



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:44 AM GMT

PDB ID : 2IS4
Title : Crystal structure of UvrD-DNA-ADPNP ternary complex
Authors : Yang, W.; Lee, J.Y.
Deposited on : 2006-10-16
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

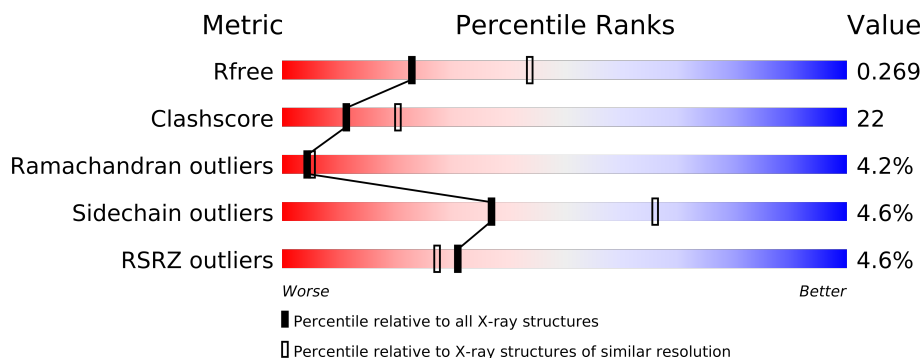
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	26	
1	D	26	
2	A	680	
2	B	680	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11148 atoms, of which 0 are hydrogen and 0 are deuterium.

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 25-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	25	Total	C	N	O	P	0	0	0
			506	244	89	150	23			
1	D	25	Total	C	N	O	P	0	0	0
			509	244	89	152	24			

- Molecule 2 is a protein called DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	646	Total	C	N	O	S	0	0	0
			5006	3140	898	942	26			
2	B	632	Total	C	N	O	S	0	0	0
			4945	3101	896	923	25			

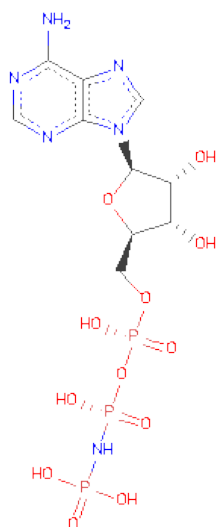
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	VAL	ALA	ENGINEERED	UNP P03018
B	399	VAL	ALA	ENGINEERED	UNP P03018

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	62	Total O 62 62	0	0
5	B	56	Total O 56 56	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: 25-MER

Chain C:



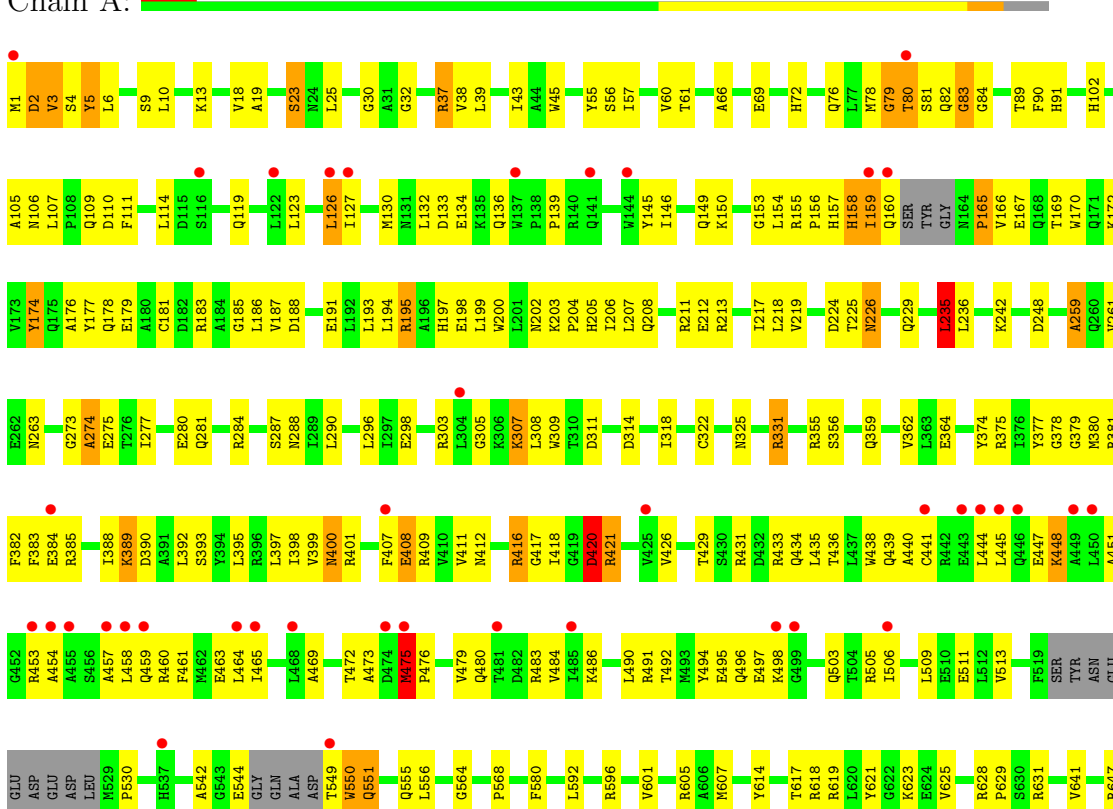
• Molecule 1: 25-MER

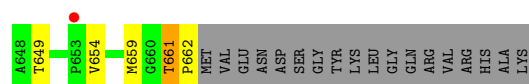
Chain D:



• Molecule 2: DNA helicase II

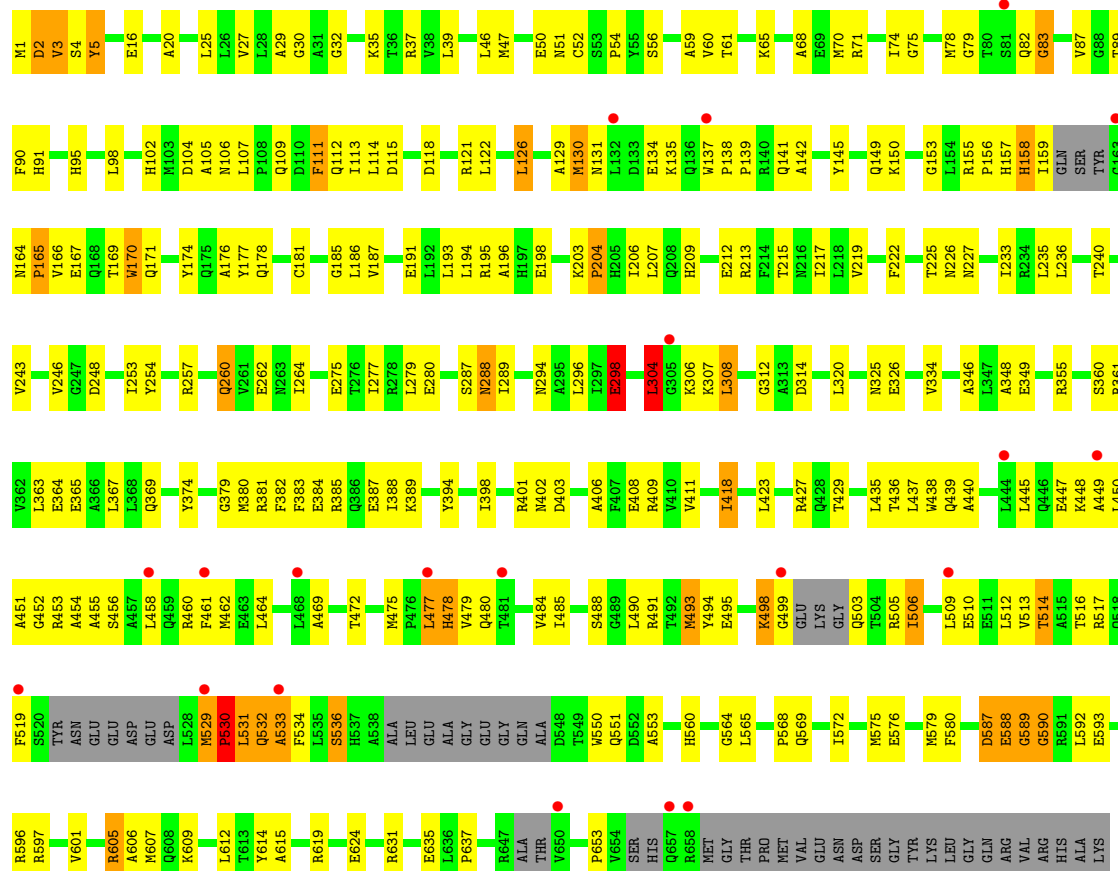
Chain A:





• Molecule 2: DNA helicase II

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.11Å 96.78Å 111.04Å 90.00° 93.85° 90.00°	Depositor
Resolution (Å)	29.84 – 2.60 48.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	85.3 (29.84-2.60) 85.2 (48.29-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.256 0.232 , 0.269	Depositor DCC
R_{free} test set	5886 reflections (10.17%)	DCC
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 60996 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11148	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	0.40	0/565	0.71	0/869
1	D	0.32	0/569	0.70	0/877
2	A	0.42	2/5099 (0.0%)	0.61	2/6913 (0.0%)
2	B	0.41	1/5032 (0.0%)	0.61	2/6807 (0.0%)
All	All	0.41	3/11265 (0.0%)	0.62	4/15466 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	134	GLU	CB-CG	-5.22	1.42	1.52
2	B	134	GLU	CB-CG	-5.17	1.42	1.52
2	A	511	GLU	CB-CG	-5.10	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	551	GLN	N-CA-C	-6.50	93.47	111.00
2	B	653	PRO	N-CA-CB	5.39	109.77	103.30
2	B	530	PRO	N-CA-CB	5.37	109.75	103.30
2	A	662	PRO	N-CA-CB	5.23	109.58	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	506	0	287	24	0
1	D	509	0	285	32	0
2	A	5006	0	4755	211	0
2	B	4945	0	4732	217	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	13	3	0
4	B	31	0	13	1	0
5	A	62	0	0	3	0
5	B	56	0	0	1	0
All	All	11148	0	10085	468	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (468) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:15:DG:H2"	1:D:16:DC:H5"	1.28	1.15
2:B:478:HIS:HB2	2:B:517:ARG:HA	1.32	1.10
1:D:5:DG:H2"	1:D:6:DC:H5"	1.34	1.09
1:D:15:DG:H2"	1:D:16:DC:C5'	1.89	1.02
1:C:13:DG:H4'	2:A:453:ARG:HD2	1.37	1.01
2:A:25:LEU:HD21	2:A:277:ILE:HD12	1.50	0.94
1:C:20:DT:HO3'	1:C:22:DG:H8	1.17	0.93
2:B:382:PHE:HA	2:B:385:ARG:NH2	1.86	0.90
2:B:155:ARG:H	2:B:158:HIS:HD2	1.17	0.89
2:A:25:LEU:HD11	2:A:277:ILE:HG13	1.55	0.88
2:B:227:ASN:HD21	2:B:260:GLN:NE2	1.71	0.88
1:C:14:DT:H2"	1:C:15:DG:C8	2.09	0.86
2:A:23:SER:HA	2:A:242:LYS:HD2	1.58	0.85
2:A:382:PHE:O	2:A:385:ARG:HG3	1.76	0.85
1:D:19:DG:H2"	1:D:20:DT:OP2	1.75	0.84
2:A:659:MET:HB3	2:A:661:THR:HG22	1.59	0.84
2:A:416:ARG:NH2	2:A:464:LEU:HD23	1.92	0.83
1:D:6:DC:H2"	1:D:7:DA:C8	2.13	0.83
1:D:15:DG:C2'	1:D:16:DC:H5"	2.08	0.82
2:A:32:GLY:H	4:A:700:ANP:HNB1	1.24	0.81
2:B:65:LYS:HD2	2:B:565:LEU:HD11	1.63	0.81
2:A:475:MET:HE2	2:A:479:VAL:HG13	1.63	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:20:DT:O3'	1:C:22:DG:H8	1.64	0.79
1:D:18:DC:H4'	1:D:19:DG:OP1	1.80	0.78
2:A:226:ASN:HD21	2:A:229:GLN:HG3	1.49	0.78
2:B:346:ALA:HB3	2:B:349:GLU:HG3	1.66	0.77
2:B:32:GLY:H	4:B:701:ANP:HNB1	1.33	0.77
1:D:7:DA:H1'	1:D:8:DC:H5''	1.66	0.77
2:B:308:LEU:H	2:B:308:LEU:HD12	1.51	0.76
1:D:5:DG:C2'	1:D:6:DC:H5''	2.13	0.76
2:A:208:GLN:O	2:A:212:GLU:HG3	1.85	0.76
2:B:227:ASN:HD21	2:B:260:GLN:HE21	1.33	0.75
2:B:381:ARG:HA	2:B:384:GLU:HG2	1.69	0.74
1:D:10:DG:H3'	2:A:421:ARG:HG3	1.69	0.74
2:B:25:LEU:HD11	2:B:277:ILE:HG13	1.70	0.74
1:C:20:DT:O3'	1:C:22:DG:H2'	1.88	0.73
2:A:476:PRO:HG2	2:A:479:VAL:HG12	1.69	0.73
2:A:429:THR:O	2:A:433:ARG:HB2	1.88	0.73
1:C:15:DG:H1	1:D:6:DC:H42	1.37	0.73
2:B:475:MET:HB3	2:B:479:VAL:HG13	1.71	0.72
2:B:222:PHE:O	2:B:225:THR:HG23	1.89	0.72
2:A:421:ARG:NH1	2:A:421:ARG:HB3	2.04	0.72
2:A:290:LEU:HD11	2:A:308:LEU:HD13	1.71	0.72
1:C:26:DA:N7	2:B:380:MET:HG2	2.05	0.72
2:A:130:MET:HG2	2:A:431:ARG:HH21	1.55	0.71
2:B:503:GLN:O	2:B:506:ILE:HG23	1.90	0.71
2:B:532:GLN:HE21	2:B:532:GLN:CA	2.03	0.71
1:D:17:DT:H4'	1:D:18:DC:OP1	1.89	0.70
2:B:532:GLN:O	2:B:534:PHE:N	2.24	0.70
2:B:532:GLN:HE21	2:B:532:GLN:HA	1.56	0.70
2:B:382:PHE:HA	2:B:385:ARG:HH21	1.56	0.69
2:A:459:GLN:O	2:A:463:GLU:HG3	1.92	0.69
2:B:592:LEU:HD21	2:B:631:ARG:NH1	2.07	0.69
2:A:411:VAL:O	2:A:416:ARG:HD3	1.93	0.69
2:B:475:MET:HB3	2:B:479:VAL:CG1	2.23	0.69
2:A:133:ASP:HB3	2:A:136:GLN:HB2	1.75	0.69
2:B:102:HIS:HB2	2:B:107:LEU:O	1.91	0.69
2:B:478:HIS:HB2	2:B:517:ARG:CA	2.17	0.68
2:A:130:MET:HG2	2:A:431:ARG:NH2	2.09	0.68
2:A:476:PRO:O	2:A:480:GLN:HB2	1.94	0.67
2:B:478:HIS:CB	2:B:517:ARG:HA	2.18	0.67
2:A:411:VAL:HA	2:A:461:PHE:CZ	2.30	0.67
2:A:25:LEU:HD12	2:A:275:GLU:O	1.95	0.67
2:B:25:LEU:HD21	2:B:277:ILE:HD12	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:149:GLN:OE1	2:A:154:LEU:HD12	1.95	0.66
2:A:421:ARG:H	2:A:421:ARG:NE	1.95	0.64
2:B:114:LEU:CD1	2:B:118:ASP:HB3	2.26	0.64
2:A:416:ARG:HH22	2:A:464:LEU:HD23	1.58	0.64
2:B:59:ALA:HB3	2:B:87:VAL:HG22	1.79	0.64
2:A:153:GLY:HA2	2:A:194:LEU:HD13	1.78	0.64
2:A:601:VAL:O	2:A:605:ARG:HD2	1.97	0.64
2:B:564:GLY:H	2:B:605:ARG:HH21	1.45	0.64
2:B:576:GLU:HG3	2:B:579:MET:HG3	1.80	0.64
2:A:431:ARG:O	2:A:431:ARG:HD3	1.98	0.63
1:C:11:DC:H42	1:D:10:DG:H1	1.47	0.63
1:C:26:DA:H5"	2:B:91:HIS:HB3	1.80	0.63
2:A:378:GLY:CA	2:A:381:ARG:HH12	2.12	0.63
2:A:218:LEU:HD12	2:A:218:LEU:N	2.13	0.63
2:A:429:THR:OG1	2:A:444:LEU:HD11	1.99	0.62
2:A:421:ARG:HH11	2:A:421:ARG:HB3	1.64	0.62
2:B:472:THR:HG22	2:B:475:MET:SD	2.39	0.62
2:A:43:ILE:HG23	2:A:57:ILE:HD13	1.81	0.62
2:A:133:ASP:HB3	2:A:136:GLN:CB	2.30	0.62
2:B:453:ARG:HG3	2:B:453:ARG:HH11	1.64	0.62
2:A:416:ARG:HH22	2:A:464:LEU:CD2	2.11	0.62
2:A:564:GLY:H	2:A:605:ARG:NH2	1.99	0.61
2:A:303:ARG:HH11	2:A:303:ARG:HB2	1.66	0.61
2:A:408:GLU:O	2:A:411:VAL:HG12	2.01	0.60
1:D:15:DG:H2"	1:D:16:DC:H5'	1.77	0.60
2:B:114:LEU:HD12	2:B:118:ASP:HB3	1.82	0.60
2:B:514:THR:O	2:B:517:ARG:HB3	2.01	0.60
2:B:104:ASP:HB3	2:B:203:LYS:HE3	1.83	0.60
2:A:377:TYR:HE2	2:A:544:GLU:H	1.50	0.60
2:A:378:GLY:O	2:A:381:ARG:NH1	2.35	0.59
2:A:217:ILE:C	2:A:218:LEU:HD12	2.22	0.59
2:B:90:PHE:HE2	2:B:233:ILE:HD11	1.67	0.59
2:A:486:LYS:HA	2:A:491:ARG:CB	2.33	0.59
2:B:56:SER:HA	2:B:213:ARG:O	2.02	0.59
2:B:153:GLY:HA2	2:B:194:LEU:HD13	1.84	0.59
2:A:416:ARG:HH11	2:A:416:ARG:HG3	1.67	0.59
1:C:20:DT:C3'	1:C:22:DG:H2'	2.32	0.58
2:A:383:PHE:HA	2:A:388:ILE:HG21	1.84	0.58
2:A:601:VAL:O	2:A:605:ARG:CD	2.50	0.58
2:A:105:ALA:O	2:A:106:ASN:HB3	2.02	0.58
2:B:485:ILE:HG22	2:B:491:ARG:HG3	1.84	0.58
2:B:156:PRO:HA	2:B:171:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:433:ARG:O	2:A:434:GLN:HB2	2.04	0.58
2:A:389:LYS:HB3	2:A:409:ARG:NE	2.19	0.58
2:A:436:THR:OG1	2:A:439:GLN:HG3	2.04	0.58
2:A:461:PHE:CZ	2:A:465:ILE:HD11	2.38	0.58
2:A:433:ARG:HB3	2:A:435:LEU:HG	1.86	0.58
2:B:47:MET:CE	2:B:54:PRO:HG3	2.34	0.58
1:D:11:DC:OP2	2:A:421:ARG:HG2	2.04	0.57
2:B:30:GLY:HA2	2:B:248:ASP:OD2	2.04	0.57
2:B:364:GLU:HG3	2:B:374:TYR:OH	2.05	0.57
2:B:2:ASP:O	2:B:5:TYR:HD2	1.88	0.57
2:A:146:ILE:HD13	2:A:177:TYR:CD2	2.40	0.57
1:C:19:DG:H4'	1:C:20:DT:OP1	2.06	0.56
2:B:126:LEU:HD21	2:B:176:ALA:HB1	1.85	0.56
2:A:130:MET:CG	2:A:431:ARG:HH21	2.19	0.56
2:B:159:ILE:HB	2:B:171:GLN:OE1	2.04	0.56
2:A:393:SER:OG	2:A:409:ARG:HD3	2.06	0.56
2:B:435:LEU:HB3	2:B:439:GLN:HB3	1.87	0.56
2:A:287:SER:HB3	2:A:314:ASP:HA	1.86	0.56
2:A:157:HIS:H	2:A:157:HIS:CD2	2.23	0.56
2:B:135:LYS:NZ	2:B:135:LYS:HB3	2.20	0.56
2:A:194:LEU:O	2:A:198:GLU:HG3	2.06	0.56
2:A:614:TYR:CE2	2:A:629:PRO:HG3	2.41	0.56
2:B:320:LEU:HD11	2:B:614:TYR:CE1	2.41	0.56
2:A:25:LEU:HD21	2:A:277:ILE:CD1	2.31	0.56
2:B:155:ARG:H	2:B:158:HIS:CD2	2.08	0.56
2:B:150:LYS:NZ	2:B:178:GLN:HE22	2.04	0.56
2:B:401:ARG:HH22	2:B:469:ALA:CB	2.19	0.55
2:B:461:PHE:O	2:B:464:LEU:HB3	2.07	0.55
2:B:170:TRP:HA	2:B:170:TRP:CE3	2.41	0.55
2:A:380:MET:O	2:A:384:GLU:HG3	2.07	0.55
1:D:17:DT:H2''	1:D:18:DC:C6	2.42	0.55
2:B:194:LEU:O	2:B:198:GLU:HG3	2.07	0.55
2:A:362:VAL:HG23	5:A:1036:HOH:O	2.05	0.55
2:B:287:SER:HB3	2:B:314:ASP:HA	1.89	0.55
2:B:369:GLN:O	2:B:369:GLN:HG2	2.07	0.55
2:A:166:VAL:HG23	2:A:167:GLU:N	2.22	0.55
1:C:16:DC:H42	1:D:5:DG:H1	1.55	0.55
2:A:401:ARG:HH22	2:A:469:ALA:CB	2.20	0.55
2:B:129:ALA:C	2:B:131:ASN:H	2.09	0.55
2:B:506:ILE:O	2:B:506:ILE:HD12	2.07	0.54
2:B:529:MET:O	2:B:531:LEU:N	2.40	0.54
2:A:503:GLN:O	2:A:506:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:387:GLU:OE2	2:B:505:ARG:NH1	2.39	0.54
2:A:165:PRO:HG2	2:A:166:VAL:H	1.71	0.54
2:B:550:TRP:CE2	2:B:551:GLN:HG3	2.42	0.54
2:B:568:PRO:HA	2:B:607:MET:HB2	1.87	0.54
2:B:320:LEU:HD11	2:B:614:TYR:HE1	1.72	0.54
1:C:16:DC:H1'	1:C:17:DT:O5'	2.07	0.54
1:D:10:DG:H3'	2:A:421:ARG:CG	2.35	0.54
2:B:164:ASN:CB	2:B:165:PRO:HD2	2.38	0.54
2:B:1:MET:O	2:B:3:VAL:N	2.40	0.54
1:C:16:DC:H2''	1:C:17:DT:OP2	2.06	0.54
2:B:637:PRO:HA	5:B:1054:HOH:O	2.08	0.54
2:A:91:HIS:CE1	2:A:193:LEU:HD11	2.43	0.54
2:A:379:GLY:HA2	2:A:542:ALA:HB1	1.89	0.54
2:B:601:VAL:O	2:B:605:ARG:HD2	2.08	0.54
2:A:72:HIS:O	2:A:76:GLN:HG2	2.09	0.53
2:B:587:ASP:O	2:B:589:GLY:N	2.39	0.53
1:D:11:DC:H2''	1:D:12:DA:C5'	2.38	0.53
1:D:22:DG:H2''	1:D:23:DT:OP2	2.07	0.53
1:D:11:DC:H2''	1:D:12:DA:H5'	1.91	0.53
2:A:378:GLY:HA2	2:A:381:ARG:HH12	1.73	0.53
2:B:203:LYS:N	2:B:204:PRO:HD3	2.24	0.53
2:B:509:LEU:O	2:B:513:VAL:HG23	2.08	0.53
2:B:423:LEU:O	2:B:427:ARG:HG3	2.09	0.53
2:A:555:GLN:C	2:A:556:LEU:HD12	2.29	0.53
2:A:126:LEU:HD21	2:A:176:ALA:HB1	1.91	0.53
2:A:5:TYR:CD2	2:A:6:LEU:N	2.77	0.53
2:A:392:LEU:HD23	2:A:395:LEU:HD12	1.91	0.52
2:A:390:ASP:OD1	2:A:409:ARG:NE	2.42	0.52
2:A:207:LEU:HD21	2:A:211:ARG:HH21	1.74	0.52
2:A:407:PHE:CE1	2:A:461:PHE:HE2	2.27	0.52
2:B:288:ASN:HB2	2:B:314:ASP:O	2.09	0.52
2:A:56:SER:HA	2:A:213:ARG:O	2.10	0.52
2:B:207:LEU:HD22	2:B:235:LEU:HD21	1.91	0.52
2:B:450:LEU:CB	2:B:455:ALA:HB2	2.40	0.52
2:A:166:VAL:HG23	2:A:167:GLU:H	1.75	0.52
2:B:493:MET:HG3	2:B:494:TYR:N	2.24	0.52
2:A:619:ARG:HA	2:A:623:LYS:O	2.09	0.52
1:C:14:DT:H2''	1:C:15:DG:N7	2.25	0.52
2:B:90:PHE:CE2	2:B:233:ILE:HD11	2.45	0.52
2:A:127:ILE:HD12	2:A:139:PRO:HG3	1.90	0.52
2:B:619:ARG:HH12	2:B:624:GLU:HB3	1.75	0.52
2:A:401:ARG:NH1	2:A:465:ILE:HG22	2.24	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:411:VAL:HA	2:B:461:PHE:CZ	2.44	0.51
2:A:592:LEU:HD11	2:A:631:ARG:NH1	2.24	0.51
2:A:30:GLY:HA2	2:A:248:ASP:OD2	2.10	0.51
2:A:79:GLY:O	2:A:80:THR:C	2.49	0.51
2:B:382:PHE:HA	2:B:385:ARG:HH22	1.71	0.51
2:B:46:LEU:O	2:B:52:CYS:HB2	2.10	0.51
2:B:95:HIS:CE1	2:B:532:GLN:HG2	2.45	0.51
2:B:187:VAL:HG13	2:B:191:GLU:HB3	1.93	0.51
2:A:475:MET:HE2	2:A:479:VAL:CG1	2.38	0.51
2:B:16:GLU:O	2:B:20:ALA:HB2	2.10	0.51
2:A:110:ASP:O	2:A:111:PHE:C	2.48	0.51
2:A:226:ASN:HD22	2:A:226:ASN:C	2.13	0.51
2:A:114:LEU:HD13	2:A:186:LEU:HD13	1.93	0.51
2:A:179:GLU:O	2:A:183:ARG:HG3	2.11	0.51
2:B:114:LEU:HD11	2:B:118:ASP:HB3	1.92	0.50
2:A:490:LEU:HD22	2:A:494:TYR:HE1	1.75	0.50
2:A:318:ILE:HB	2:A:641:VAL:HG22	1.94	0.50
2:A:445:LEU:C	2:A:447:GLU:H	2.13	0.50
2:B:529:MET:O	2:B:530:PRO:C	2.49	0.50
2:B:408:GLU:HG2	2:B:437:LEU:CD1	2.42	0.50
2:B:217:ILE:HB	2:B:243:VAL:HG22	1.92	0.50
2:A:509:LEU:O	2:A:513:VAL:HG23	2.11	0.50
2:B:145:TYR:O	2:B:149:GLN:HG2	2.12	0.50
2:B:91:HIS:CE1	2:B:193:LEU:HD11	2.46	0.50
2:A:187:VAL:HG13	2:A:191:GLU:HB3	1.94	0.50
2:A:472:THR:HG22	2:A:483:ARG:HD2	1.94	0.50
2:A:205:HIS:CE1	2:A:206:ILE:HG13	2.47	0.50
1:D:12:DA:OP1	2:A:417:GLY:HA2	2.11	0.50
2:B:361:ARG:O	2:B:365:GLU:HG3	2.11	0.50
2:B:385:ARG:HB3	2:B:387:GLU:OE1	2.12	0.50
2:B:27:VAL:HB	2:B:246:VAL:HG12	1.94	0.50
2:A:364:GLU:HG3	2:A:374:TYR:CZ	2.47	0.50
2:B:82:GLN:O	2:B:83:GLY:C	2.50	0.50
2:A:61:THR:O	2:A:89:THR:HA	2.12	0.49
2:A:429:THR:HG22	2:A:440:ALA:HB1	1.93	0.49
2:B:530:PRO:O	2:B:531:LEU:O	2.30	0.49
2:A:458:LEU:HD12	2:A:458:LEU:O	2.12	0.49
2:A:480:GLN:O	2:A:484:VAL:HG23	2.12	0.49
2:A:226:ASN:ND2	2:A:229:GLN:HG3	2.23	0.49
2:B:569:GLN:NE2	2:B:609:LYS:HB3	2.27	0.49
2:B:47:MET:HE2	2:B:54:PRO:HG3	1.94	0.49
2:B:512:LEU:O	2:B:516:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:498:LYS:O	2:B:499:GLY:C	2.51	0.49
2:A:23:SER:CA	2:A:242:LYS:HD2	2.36	0.49
2:B:564:GLY:H	2:B:605:ARG:NH2	2.09	0.49
2:B:170:TRP:HA	2:B:170:TRP:HE3	1.77	0.49
2:B:141:GLN:HG3	2:B:170:TRP:CZ2	2.48	0.49
2:B:187:VAL:HG13	2:B:191:GLU:CG	2.43	0.49
2:B:588:GLU:O	2:B:590:GLY:N	2.46	0.49
2:B:155:ARG:N	2:B:158:HIS:HD2	1.99	0.49
2:A:78:MET:O	2:A:79:GLY:O	2.31	0.49
2:A:109:GLN:HG2	2:A:109:GLN:O	2.13	0.49
2:B:289:ILE:HD13	2:B:606:ALA:HB3	1.95	0.49
2:B:438:TRP:CZ3	2:B:462:MET:HG2	2.48	0.48
1:D:12:DA:H2''	1:D:13:DG:H8	1.77	0.48
2:B:112:GLN:HB3	2:B:186:LEU:HD23	1.95	0.48
2:A:303:ARG:CB	2:A:303:ARG:NH1	2.76	0.48
2:A:191:GLU:OE2	2:A:195:ARG:HD3	2.13	0.48
2:A:55:TYR:HA	2:A:84:GLY:O	2.13	0.48
1:C:6:DC:H2''	1:C:7:DA:OP2	2.13	0.48
2:A:411:VAL:HG13	2:A:412:ASN:N	2.28	0.48
2:A:296:LEU:O	2:A:596:ARG:HD3	2.12	0.48
1:C:20:DT:HO3'	1:C:22:DG:H2'	1.77	0.48
2:A:401:ARG:HH12	2:A:465:ILE:HG22	1.78	0.48
2:B:107:LEU:HB3	2:B:111:PHE:HD2	1.78	0.48
2:A:389:LYS:HB3	2:A:409:ARG:CZ	2.44	0.48
2:A:2:ASP:O	2:A:3:VAL:C	2.51	0.48
2:B:348:ALA:HA	2:B:553:ALA:O	2.13	0.48
2:A:150:LYS:NZ	2:A:178:GLN:HE22	2.12	0.48
2:B:394:TYR:O	2:B:398:ILE:HG13	2.14	0.48
2:A:10:LEU:HD13	2:A:18:VAL:HG21	1.96	0.47
2:A:436:THR:HG23	2:A:439:GLN:OE1	2.14	0.47
1:D:15:DG:C2'	1:D:16:DC:C5'	2.76	0.47
2:B:532:GLN:CD	2:B:536:SER:HB2	2.34	0.47
2:A:378:GLY:CA	2:A:381:ARG:NH1	2.77	0.47
2:B:491:ARG:O	2:B:495:GLU:HG3	2.14	0.47
2:B:126:LEU:HD11	2:B:177:TYR:N	2.29	0.47
2:A:181:CYS:O	2:A:185:GLY:N	2.47	0.47
2:B:61:THR:O	2:B:89:THR:HA	2.14	0.47
2:A:155:ARG:HB3	2:A:156:PRO:HD2	1.97	0.47
2:A:407:PHE:O	2:A:411:VAL:HB	2.14	0.47
2:A:397:LEU:HD13	2:A:465:ILE:HD13	1.97	0.47
2:A:457:ALA:O	2:A:460:ARG:N	2.47	0.47
2:A:10:LEU:CD1	2:A:18:VAL:HG21	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:355:ARG:HD3	2:B:580:PHE:CD2	2.49	0.47
2:A:383:PHE:HA	2:A:388:ILE:CG2	2.45	0.47
2:B:95:HIS:CE1	2:B:113:ILE:HD11	2.50	0.47
2:A:200:TRP:HB3	2:A:207:LEU:HD13	1.97	0.47
2:A:102:HIS:HB2	2:A:107:LEU:O	2.15	0.47
2:A:126:LEU:O	2:A:130:MET:HG3	2.15	0.47
2:A:399:VAL:O	2:A:400:ASN:HB2	2.16	0.46
2:A:90:PHE:CZ	2:A:225:THR:HG22	2.50	0.46
2:B:304:LEU:N	2:B:304:LEU:HD23	2.30	0.46
2:A:159:ILE:O	2:A:160:GLN:CB	2.64	0.46
2:B:418:ILE:HD13	2:B:458:LEU:HD23	1.97	0.46
2:B:104:ASP:HB3	2:B:203:LYS:HG3	1.96	0.46
2:A:2:ASP:O	2:A:4:SER:N	2.48	0.46
2:A:203:LYS:N	2:A:204:PRO:HD3	2.31	0.46
2:B:254:TYR:HB3	2:B:257:ARG:HH21	1.79	0.46
2:A:438:TRP:HZ3	2:A:465:ILE:HD12	1.80	0.46
2:B:436:THR:OG1	2:B:439:GLN:HB2	2.15	0.46
2:A:420:ASP:HB3	2:A:421:ARG:HH21	1.81	0.46
2:A:191:GLU:O	2:A:195:ARG:HB2	2.16	0.46
2:A:549:THR:O	2:A:551:GLN:N	2.49	0.46
2:A:325:ASN:HA	2:A:617:THR:O	2.16	0.46
2:B:490:LEU:HA	2:B:493:MET:HG2	1.98	0.46
2:B:294:ASN:O	2:B:298:GLU:HB2	2.16	0.46
2:B:126:LEU:O	2:B:130:MET:HG3	2.16	0.45
2:B:530:PRO:O	2:B:531:LEU:C	2.54	0.45
2:A:397:LEU:HD21	2:A:407:PHE:N	2.31	0.45
2:A:202:ASN:O	2:A:203:LYS:HG2	2.16	0.45
2:A:618:ARG:O	2:A:625:VAL:HG22	2.16	0.45
2:B:56:SER:HB2	2:B:215:THR:OG1	2.16	0.45
2:B:402:ASN:HB3	2:B:436:THR:HG21	1.96	0.45
1:D:26:DA:N7	2:A:380:MET:HG3	2.32	0.45
2:B:389:LYS:HB3	2:B:409:ARG:NE	2.32	0.45
1:C:11:DC:N4	1:D:10:DG:H1	2.11	0.45
2:B:532:GLN:CA	2:B:532:GLN:NE2	2.75	0.45
2:B:532:GLN:C	2:B:532:GLN:HE21	2.20	0.45
2:B:445:LEU:C	2:B:447:GLU:H	2.19	0.45
2:B:209:HIS:O	2:B:212:GLU:HB2	2.16	0.45
2:B:418:ILE:CD1	2:B:458:LEU:HD23	2.47	0.45
2:B:95:HIS:HE1	2:B:532:GLN:HG2	1.80	0.45
2:A:217:ILE:HD11	2:A:236:LEU:HG	1.98	0.45
2:A:303:ARG:NH1	2:A:303:ARG:HB2	2.32	0.45
2:A:309:TRP:HZ3	2:A:311:ASP:OD2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:375:ARG:HH12	2:A:544:GLU:HA	1.81	0.45
2:A:496:GLN:O	2:A:498:LYS:N	2.49	0.45
2:A:1:MET:O	2:A:3:VAL:N	2.50	0.45
2:A:356:SER:H	2:A:359:GLN:NE2	2.15	0.45
1:D:8:DC:H2'	1:D:9:DT:H71	1.99	0.45
2:B:105:ALA:O	2:B:107:LEU:HG	2.17	0.45
2:B:121:ARG:CZ	2:B:409:ARG:HH22	2.30	0.45
2:B:181:CYS:O	2:B:185:GLY:N	2.49	0.45
2:A:197:HIS:CD2	2:A:235:LEU:HD12	2.52	0.45
2:A:32:GLY:N	4:A:700:ANP:HNB1	2.04	0.44
2:B:374:TYR:HA	2:B:553:ALA:HB1	1.98	0.44
2:B:60:VAL:O	2:B:219:VAL:HA	2.17	0.44
1:C:13:DG:H2''	1:C:14:DT:H5'	1.99	0.44
2:B:381:ARG:HA	2:B:384:GLU:CG	2.45	0.44
2:B:361:ARG:HH11	2:B:361:ARG:HG2	1.82	0.44
2:A:281:GLN:HB2	2:A:309:TRP:CZ2	2.52	0.44
2:A:130:MET:HB2	2:A:132:LEU:HD12	1.99	0.44
2:B:477:LEU:HG	2:B:516:THR:HB	2.00	0.44
2:A:39:LEU:C	2:A:39:LEU:HD23	2.37	0.44
2:B:29:ALA:HB3	2:B:35:LYS:HD3	1.99	0.44
2:B:480:GLN:O	2:B:484:VAL:HG23	2.16	0.44
2:B:126:LEU:O	2:B:126:LEU:HD23	2.17	0.44
2:A:355:ARG:HD3	2:A:580:PHE:CD2	2.53	0.44
2:B:334:VAL:HG22	2:B:367:LEU:HD23	1.99	0.44
2:A:429:THR:CG2	2:A:440:ALA:HB1	2.48	0.43
2:A:307:LYS:O	2:A:308:LEU:HB2	2.18	0.43
2:B:217:ILE:HD11	2:B:236:LEU:HG	1.99	0.43
2:B:447:GLU:C	2:B:449:ALA:H	2.21	0.43
2:A:398:ILE:HG23	2:A:469:ALA:HA	2.00	0.43
2:A:303:ARG:C	2:A:305:GLY:H	2.21	0.43
2:B:203:LYS:O	2:B:206:ILE:N	2.47	0.43
2:B:325:ASN:HB2	2:B:326:GLU:OE1	2.18	0.43
2:A:207:LEU:HD21	2:A:211:ARG:NH2	2.33	0.43
2:A:123:LEU:O	2:A:127:ILE:HG13	2.19	0.43
2:A:150:LYS:NZ	2:A:188:ASP:OD2	2.52	0.43
2:B:29:ALA:CB	2:B:279:LEU:HB2	2.48	0.43
2:B:387:GLU:CD	2:B:387:GLU:H	2.17	0.43
1:D:12:DA:H2''	1:D:13:DG:C8	2.53	0.43
2:B:107:LEU:HD21	2:B:195:ARG:CZ	2.49	0.43
2:A:491:ARG:O	2:A:495:GLU:HB2	2.18	0.43
2:A:119:GLN:HG3	2:A:177:TYR:OH	2.18	0.43
2:B:142:ALA:HB2	2:B:170:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:325:ASN:HA	2:B:615:ALA:HB1	1.99	0.43
2:B:25:LEU:HD12	2:B:275:GLU:O	2.19	0.43
2:B:113:ILE:HD12	2:B:532:GLN:OE1	2.17	0.43
2:B:114:LEU:HD12	2:B:118:ASP:CB	2.48	0.43
2:B:129:ALA:C	2:B:131:ASN:N	2.71	0.43
2:A:13:LYS:NZ	5:A:1026:HOH:O	2.44	0.43
2:A:303:ARG:HH11	2:A:303:ARG:CB	2.30	0.43
2:A:157:HIS:CD2	2:A:157:HIS:N	2.85	0.43
2:B:383:PHE:HA	2:B:388:ILE:HG21	2.00	0.43
1:D:16:DC:H2"	1:D:17:DT:C6	2.53	0.43
1:D:20:DT:C2	2:A:621:TYR:HD2	2.35	0.43
2:B:157:HIS:O	2:B:159:ILE:N	2.52	0.43
2:B:532:GLN:O	2:B:533:ALA:C	2.57	0.43
2:B:488:SER:OG	2:B:490:LEU:HG	2.19	0.43
2:A:475:MET:HE3	2:A:483:ARG:CZ	2.49	0.42
2:B:516:THR:HG22	2:B:534:PHE:CE2	2.54	0.42
2:B:111:PHE:C	2:B:111:PHE:CD1	2.92	0.42
2:B:203:LYS:N	2:B:204:PRO:CD	2.82	0.42
2:B:206:ILE:O	2:B:209:HIS:HB3	2.19	0.42
2:B:50:GLU:O	2:B:51:ASN:C	2.57	0.42
2:A:654:VAL:O	2:A:654:VAL:HG13	2.18	0.42
2:A:145:TYR:CD2	2:A:170:TRP:HB3	2.54	0.42
2:A:226:ASN:HA	2:A:259:ALA:HA	2.02	0.42
2:B:429:THR:HB	2:B:440:ALA:HB1	2.01	0.42
2:A:445:LEU:HD13	2:A:459:GLN:OE1	2.19	0.42
2:A:284:ARG:HH22	4:A:700:ANP:HNB1	1.67	0.42
2:B:47:MET:O	2:B:51:ASN:HA	2.20	0.42
2:A:273:GLY:O	2:A:274:ALA:C	2.57	0.42
2:A:174:TYR:C	2:A:174:TYR:CD1	2.93	0.42
2:A:169:THR:O	2:A:172:LYS:N	2.51	0.42
1:C:13:DG:H5"	2:A:453:ARG:NH1	2.35	0.42
2:A:397:LEU:HD11	2:A:407:PHE:HA	2.01	0.42
2:A:647:ARG:NE	2:A:649:THR:O	2.51	0.42
2:A:661:THR:HG23	2:A:661:THR:O	2.20	0.42
2:B:129:ALA:O	2:B:131:ASN:N	2.52	0.42
2:A:38:VAL:HG12	2:A:39:LEU:N	2.34	0.42
2:A:568:PRO:HA	2:A:607:MET:HB2	2.02	0.42
2:A:395:LEU:HD23	2:A:484:VAL:HG21	2.00	0.42
2:A:224:ASP:O	2:A:259:ALA:HB2	2.20	0.42
2:A:457:ALA:C	2:A:459:GLN:N	2.73	0.42
2:A:2:ASP:O	2:A:5:TYR:CD2	2.72	0.42
2:B:115:ASP:OD2	2:B:115:ASP:C	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:226:ASN:ND2	2:A:226:ASN:H	2.18	0.42
2:B:104:ASP:CB	2:B:203:LYS:HE3	2.48	0.42
2:B:70:MET:O	2:B:74:ILE:HG13	2.19	0.42
2:B:137:TRP:CZ3	2:B:169:THR:OG1	2.73	0.42
2:A:199:LEU:O	2:A:203:LYS:HB2	2.20	0.42
2:A:60:VAL:HG22	2:A:61:THR:N	2.34	0.42
2:A:242:LYS:HD3	2:A:242:LYS:HA	1.77	0.41
1:D:11:DC:H5''	2:A:417:GLY:O	2.19	0.41
2:B:304:LEU:HD11	2:B:306:LYS:CE	2.50	0.41
2:B:253:ILE:HD12	2:B:560:HIS:CD2	2.55	0.41
2:B:575:MET:HG3	2:B:612:LEU:HB3	2.02	0.41
2:B:514:THR:HG23	2:B:517:ARG:HH11	1.85	0.41
1:C:15:DG:H1	1:D:6:DC:N4	2.12	0.41
1:C:20:DT:H2''	1:C:22:DG:C2'	2.50	0.41
2:B:260:GLN:HG3	2:B:260:GLN:H	1.55	0.41
2:A:82:GLN:O	2:A:83:GLY:O	2.38	0.41
2:B:296:LEU:O	2:B:596:ARG:HD3	2.19	0.41
2:A:331:ARG:HB3	2:A:331:ARG:HH21	1.84	0.41
2:A:447:GLU:O	2:A:448:LYS:C	2.58	0.41
2:B:631:ARG:HG3	2:B:635:GLU:OE2	2.21	0.41
2:B:593:GLU:O	2:B:597:ARG:HG3	2.19	0.41
2:A:130:MET:CG	2:A:431:ARG:NH2	2.81	0.41
2:B:532:GLN:HA	2:B:532:GLN:NE2	2.31	0.41
2:B:453:ARG:NH1	2:B:453:ARG:HG3	2.33	0.41
2:A:375:ARG:HD3	2:A:377:TYR:CZ	2.55	0.41
2:B:550:TRP:CD2	2:B:551:GLN:HG3	2.55	0.41
2:A:37:ARG:HD3	5:A:1005:HOH:O	2.19	0.41
2:B:138:PRO:HA	2:B:139:PRO:HD3	1.84	0.41
2:B:159:ILE:HB	2:B:171:GLN:CD	2.41	0.41
2:A:60:VAL:O	2:A:219:VAL:HA	2.21	0.41
2:B:452:GLY:C	2:B:454:ALA:H	2.22	0.41
2:B:403:ASP:HB3	2:B:406:ALA:HB3	2.02	0.41
2:B:519:PHE:HZ	2:B:533:ALA:HB1	1.85	0.41
2:B:532:GLN:O	2:B:532:GLN:NE2	2.53	0.41
2:B:364:GLU:HG3	2:B:374:TYR:CZ	2.55	0.41
2:B:2:ASP:O	2:B:3:VAL:C	2.58	0.41
2:B:122:LEU:O	2:B:126:LEU:HB2	2.20	0.41
2:A:157:HIS:O	2:A:158:HIS:C	2.59	0.41
2:B:360:SER:HA	2:B:363:LEU:HD12	2.02	0.41
2:B:2:ASP:O	2:B:5:TYR:N	2.47	0.41
2:B:510:GLU:O	2:B:513:VAL:HB	2.21	0.41
2:B:39:LEU:C	2:B:39:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:114:LEU:HD13	2:B:186:LEU:HD13	2.03	0.41
2:B:2:ASP:O	2:B:4:SER:N	2.53	0.41
2:B:572:ILE:HB	2:B:612:LEU:HD23	2.03	0.41
2:B:452:GLY:C	2:B:454:ALA:N	2.73	0.41
2:B:68:ALA:HA	2:B:71:ARG:NH2	2.35	0.41
1:C:16:DC:HI'	1:C:17:DT:C5'	2.50	0.41
2:B:477:LEU:HD12	2:B:477:LEU:O	2.21	0.41
2:A:203:LYS:O	2:A:206:ILE:N	2.54	0.41
1:C:25:DT:H2'	1:C:25:DT:H6	1.51	0.41
2:B:456:SER:O	2:B:460:ARG:CG	2.69	0.41
2:B:75:GLY:O	2:B:79:GLY:N	2.54	0.41
2:A:19:ALA:HA	2:A:45:TRP:CE2	2.56	0.41
2:B:98:LEU:HD21	2:B:196:ALA:HA	2.03	0.41
2:B:550:TRP:CZ2	2:B:551:GLN:HG3	2.56	0.41
2:B:106:ASN:CG	2:B:106:ASN:O	2.59	0.41
2:A:426:VAL:HG11	2:A:441:CYS:SG	2.61	0.40
2:B:98:LEU:HD21	2:B:196:ALA:CA	2.51	0.40
2:B:78:MET:O	2:B:79:GLY:C	2.60	0.40
2:B:576:GLU:HG3	2:B:579:MET:CG	2.50	0.40
2:A:322:CYS:HB2	2:A:614:TYR:CZ	2.57	0.40
2:A:2:ASP:O	2:A:5:TYR:HD2	2.05	0.40
2:B:262:GLU:C	2:B:264:ILE:N	2.75	0.40
2:B:98:LEU:HD11	2:B:195:ARG:HB3	2.04	0.40
2:A:469:ALA:O	2:A:473:ALA:HB2	2.22	0.40
2:B:288:ASN:HA	2:B:288:ASN:HD22	1.63	0.40
2:A:66:ALA:O	2:A:69:GLU:HB3	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
2	A	638/680 (94%)	541 (85%)	72 (11%)	25 (4%)	5 6
2	B	618/680 (91%)	531 (86%)	59 (10%)	28 (4%)	4 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1256/1360 (92%)	1072 (85%)	131 (10%)	53 (4%)	4	5

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2	ASP
2	A	81	SER
2	A	307	LYS
2	A	451	ALA
2	A	497	GLU
2	A	550	TRP
2	A	661	THR
2	B	2	ASP
2	B	307	LYS
2	B	418	ILE
2	B	529	MET
2	B	530	PRO
2	B	531	LEU
2	B	533	ALA
2	B	536	SER
2	B	589	GLY
2	A	3	VAL
2	A	79	GLY
2	A	83	GLY
2	A	400	ASN
2	A	475	MET
2	B	83	GLY
2	B	130	MET
2	B	158	HIS
2	B	165	PRO
2	B	304	LEU
2	B	312	GLY
2	B	379	GLY
2	B	451	ALA
2	B	477	LEU
2	A	80	THR
2	A	259	ALA
2	A	274	ALA
2	A	420	ASP
2	A	448	LYS
2	A	454	ALA
2	B	109	GLN

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Mol	Chain	Res	Type
2	B	448	LYS
2	B	587	ASP
2	A	408	GLU
2	B	498	LYS
2	A	158	HIS
2	A	235	LEU
2	A	263	ASN
2	B	298	GLU
2	B	590	GLY
2	A	165	PRO
2	B	588	GLU
2	B	3	VAL
2	B	204	PRO
2	A	159	ILE
2	A	418	ILE
2	B	166	VAL

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	496/574 (86%)	472 (95%)	24 (5%)	35	64
2	B	493/574 (86%)	472 (96%)	21 (4%)	40	69
All	All	989/1148 (86%)	944 (95%)	45 (5%)	37	66

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	TYR
2	A	9	SER
2	A	23	SER
2	A	37	ARG
2	A	126	LEU
2	A	174	TYR
2	A	195	ARG
2	A	226	ASN
2	A	235	LEU

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Mol	Chain	Res	Type
2	A	261	VAL
2	A	280	GLU
2	A	288	ASN
2	A	298	GLU
2	A	331	ARG
2	A	389	LYS
2	A	416	ARG
2	A	420	ASP
2	A	421	ARG
2	A	475	MET
2	A	492	THR
2	A	505	ARG
2	A	530	PRO
2	A	550	TRP
2	A	628	ARG
2	B	5	TYR
2	B	37	ARG
2	B	111	PHE
2	B	126	LEU
2	B	167	GLU
2	B	170	TRP
2	B	174	TYR
2	B	226	ASN
2	B	240	THR
2	B	260	GLN
2	B	280	GLU
2	B	288	ASN
2	B	298	GLU
2	B	304	LEU
2	B	308	LEU
2	B	478	HIS
2	B	493	MET
2	B	506	ILE
2	B	514	THR
2	B	532	GLN
2	B	605	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	119	GLN
2	A	136	GLN

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Mol	Chain	Res	Type
2	A	147	ASN
2	A	157	HIS
2	A	178	GLN
2	A	197	HIS
2	A	205	HIS
2	A	226	ASN
2	A	227	ASN
2	A	288	ASN
2	A	359	GLN
2	A	508	ASN
2	B	119	GLN
2	B	147	ASN
2	B	158	HIS
2	B	178	GLN
2	B	226	ASN
2	B	260	GLN
2	B	288	ASN
2	B	359	GLN
2	B	508	ASN
2	B	518	GLN
2	B	560	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ANP	A	700	3	33,33,33	3.96	15 (45%)	51,52,52	2.30	15 (29%)
4	ANP	B	701	3	33,33,33	4.04	14 (42%)	51,52,52	2.26	14 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	700	3	-	0/18/38/38	0/1/3/3
4	ANP	B	701	3	-	0/18/38/38	0/1/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	ANP	PG-O1G	17.99	1.68	1.46
4	B	701	ANP	PG-O1G	17.88	1.68	1.46
4	B	701	ANP	PB-N3B	7.13	1.70	1.64
4	B	701	ANP	C2'-C1'	-5.34	1.45	1.53
4	A	700	ANP	C2'-C1'	-5.24	1.46	1.53
4	A	700	ANP	C4-N9	-5.24	1.30	1.37
4	B	701	ANP	C4-N9	-4.78	1.30	1.37
4	A	700	ANP	PB-N3B	4.77	1.68	1.64
4	A	700	ANP	C5-C4	4.09	1.49	1.40
4	B	701	ANP	C2-N3	4.03	1.40	1.32
4	B	701	ANP	C5-C4	4.00	1.49	1.40
4	B	701	ANP	PG-O3G	-3.65	1.44	1.55
4	A	700	ANP	C4-N3	3.63	1.41	1.35
4	B	701	ANP	C4-N3	3.56	1.41	1.35
4	A	700	ANP	C2-N3	3.51	1.39	1.32
4	A	700	ANP	PG-O3G	-3.02	1.46	1.55
4	A	700	ANP	PB-O2B	-2.85	1.46	1.55
4	B	701	ANP	PB-O2B	-2.73	1.47	1.55
4	A	700	ANP	PG-N3B	-2.58	1.62	1.64
4	A	700	ANP	O4'-C1'	2.52	1.45	1.41
4	A	700	ANP	C5-N7	-2.42	1.31	1.40
4	B	701	ANP	C2-N1	2.39	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ANP	PA-O2A	-2.35	1.44	1.55
4	B	701	ANP	C5-N7	-2.35	1.31	1.40
4	A	700	ANP	PA-O2A	-2.35	1.44	1.55
4	A	700	ANP	C2-N1	2.28	1.38	1.33
4	B	701	ANP	O4'-C1'	2.06	1.44	1.41
4	B	701	ANP	O4'-C4'	-2.03	1.40	1.45
4	A	700	ANP	O3'-C3'	2.02	1.47	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	ANP	N3-C2-N1	-8.49	121.61	128.71
4	B	701	ANP	N3-C2-N1	-8.19	121.86	128.71
4	A	700	ANP	O4'-C1'-N9	-7.03	101.90	108.44
4	B	701	ANP	O4'-C1'-N9	-6.77	102.14	108.44
4	B	701	ANP	N3-C4-N9	5.54	135.43	125.43
4	A	700	ANP	N3-C4-N9	5.27	134.95	125.43
4	A	700	ANP	O2B-PB-O1B	4.47	120.20	109.89
4	B	701	ANP	O2B-PB-O1B	4.30	119.81	109.89
4	B	701	ANP	PB-N3B-PG	2.86	134.88	130.07
4	A	700	ANP	C1'-N9-C4	-2.80	121.79	126.64
4	B	701	ANP	C5-C4-N3	-2.74	119.73	125.70
4	B	701	ANP	C2-N3-C4	2.71	121.72	114.01
4	A	700	ANP	C2-N3-C4	2.68	121.64	114.01
4	A	700	ANP	C8-N9-C4	2.65	108.92	106.90
4	B	701	ANP	C8-N9-C4	2.62	108.90	106.90
4	B	701	ANP	C1'-N9-C4	-2.61	122.13	126.64
4	A	700	ANP	C5-C4-N3	-2.61	120.02	125.70
4	A	700	ANP	O1B-PB-N3B	-2.56	107.96	111.83
4	B	701	ANP	C2'-C1'-N9	2.55	119.81	113.27
4	B	701	ANP	C4-C5-N7	-2.49	107.39	109.52
4	A	700	ANP	C4-C5-N7	-2.46	107.42	109.52
4	B	701	ANP	O2G-PG-O1G	-2.44	107.33	113.60
4	A	700	ANP	O3'-C3'-C4'	-2.30	104.29	111.08
4	A	700	ANP	C2'-C1'-N9	2.30	119.17	113.27
4	A	700	ANP	O3G-PG-O2G	2.29	114.22	107.66
4	B	701	ANP	O3'-C3'-C4'	-2.26	104.41	111.08
4	A	700	ANP	O2G-PG-O1G	-2.13	108.14	113.60
4	A	700	ANP	PB-N3B-PG	2.08	133.57	130.07
4	B	701	ANP	O3G-PG-O2G	2.05	113.54	107.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å ²)	Q<0.9
1	C	25/26 (96%)	-0.04	0	100 100	51, 117, 165, 171	0
1	D	25/26 (96%)	-0.09	0	100 100	59, 117, 150, 153	0
2	A	646/680 (95%)	0.21	41 (6%)	19 16	31, 73, 126, 140	1 (0%)
2	B	632/680 (92%)	0.15	20 (3%)	45 42	36, 68, 122, 179	1 (0%)
All	All	1328/1412 (94%)	0.17	61 (4%)	31 27	31, 72, 126, 179	2 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	658	ARG	12.1
2	B	657	GLN	10.0
2	A	499	GLY	6.6
2	B	519	PHE	4.9
2	A	137	TRP	4.3
2	A	453	ARG	4.1
2	A	1	MET	4.1
2	B	458	LEU	4.1
2	A	454	ALA	3.8
2	B	499	GLY	3.7
2	A	446	GLN	3.7
2	A	464	LEU	3.5
2	B	81	SER	3.4
2	A	468	LEU	3.4
2	B	132	LEU	3.4
2	A	481	THR	3.3
2	A	144	TRP	3.3
2	A	445	LEU	3.3
2	A	458	LEU	3.3
2	A	449	ALA	3.2
2	B	163	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	A	80	THR	3.2
2	B	444	LEU	3.1
2	A	474	ASP	3.1
2	B	509	LEU	3.0
2	A	506	ILE	3.0
2	A	116	SER	3.0
2	A	159	ILE	3.0
2	A	465	ILE	2.9
2	B	650	VAL	2.9
2	B	529	MET	2.7
2	B	477	LEU	2.7
2	B	449	ALA	2.7
2	A	443	GLU	2.7
2	A	444	LEU	2.6
2	A	425	VAL	2.6
2	A	549	THR	2.6
2	A	160	GLN	2.6
2	B	468	LEU	2.5
2	A	441	CYS	2.5
2	A	141	GLN	2.5
2	A	485	ILE	2.5
2	A	450	LEU	2.5
2	B	137	TRP	2.5
2	A	455	ALA	2.5
2	A	537	HIS	2.5
2	B	461	PHE	2.5
2	B	305	GLY	2.5
2	A	459	GLN	2.4
2	B	481	THR	2.4
2	B	533	ALA	2.4
2	A	457	ALA	2.3
2	A	653	PRO	2.3
2	A	126	LEU	2.2
2	A	304	LEU	2.1
2	A	498	LYS	2.1
2	A	384	GLU	2.1
2	A	122	LEU	2.1
2	A	475	MET	2.0
2	A	407	PHE	2.0
2	A	127	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ANP	A	700	31/31	0.18	1.47	43,48,56,58	0
4	ANP	B	701	31/31	0.19	0.38	45,52,58,61	0
3	MG	B	1002	1/1	0.21	0.24	40,40,40,40	0
3	MG	A	1001	1/1	0.16	0.04	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.