASP:O	3:B:258:ILE:N	2.54	0.41
2:A:324:ALA:CA	2:A:342:PRO:HD3	2.49	0.41
3:B:191:ARG:CD	3:B:216:PRO:HG3	2.51	0.41
2:A:301:LEU:HD23	2:A:302:LEU:O	2.20	0.41
2:A:95:VAL:HG22	2:A:95:VAL:O	2.21	0.41
1:C:8:DT:C2'	1:C:9:DT:H71	2.51	0.41
2:A:133:GLU:HG3	2:A:134:SER:H	1.86	0.41
2:A:350:SER:HB2	2:A:351:GLU:H	1.67	0.41
3:B:52:ARG:CA	3:B:220:SER:HB3	2.51	0.41
3:B:142:THR:OG1	3:B:145:ASN:HB2	2.21	0.40
2:A:239:VAL:HG23	2:A:241:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:125:GLY:O	3:B:129:MET:CE	2.69	0.40
3:B:54:ARG:HG3	3:B:58:GLU:OE1	2.21	0.40
2:A:339:PHE:CD1	2:A:339:PHE:N	2.89	0.40
3:B:303:VAL:O	3:B:325:TYR:HB2	2.20	0.40
1:C:8:DT:H2'	1:C:9:DT:H71	2.02	0.40
3:B:186:ASP:CG	3:B:189:ILE:HG22	2.41	0.40
3:B:186:ASP:HB3	3:B:189:ILE:CG2	2.51	0.40
3:B:189:ILE:HD11	3:B:216:PRO:HB3	2.02	0.40
2:A:283:ILE:HG12	2:A:359:LEU:HD11	2.01	0.40
1:D:13:DC:O5'	2:A:125:ARG:HD2	2.22	0.40
3:B:51:PHE:CD1	3:B:65:LEU:HD13	2.57	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	
2	A	294/296 (99%)	187 (64%)	71 (24%)	36 (12%)	0	1
3	B	291/293 (99%)	187 (64%)	69 (24%)	35 (12%)	0	2
All	All	585/589 (99%)	374 (64%)	140 (24%)	71 (12%)	0	2

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	99	PRO
2	A	133	GLU
2	A	164	TRP
2	A	193	HIS
2	A	194	VAL
2	A	213	ILE
2	A	235	ASN

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Mol	Chain	Res	Type
2	A	269	PRO
2	A	287	ASN
2	A	324	ALA
2	A	350	SER
3	B	104	ALA
3	B	134	ASN
3	B	206	SER
3	B	226	SER
3	B	234	ASP
3	B	240	VAL
3	B	241	ARG
3	B	264	GLU
3	B	270	TRP
3	B	279	THR
2	A	95	VAL
2	A	98	GLY
2	A	113	GLN
2	A	124	GLY
2	A	130	ILE
2	A	169	HIS
2	A	349	ILE
2	A	362	LEU
3	B	116	GLU
3	B	216	PRO
3	B	220	SER
3	B	274	GLY
3	B	299	ILE
3	B	300	GLU
2	A	100	CYS
2	A	101	PRO
2	A	136	THR
2	A	167	TRP
2	A	192	PRO
2	A	202	ASN
2	A	211	LYS
2	A	227	PRO
2	A	279	SER
2	A	309	GLU
2	A	310	ASP
3	B	78	PRO
3	B	128	ASP
3	B	162	ARG

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Mol	Chain	Res	Type
3	B	168	GLU
3	B	201	SER
3	B	228	LEU
3	B	317	VAL
2	A	262	MET
3	B	115	SER
3	B	165	GLY
3	B	208	PRO
3	B	239	SER
3	B	263	TYR
3	B	312	LYS
2	A	93	ARG
2	A	138	ALA
2	A	223	LEU
2	A	366	VAL
3	B	72	LYS
3	B	186	ASP
3	B	255	LYS
2	A	141	THR
3	B	243	GLY
3	B	238	GLY
3	B	91	ILE

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	
2	A	262/265 (99%)	237 (90%)	25 (10%)	11	36
3	B	247/256 (96%)	226 (92%)	21 (8%)	13	43
All	All	509/521 (98%)	463 (91%)	46 (9%)	12	39

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	102	ARG

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Mol	Chain	Res	Type
2	A	105	LEU
2	A	109	GLU
2	A	114	ARG
2	A	122	CYS
2	A	140	LYS
2	A	187	ARG
2	A	203	LEU
2	A	206	GLN
2	A	209	ARG
2	A	235	ASN
2	A	238	GLU
2	A	241	MET
2	A	246	ILE
2	A	268	GLU
2	A	269	PRO
2	A	277	ASN
2	A	287	ASN
2	A	289	GLU
2	A	301	LEU
2	A	309	GLU
2	A	311	ILE
2	A	317	THR
2	A	326	PHE
2	A	347	LEU
3	B	45	GLN
3	B	54	ARG
3	B	72	LYS
3	B	112	LYS
3	B	133	PHE
3	B	134	ASN
3	B	160	ARG
3	B	166	LEU
3	B	181	LEU
3	B	192	LEU
3	B	193	ARG
3	B	209	LEU
3	B	229	LYS
3	B	244	ASP
3	B	251	ASP
3	B	256	ASP
3	B	276	PHE
3	B	299	ILE

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Mol	Chain	Res	Type
3	B	313	ARG
3	B	322	GLN
3	B	328	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	113	GLN
2	A	142	GLN
2	A	172	HIS
2	A	193	HIS
2	A	206	GLN
2	A	222	GLN
2	A	235	ASN
2	A	236	HIS
2	A	237	GLN
2	A	249	GLN
2	A	255	GLN
2	A	328	GLN
3	B	45	GLN
3	B	48	GLN
3	B	107	HIS
3	B	113	GLN
3	B	135	ASN
3	B	145	ASN
3	B	155	GLN
3	B	157	GLN
3	B	171	GLN
3	B	176	GLN
3	B	215	GLN
3	B	218	HIS
3	B	271	GLN
3	B	308	GLN
3	B	322	GLN

5.3.3 RNA ⓘ

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 ⓘ

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, 95th 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(Å²)	Q<0.9	
1	C	10/11 (90%)	-0.18	0	100	100	38, 49, 78, 80	0
1	D	11/11 (100%)	-0.44	0	100	100	38, 56, 68, 75	0
1	E	11/11 (100%)	-0.49	0	100	100	54, 66, 90, 133	0
2	A	296/296 (100%)	-0.17	9 (3%)	54	27	42, 105, 137, 141	0
3	B	293/293 (100%)	-0.31	7 (2%)	62	37	45, 103, 137, 141	0
All	All	621/622 (99%)	-0.25	16 (2%)	59	33	38, 102, 137, 141	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	89	CYS	4.8
2	A	250	ALA	4.3
3	B	272	ALA	3.5
2	A	88	SER	3.4
2	A	92	GLY	3.4
3	B	303	VAL	3.2
3	B	260	VAL	2.8
3	B	259	GLU	2.8
2	A	383	TYR	2.4
2	A	90	THR	2.4
3	B	297	MET	2.3
3	B	302	PRO	2.2
2	A	346	ASP	2.2
2	A	382	SER	2.1
2	A	375	TYR	2.1
3	B	295	HIS	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.