



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:04 PM UTC

PDB ID : 2IS4 / pdb_00002is4
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

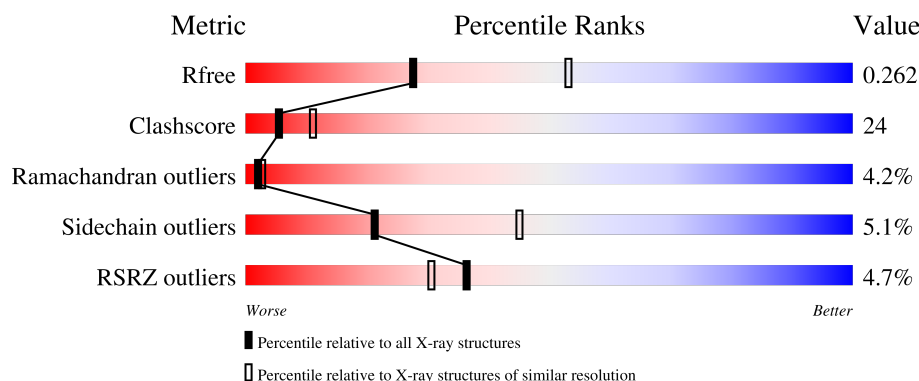
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. 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	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 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 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			

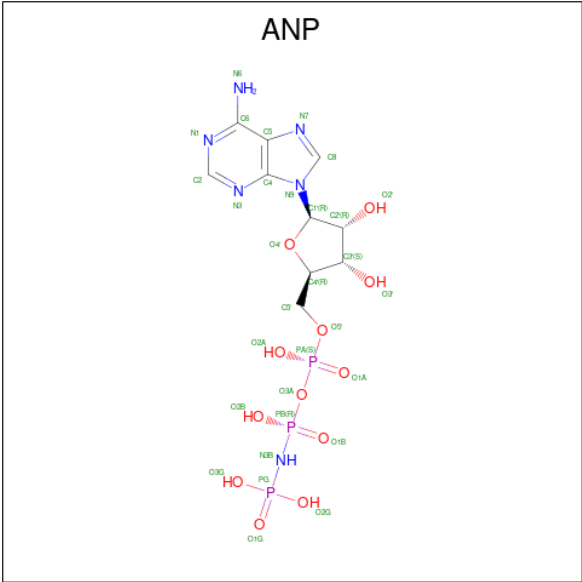
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

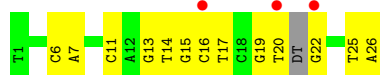
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	56	Total	O	0	0
			56	56		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

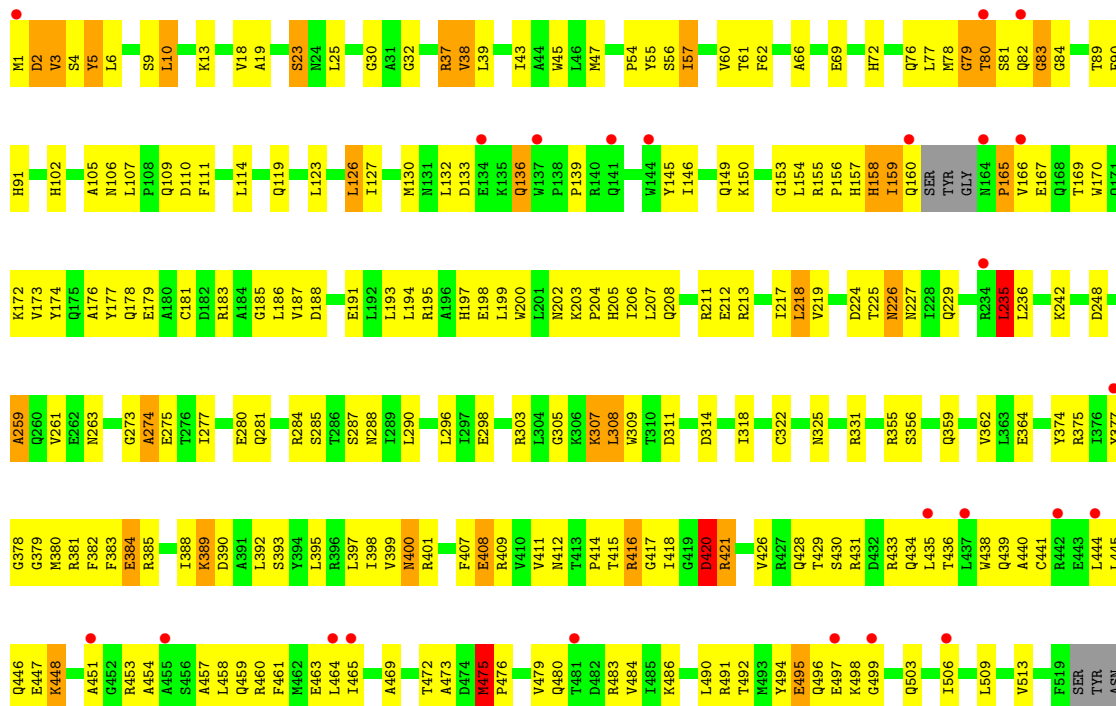
• Molecule 1: 25-MER

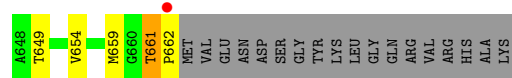


• Molecule 1: 25-MER

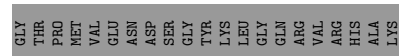
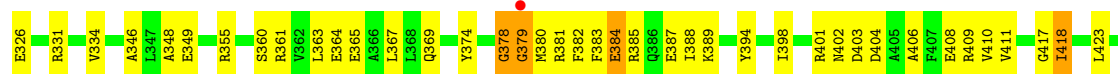


• Molecule 2: DNA helicase II





● Molecule 2: DNA helicase II



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 29.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	85.3 (29.84-2.60) 85.3 (29.84-2.60)	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 0.224 , 0.262	Depositor DCC
R_{free} test set	5887 reflections (9.65%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

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	0.30	0/565	0.70	0/869
1	D	0.28	0/569	0.66	0/877
2	A	0.48	0/5099	0.94	16/6913 (0.2%)
2	B	0.48	0/5032	0.99	22/6807 (0.3%)
All	All	0.46	0/11265	0.94	38/15466 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	SER	N-CA-C	-8.59	102.36	112.92
2	B	243	VAL	N-CA-C	8.35	120.50	108.48
2	A	499	GLY	N-CA-C	-8.11	100.98	114.76
2	B	270	ASP	N-CA-C	7.73	121.20	111.69
2	B	653	PRO	N-CA-CB	7.68	109.77	103.32
2	B	378	GLY	N-CA-C	-7.42	103.37	115.46
2	B	504	THR	N-CA-C	-7.27	103.34	111.71
2	A	10	LEU	N-CA-C	7.16	119.55	110.24
2	A	227	ASN	N-CA-C	7.09	118.80	111.14
2	A	551	GLN	N-CA-C	-7.08	93.47	107.69
2	B	227	ASN	N-CA-C	6.98	118.89	111.28
2	B	168	GLN	N-CA-C	-6.92	104.09	112.54
2	A	136	GLN	N-CA-C	-6.80	105.14	113.50
2	B	285	SER	N-CA-C	6.78	120.57	109.85
2	B	62	PHE	N-CA-C	6.52	119.65	111.24
2	B	239	ASP	N-CA-C	-6.26	105.42	114.12
2	B	488	SER	N-CA-C	-6.23	105.62	113.72
2	A	628	ARG	N-CA-C	-6.20	101.73	110.29
2	A	285	SER	N-CA-C	6.19	120.01	110.42
2	B	530	PRO	N-CA-CB	6.19	109.75	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	662	PRO	N-CA-CB	5.98	109.58	103.00
2	B	8	ASP	N-CA-C	5.89	118.18	111.11
2	B	384	GLU	N-CA-C	-5.88	106.24	113.41
2	B	578	GLY	N-CA-C	-5.81	107.56	114.48
2	A	446	GLN	N-CA-C	-5.69	105.47	113.20
2	B	57	ILE	N-CA-C	5.68	116.04	107.75
2	A	384	GLU	N-CA-C	-5.53	106.70	113.50
2	A	62	PHE	N-CA-C	5.51	118.12	111.40
2	A	641	VAL	N-CA-C	5.41	116.28	108.48
2	B	284	ARG	N-CA-C	5.40	118.33	111.69
2	A	57	ILE	N-CA-C	5.33	115.77	107.99
2	B	475	MET	N-CA-C	5.32	115.72	109.60
2	B	222	PHE	N-CA-C	5.23	118.44	111.75
2	B	579	MET	N-CA-C	-5.18	105.03	112.13
2	A	529	MET	CA-C-N	5.17	126.31	119.84
2	A	529	MET	C-N-CA	5.17	126.31	119.84
2	B	10	LEU	N-CA-C	5.05	116.80	110.24
2	A	605	ARG	N-CA-C	-5.02	107.00	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	506	0	287	24	0
1	D	509	0	285	32	0
2	A	5006	0	4755	229	0
2	B	4945	0	4732	233	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	502	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 24.

All (502) 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: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:B:47:MET:HE3	2:B:54:PRO:HG3	1.46	0.98
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:550:TRP:H	2:A:550:TRP:CD1	2.08	0.71
2:A:130:MET:HG2	2:A:431:ARG:HH21	1.55	0.71
2:A:475:MET:HE2	2:A:479:VAL:HG13	1.71	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:A:659:MET:HE3	2:A:661:THR:HG21	1.72	0.70
2:B:532:GLN:HE21	2:B:532:GLN:HA	1.56	0.70
2:B:438:TRP:CE2	2:B:462:MET:HE3	2.27	0.70
2:A:459:GLN:O	2:A:463:GLU:HG3	1.92	0.69
2:B:382:PHE:HA	2:B:385:ARG:HH21	1.56	0.69
2:B:592:LEU:HD21	2:B:631:ARG:NH1	2.07	0.69
2:A:133:ASP:HB3	2:A:136:GLN:HB2	1.75	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: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:A:149:GLN:OE1	2:A:154:LEU:HD12	1.95	0.66
2:B:25:LEU:HD21	2:B:277:ILE:HD12	1.78	0.66
2:A:421:ARG:NE	2:A:421:ARG:H	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:A:77:LEU:HD23	2:A:78:MET:HE2	1.80	0.64
2:A:217:ILE:C	2:A:218:LEU:HD12	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:MET:HE3	2:A:132:LEU:HD12	1.81	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:HB3	2:A:421:ARG:HH11	1.64	0.62
2:A:43:ILE:HG23	2:A:57:ILE:HD13	1.81	0.62
2:B:472:THR:HG22	2:B:475:MET:SD	2.39	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:A:130:MET:HE1	2:A:173:VAL:HG13	1.84	0.60
2:B:104:ASP:HB3	2:B:203:LYS:HE3	1.83	0.60
2:B:514:THR:O	2:B:517:ARG:HB3	2.01	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: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:129:ALA:C	2:B:131:ASN:H	2.09	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:HG3	2:A:416:ARG:HH11	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:105:ALA:O	2:A:106:ASN:HB3	2.02	0.58
2:A:601:VAL:O	2:A:605:ARG:CD	2.50	0.58
2:B:156:PRO:HA	2:B:171:GLN:NE2	2.19	0.58
2:B:485:ILE:HG22	2:B:491:ARG:HG3	1.84	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:O	2:A:434:GLN:HB2	2.04	0.58
2:A:433:ARG:HB3	2:A:435:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:475:MET:HE3	2:A:483:ARG:CZ	2.34	0.58
1:D:11:DC:OP2	2:A:421:ARG:HG2	2.04	0.57
2:A:555:GLN:C	2:A:556:LEU:HD12	2.29	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:A:146:ILE:HD13	2:A:177:TYR:CD2	2.40	0.57
2:B:2:ASP:O	2:B:5:TYR:HD2	1.88	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:A:287:SER:HB3	2:A:314:ASP:HA	1.86	0.56
2:A:393:SER:OG	2:A:409:ARG:HD3	2.06	0.56
2:B:159:ILE:HB	2:B:171:GLN:OE1	2.04	0.56
2:B:435:LEU:HB3	2:B:439:GLN:HB3	1.87	0.56
2:A:157:HIS:CD2	2:A:157:HIS:H	2.23	0.56
2:B:135:LYS:NZ	2:B:135:LYS:HB3	2.20	0.56
2:A:79:GLY:O	2:A:80:THR:C	2.49	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:A:110:ASP:O	2:A:111:PHE:C	2.48	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:A:226:ASN:C	2:A:226:ASN:HD22	2.13	0.55
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:A:380:MET:O	2:A:384:GLU:HG3	2.07	0.55
2:A:445:LEU:C	2:A:447:GLU:H	2.13	0.55
2:B:170:TRP:HA	2:B:170:TRP:CE3	2.41	0.55
1:D:17:DT:H2''	1:D:18:DC:C6	2.42	0.55
2:A:362:VAL:HG23	5:A:1036:HOH:O	2.05	0.55
2:B:194:LEU:O	2:B:198:GLU:HG3	2.07	0.55
2:B:287:SER:HB3	2:B:314:ASP:HA	1.89	0.55
2:B:529:MET:O	2:B:530:PRO:C	2.49	0.55
2:A:47:MET:HE3	2:A:54:PRO:HG3	1.88	0.55
2:A:166:VAL:HG23	2:A:167:GLU:N	2.22	0.55
2:B:369:GLN:O	2:B:369:GLN:HG2	2.07	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:A:503:GLN:O	2:A:506:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:ILE:HD12	2:B:506:ILE:O	2.07	0.54
2:B:529:MET:O	2:B:531:LEU:N	2.40	0.54
2:A:165:PRO:HG2	2:A:166:VAL:H	1.71	0.54
2:B:82:GLN:O	2:B:83:GLY:C	2.50	0.54
2:B:387:GLU:OE2	2:B:505:ARG:NH1	2.39	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:B:498:LYS:O	2:B:499:GLY:C	2.51	0.53
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:423:LEU:O	2:B:427:ARG:HG3	2.09	0.53
2:B:509:LEU:O	2:B:513:VAL:HG23	2.08	0.53
2:A:5:TYR:CD2	2:A:6:LEU:N	2.77	0.53
2:A:126:LEU:HD21	2:A:176:ALA:HB1	1.91	0.53
2:A:2:ASP:O	2:A:3:VAL:C	2.51	0.53
2:A:130:MET:HE3	2:A:132:LEU:CD1	2.39	0.52
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:56:SER:HA	2:A:213:ARG:O	2.10	0.52
2:A:407:PHE:CE1	2:A:461:PHE:HE2	2.27	0.52
2:B:207:LEU:HD22	2:B:235:LEU:HD21	1.91	0.52
2:B:288:ASN:HB2	2:B:314:ASP:O	2.09	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:A:619:ARG:HA	2:A:623:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:MET:HG3	2:B:494:TYR:N	2.24	0.52
2:B:532:GLN:CD	2:B:536:SER:HB2	2.34	0.52
1:C:14:DT:H2"	1:C:15:DG:N7	2.25	0.52
2:A:127:ILE:HD12	2:A:139:PRO:HG3	1.90	0.52
2:B:90:PHE:CE2	2:B:233:ILE:HD11	2.45	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
2:A:592:LEU:HD11	2:A:631:ARG:NH1	2.24	0.51
2:B:411:VAL:HA	2:B:461:PHE:CZ	2.44	0.51
2:A:30:GLY:HA2	2:A:248:ASP:OD2	2.10	0.51
2:B:46:LEU:O	2:B:52:CYS:HB2	2.10	0.51
2:B:382:PHE:HA	2:B:385:ARG:HH22	1.71	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:B:16:GLU:O	2:B:20:ALA:HB2	2.10	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:A:318:ILE:HB	2:A:641:VAL:HG22	1.94	0.50
2:A:490:LEU:HD22	2:A:494:TYR:HE1	1.75	0.50
2:B:114:LEU:HD11	2:B:118:ASP:HB3	1.92	0.50
2:B:445:LEU:C	2:B:447:GLU:H	2.19	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:217:ILE:HB	2:B:243:VAL:HG22	1.92	0.50
2:B:408:GLU:HG2	2:B:437:LEU:CD1	2.42	0.50
2:B:91:HIS:CE1	2:B:193:LEU:HD11	2.46	0.50
2:B:530:PRO:O	2:B:531:LEU:C	2.54	0.50
2:A:13:LYS:NZ	5:A:1026:HOH:O	2.44	0.50
2:A:187:VAL:HG13	2:A:191:GLU:HB3	1.94	0.50
2:A:205:HIS:CE1	2:A:206:ILE:HG13	2.47	0.50
2:A:472:THR:HG22	2:A:483:ARG:HD2	1.94	0.50
2:B:532:GLN:HE21	2:B:532:GLN:C	2.20	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:A:364:GLU:HG3	2:A:374:TYR:CZ	2.47	0.50
2:B:27:VAL:HB	2:B:246:VAL:HG12	1.94	0.50
2:B:385:ARG:HB3	2:B:387:GLU:OE1	2.12	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:A:458:LEU:HD12	2:A:458:LEU:O	2.12	0.49
2:B:530:PRO:O	2:B:531:LEU:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:226:ASN:ND2	2:A:229:GLN:HG3	2.23	0.49
2:A:480:GLN:O	2:A:484:VAL:HG23	2.12	0.49
2:B:569:GLN:NE2	2:B:609:LYS:HB3	2.27	0.49
2:A:39:LEU:C	2:A:39:LEU:HD23	2.37	0.49
2:B:512:LEU:O	2:B:516:THR:HG23	2.12	0.49
2:A:23:SER:CA	2:A:242:LYS:HD2	2.36	0.49
2:B:170:TRP:HA	2:B:170:TRP:HE3	1.77	0.49
2:B:564:GLY:H	2:B:605:ARG:NH2	2.09	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:A:78:MET:O	2:A:79:GLY:O	2.31	0.49
2:A:109:GLN:O	2:A:109:GLN:HG2	2.13	0.49
2:B:155:ARG:N	2:B:158:HIS:HD2	1.99	0.49
2:B:289:ILE:HD13	2:B:606:ALA:HB3	1.95	0.49
2:B:82:GLN:HB2	2:B:85:MET:HE3	1.94	0.48
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:A:191:GLU:OE2	2:A:195:ARG:HD3	2.13	0.48
2:A:303:ARG:NH1	2:A:303:ARG:CB	2.76	0.48
2:B:112:GLN:HB3	2:B:186:LEU:HD23	1.95	0.48
1:C:6:DC:H2''	1:C:7:DA:OP2	2.13	0.48
2:A:55:TYR:HA	2:A:84:GLY:O	2.13	0.48
2:B:447:GLU:C	2:B:449:ALA:H	2.21	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:B:387:GLU:H	2:B:387:GLU:CD	2.17	0.48
2:A:389:LYS:HB3	2:A:409:ARG:CZ	2.44	0.48
2:A:150:LYS:NZ	2:A:178:GLN:HE22	2.12	0.48
2:B:111:PHE:CD1	2:B:111:PHE:C	2.92	0.48
2:B:348:ALA:HA	2:B:553:ALA:O	2.13	0.48
2:B:394:TYR:O	2:B:398:ILE:HG13	2.14	0.48
2:A:303:ARG:C	2:A:305:GLY:H	2.21	0.47
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
2:B:532:GLN:O	2:B:533:ALA:C	2.57	0.47
1:D:15:DG:C2'	1:D:16:DC:C5'	2.76	0.47
2:A:378:GLY:CA	2:A:381:ARG:NH1	2.77	0.47
2:A:411:VAL:HG13	2:A:412:ASN:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:GLU:O	2:B:51:ASN:C	2.57	0.47
2:B:126:LEU:HD11	2:B:177:TYR:N	2.29	0.47
2:B:491:ARG:O	2:B:495:GLU:HG3	2.14	0.47
2:A:155:ARG:HB3	2:A:156:PRO:HD2	1.97	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:10:LEU:CD1	2:A:18:VAL:HG21	2.45	0.47
2:A:174:TYR:CD1	2:A:174:TYR:C	2.93	0.47
2:A:397:LEU:HD13	2:A:465:ILE:HD13	1.97	0.47
2:A:407:PHE:O	2:A:411:VAL:HB	2.14	0.47
2:A:457:ALA:O	2:A:460:ARG:N	2.47	0.47
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:A:102:HIS:HB2	2:A:107:LEU:O	2.15	0.47
2:A:200:TRP:HB3	2:A:207:LEU:HD13	1.97	0.47
2:B:95:HIS:CE1	2:B:113:ILE:HD11	2.50	0.47
2:A:126:LEU:O	2:A:130:MET:HG3	2.15	0.47
2:A:457:ALA:C	2:A:459:GLN:N	2.73	0.47
2:B:115:ASP:OD2	2:B:115:ASP:C	2.57	0.47
2:A:90:PHE:CZ	2:A:225:THR:HG22	2.50	0.46
2:A:399:VAL:O	2:A:400:ASN:HB2	2.16	0.46
2:A:159:ILE:O	2:A:160:GLN:CB	2.64	0.46
2:B:304:LEU:N	2:B:304:LEU:HD23	2.30	0.46
2:B:418:ILE:HD13	2:B:458:LEU:HD23	1.97	0.46
2:B:438:TRP:CZ2	2:B:462:MET:HE3	2.50	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:104:ASP:HB3	2:B:203:LYS:HG3	1.96	0.46
2:B:254:TYR:HB3	2:B:257:ARG:HH21	1.79	0.46
2:A:273:GLY:O	2:A:274:ALA:C	2.57	0.46
2:A:438:TRP:HZ3	2:A:465:ILE:HD12	1.80	0.46
2:A:447:GLU:O	2:A:448:LYS:C	2.58	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:B:159:ILE:HB	2:B:171:GLN:CD	2.41	0.46
2:B:452:GLY:C	2:B:454:ALA:H	2.22	0.46
2:A:191:GLU:O	2:A:195:ARG:HB2	2.16	0.46
2:A:325:ASN:HA	2:A:617:THR:O	2.16	0.46
2:A:549:THR:O	2:A:551:GLN:N	2.49	0.46
2:B:39:LEU:C	2:B:39:LEU:HD23	2.41	0.46
2:B:490:LEU:HA	2:B:493:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:202:ASN:O	2:A:203:LYS:HG2	2.16	0.45
2:A:397:LEU:HD21	2:A:407:PHE:N	2.31	0.45
2:A:618:ARG:O	2:A:625:VAL:HG22	2.16	0.45
1:D:26:DA:N7	2:A:380:MET:HG3	2.32	0.45
2:A:157:HIS:O	2:A:158:HIS:C	2.59	0.45
2:B:56:SER:HB2	2:B:215:THR:OG1	2.16	0.45
2:B:106:ASN:CG	2:B:106:ASN:O	2.59	0.45
2:B:389:LYS:HB3	2:B:409:ARG:NE	2.32	0.45
2:B:402:ASN:HB3	2:B:436:THR:HG21	1.96	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:78:MET:O	2:B:79:GLY:C	2.60	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:A:217:ILE:HD11	2:A:236:LEU:HG	1.98	0.45
2:A:303:ARG:HB2	2:A:303:ARG:NH1	2.32	0.45
2:A:309:TRP:HZ3	2:A:311:ASP:OD2	1.99	0.45
2:B:95:HIS:HE1	2:B:532:GLN:HG2	1.80	0.45
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:A:197:HIS:CD2	2:A:235:LEU:HD12	2.52	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:32:GLY:N	4:A:700:ANP:HNB1	2.04	0.44
2:B:60:VAL:O	2:B:219:VAL:HA	2.17	0.44
2:B:226:ASN:C	2:B:226:ASN:HD22	2.25	0.44
2:B:374:TYR:HA	2:B:553:ALA:HB1	1.98	0.44
2:B:2:ASP:O	2:B:3:VAL:C	2.58	0.44
1:C:13:DG:H2''	1:C:14:DT:H5'	1.99	0.44
2:A:281:GLN:HB2	2:A:309:TRP:CZ2	2.52	0.44
2:B:361:ARG:HG2	2:B:361:ARG:HH11	1.82	0.44
2:B:381:ARG:HA	2:B:384:GLU:CG	2.45	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:B:29:ALA:HB3	2:B:35:LYS:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:651:SER:O	2:B:652:ARG:C	2.61	0.44
2:A:188:ASP:OD1	2:A:188:ASP:C	2.60	0.43
2:A:429:THR:CG2	2:A:440:ALA:HB1	2.48	0.43
2:B:217:ILE:HD11	2:B:236:LEU:HG	1.99	0.43
2:B:452:GLY:C	2:B:454:ALA:N	2.73	0.43
2:A:398:ILE:HG23	2:A:469:ALA:HA	2.00	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:A:475:MET:HE2	2:A:479:VAL:CG1	2.43	0.43
2:B:29:ALA:CB	2:B:279:LEU:HB2	2.48	0.43
1:D:12:DA:H2"	1:D:13:DG:C8	2.53	0.43
2:A:119:GLN:HG3	2:A:177:TYR:OH	2.18	0.43
2:A:226:ASN:C	2:A:226:ASN:ND2	2.75	0.43
2:A:445:LEU:C	2:A:447:GLU:N	2.77	0.43
2:A:491:ARG:O	2:A:495:GLU:HB2	2.18	0.43
2:B:107:LEU:HD21	2:B:195:ARG:CZ	2.49	0.43
2:B:142:ALA:HB2	2:B:170:TRP:CZ3	2.54	0.43
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:494:TYR:O	2:B:495:GLU:C	2.59	0.43
2:B:114:LEU:HD12	2:B:118:ASP:CB	2.48	0.43
2:A:157:HIS:CD2	2:A:157:HIS:N	2.85	0.43
2:A:303:ARG:HH11	2:A:303:ARG:CB	2.30	0.43
2:A:307:LYS:O	2:A:308:LEU:HB2	2.18	0.43
2:B:111:PHE:C	2:B:111:PHE:HD1	2.27	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:488:SER:OG	2:B:490:LEU:HG	2.19	0.43
2:B:536:SER:O	2:B:537:HIS:C	2.61	0.43
2:B:135:LYS:HB3	2:B:135:LYS:HZ3	1.83	0.42
2:B:262:GLU:C	2:B:264:ILE:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:THR:HG22	2:B:534:PHE:CE2	2.54	0.42
2:A:145:TYR:CD2	2:A:170:TRP:HB3	2.54	0.42
2:A:654:VAL:HG13	2:A:654:VAL:O	2.18	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: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:B:410:VAL:O	2:B:411:VAL:C	2.63	0.42
2:A:169:THR:O	2:A:172:LYS:N	2.51	0.42
2:A:284:ARG:HH22	4:A:700:ANP:HNB1	1.67	0.42
2:A:414:PRO:O	2:A:415:THR:C	2.63	0.42
2:B:47:MET:O	2:B:51:ASN:HA	2.20	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: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: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:2:ASP:O	2:A:5:TYR:CD2	2.72	0.42
2:A:224:ASP:O	2:A:259:ALA:HB2	2.20	0.42
2:A:395:LEU:HD23	2:A:484:VAL:HG21	2.00	0.42
2:A:226:ASN:ND2	2:A:226:ASN:H	2.18	0.42
2:A:428:GLN:C	2:A:430:SER:N	2.77	0.42
2:B:70:MET:O	2:B:74:ILE:HG13	2.19	0.42
2:B:104:ASP:CB	2:B:203:LYS:HE3	2.48	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
1:D:11:DC:H5''	2:A:417:GLY:O	2.19	0.41
2:A:242:LYS:HD3	2:A:242:LYS:HA	1.77	0.41
2:A:303:ARG:C	2:A:305:GLY:N	2.78	0.41
2:B:253:ILE:HD12	2:B:560:HIS:CD2	2.55	0.41
2:B:304:LEU:HD11	2:B:306:LYS:CE	2.50	0.41
2:B:575:MET:HG3	2:B:612:LEU:HB3	2.02	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:A:82:GLN:O	2:A:83:GLY:O	2.38	0.41
2:A:331:ARG:HB3	2:A:331:ARG:HH21	1.84	0.41
2:B:260:GLN:H	2:B:260:GLN:HG3	1.55	0.41
2:B:296:LEU:O	2:B:596:ARG:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:GLY:O	2:B:379:GLY:C	2.63	0.41
2:B:514:THR:HG23	2:B:517:ARG:HH11	1.85	0.41
2:B:593:GLU:O	2:B:597:ARG:HG3	2.19	0.41
2:B:631:ARG:HG3	2:B:635:GLU:OE2	2.21	0.41
2:A:37:ARG:HD3	5:A:1005:HOH:O	2.19	0.41
2:A:130:MET:CG	2:A:431:ARG:NH2	2.81	0.41
2:A:375:ARG:HD3	2:A:377:TYR:CZ	2.55	0.41
2:B:138:PRO:HA	2:B:139:PRO:HD3	1.84	0.41
2:B:453:ARG:HG3	2:B:453:ARG:NH1	2.33	0.41
2:B:532:GLN:HA	2:B:532:GLN:NE2	2.31	0.41
2:B:550:TRP:CD2	2:B:551:GLN:HG3	2.55	0.41
2:A:60:VAL:O	2:A:219:VAL:HA	2.21	0.41
2:B:403:ASP:HB3	2:B:406:ALA:HB3	2.02	0.41
2:B:122:LEU:O	2:B:126:LEU:HB2	2.20	0.41
2:B:360:SER:HA	2:B:363:LEU:HD12	2.02	0.41
2:B:364:GLU:HG3	2:B:374:TYR:CZ	2.55	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:A:82:GLN:O	2:A:83:GLY:C	2.63	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:2:ASP:O	2:B:4:SER:N	2.53	0.41
2:B:68:ALA:HA	2:B:71:ARG:NH2	2.35	0.41
2:B:114:LEU:HD13	2:B:186:LEU:HD13	2.03	0.41
2:B:417:GLY:O	2:B:418:ILE:C	2.64	0.41
2:B:572:ILE:HB	2:B:612:LEU:HD23	2.03	0.41
1:C:16:DC:H1'	1:C:17:DT:C5'	2.50	0.41
1:C:25:DT:H6	1:C:25:DT:H2'	1.51	0.41
2:A:19:ALA:HA	2:A:45:TRP:CE2	2.56	0.41
2:A:203:LYS:O	2:A:206:ILE:N	2.54	0.41
2:A:541:GLU:C	2:A:543:GLY:H	2.28	0.41
2:B:75:GLY:O	2:B:79:GLY:N	2.54	0.41
2:B:403:ASP:O	2:B:404:ASP:C	2.64	0.41
2:B:456:SER:O	2:B:460:ARG:CG	2.69	0.41
2:B:477:LEU:O	2:B:477:LEU:HD12	2.21	0.41
2:B:569:GLN:CD	2:B:609:LYS:HB3	2.46	0.41
2:A:60:VAL:HG22	2:A:61:THR:N	2.34	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:639:GLU:H	2:B:639:GLU:CD	2.29	0.41
2:A:426:VAL:HG11	2:A:441:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:PHE:C	2:B:224:ASP:H	2.29	0.40
2:B:98:LEU:HD21	2:B:196:ALA:CA	2.51	0.40
2:A:2:ASP:O	2:A:5:TYR:HD2	2.05	0.40
2:A:156:PRO:O	2:A:157:HIS:C	2.64	0.40
2:A:322:CYS:HB2	2:A:614:TYR:CZ	2.57	0.40
2:A:659:MET:HE3	2:A:661:THR:CG2	2.48	0.40
2:B:576:GLU:HG3	2:B:579:MET:CG	2.50	0.40
2:A:3:VAL:O	2:A:4:SER:C	2.64	0.40
2:B:98:LEU:HD11	2:B:195:ARG:HB3	2.04	0.40
2:B:519:PHE:O	2:B:520:SER:C	2.63	0.40
2:A:66:ALA:O	2:A:69:GLU:HB3	2.22	0.40
2:A:469:ALA:O	2:A:473:ALA:HB2	2.22	0.40
2:B:47:MET:CE	2:B:54:PRO:HG3	2.34	0.40
2:B:288:ASN:HD22	2:B:288:ASN:HA	1.63	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	638/680 (94%)	541 (85%)	72 (11%)	25 (4%)	2	3
2	B	618/680 (91%)	531 (86%)	59 (10%)	28 (4%)	2	2
All	All	1256/1360 (92%)	1072 (85%)	131 (10%)	53 (4%)	2	3

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	23	47
2	B	493/574 (86%)	467 (95%)	26 (5%)	20	43
All	All	989/1148 (86%)	939 (95%)	50 (5%)	21	45

All (50) 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	38	VAL
2	A	126	LEU
2	A	218	LEU
2	A	226	ASN
2	A	235	LEU
2	A	261	VAL
2	A	280	GLU
2	A	288	ASN
2	A	298	GLU
2	A	308	LEU
2	A	389	LYS
2	A	416	ARG

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Mol	Chain	Res	Type
2	A	420	ASP
2	A	421	ARG
2	A	475	MET
2	A	492	THR
2	A	495	GLU
2	A	530	PRO
2	A	550	TRP
2	A	628	ARG
2	B	5	TYR
2	B	26	LEU
2	B	37	ARG
2	B	126	LEU
2	B	167	GLU
2	B	170	TRP
2	B	204	PRO
2	B	225	THR
2	B	226	ASN
2	B	240	THR
2	B	260	GLN
2	B	261	VAL
2	B	280	GLU
2	B	288	ASN
2	B	298	GLU
2	B	304	LEU
2	B	308	LEU
2	B	331	ARG
2	B	478	HIS
2	B	493	MET
2	B	506	ILE
2	B	514	THR
2	B	532	GLN
2	B	576	GLU
2	B	605	ARG
2	B	641	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	119	GLN
2	A	136	GLN
2	A	141	GLN
2	A	147	ASN

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Mol	Chain	Res	Type
2	A	157	HIS
2	A	178	GLN
2	A	197	HIS
2	A	205	HIS
2	A	208	GLN
2	A	226	ASN
2	A	227	ASN
2	A	251	GLN
2	A	265	GLN
2	A	269	ASN
2	A	288	ASN
2	A	357	ASN
2	A	359	GLN
2	A	434	GLN
2	A	508	ASN
2	A	583	GLN
2	B	41	HIS
2	B	51	ASN
2	B	119	GLN
2	B	147	ASN
2	B	158	HIS
2	B	178	GLN
2	B	202	ASN
2	B	208	GLN
2	B	226	ASN
2	B	227	ASN
2	B	260	GLN
2	B	265	GLN
2	B	288	ASN
2	B	359	GLN
2	B	369	GLN
2	B	402	ASN
2	B	459	GLN
2	B	508	ASN
2	B	518	GLN
2	B	555	GLN
2	B	560	HIS
2	B	608	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	3.50	13 (39%)	45,52,52	2.16	16 (35%)
4	ANP	B	701	3	33,33,33	3.52	15 (45%)	45,52,52	2.14	14 (31%)

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	-	3/18/38/38	0/3/3/3
4	ANP	B	701	3	-	3/18/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	ANP	PG-O1G	14.75	1.68	1.46
4	B	701	ANP	PG-O1G	14.66	1.68	1.46
4	A	700	ANP	C5-C4	5.96	1.49	1.39
4	B	701	ANP	C5-C4	5.85	1.49	1.39
4	B	701	ANP	PG-O3G	-4.63	1.44	1.56
4	A	700	ANP	C5-N7	-4.31	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ANP	C5-N7	-4.17	1.31	1.39
4	A	700	ANP	PG-O3G	-3.94	1.46	1.56
4	A	700	ANP	PB-O2B	-3.75	1.46	1.56
4	B	701	ANP	C5-C6	3.67	1.51	1.41
4	A	700	ANP	C4-N9	-3.65	1.30	1.37
4	B	701	ANP	PB-O2B	-3.62	1.47	1.56
4	A	700	ANP	C4-N3	3.60	1.41	1.34
4	B	701	ANP	C4-N3	3.54	1.41	1.34
4	A	700	ANP	C5-C6	3.52	1.50	1.41
4	B	701	ANP	C2-N3	3.50	1.40	1.33
4	B	701	ANP	C4-N9	-3.33	1.30	1.37
4	A	700	ANP	C2-N3	2.91	1.39	1.33
4	B	701	ANP	PB-N3B	2.74	1.70	1.63
4	B	701	ANP	C2-N1	2.64	1.38	1.33
4	A	700	ANP	C2-N1	2.52	1.38	1.33
4	B	701	ANP	C2'-C1'	-2.43	1.45	1.53
4	A	700	ANP	C2'-C1'	-2.38	1.46	1.53
4	B	701	ANP	PA-O2A	-2.33	1.44	1.55
4	A	700	ANP	PA-O2A	-2.33	1.44	1.55
4	B	701	ANP	C6-N1	2.14	1.41	1.35
4	A	700	ANP	C6-N1	2.13	1.41	1.35
4	B	701	ANP	O4'-C4'	-2.12	1.40	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	ANP	C5-C4-N3	-5.07	119.73	126.72
4	A	700	ANP	C5-C4-N3	-4.86	120.02	126.72
4	B	701	ANP	N3-C4-N9	4.86	135.43	127.17
4	A	700	ANP	O2B-PB-O1B	4.82	120.20	109.87
4	B	701	ANP	O2B-PB-O1B	4.63	119.81	109.87
4	A	700	ANP	N3-C2-N1	-4.60	121.61	128.58
4	A	700	ANP	N3-C4-N9	4.58	134.95	127.17
4	B	701	ANP	N3-C2-N1	-4.44	121.86	128.58
4	B	701	ANP	C2-N3-C4	4.05	121.72	111.83
4	A	700	ANP	C2-N3-C4	4.02	121.64	111.83
4	A	700	ANP	O4'-C1'-N9	-3.22	101.90	108.09
4	B	701	ANP	O4'-C1'-N9	-3.10	102.14	108.09
4	A	700	ANP	C4-N9-C8	3.03	108.92	105.74
4	B	701	ANP	C4-N9-C8	3.01	108.90	105.74
4	B	701	ANP	C4-C5-N7	-2.79	107.39	110.58
4	A	700	ANP	C4-C5-N7	-2.77	107.42	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	ANP	C6-C5-N7	2.63	137.15	132.09
4	B	701	ANP	C2'-C1'-N9	2.62	119.81	113.30
4	A	700	ANP	O1B-PB-N3B	-2.59	107.96	111.77
4	B	701	ANP	C5-N7-C8	2.57	107.49	103.45
4	B	701	ANP	C6-C5-N7	2.53	136.96	132.09
4	A	700	ANP	O2G-PG-O3G	2.47	114.22	107.59
4	B	701	ANP	O2G-PG-O1G	-2.44	107.33	113.45
4	A	700	ANP	C5-N7-C8	2.41	107.23	103.45
4	A	700	ANP	O3'-C3'-C4'	-2.36	104.29	111.08
4	A	700	ANP	C2'-C1'-N9	2.36	119.17	113.30
4	B	701	ANP	O3'-C3'-C4'	-2.32	104.41	111.08
4	B	701	ANP	O2G-PG-O3G	2.21	113.54	107.59
4	A	700	ANP	O2G-PG-O1G	-2.12	108.14	113.45
4	A	700	ANP	C4-N9-C1'	-2.07	121.79	126.63

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	700	ANP	PB-N3B-PG-O1G
4	A	700	ANP	PA-O3A-PB-O2B
4	B	701	ANP	PB-N3B-PG-O1G
4	B	701	ANP	PA-O3A-PB-O2B
4	A	700	ANP	PA-O3A-PB-O1B
4	B	701	ANP	PA-O3A-PB-O1B

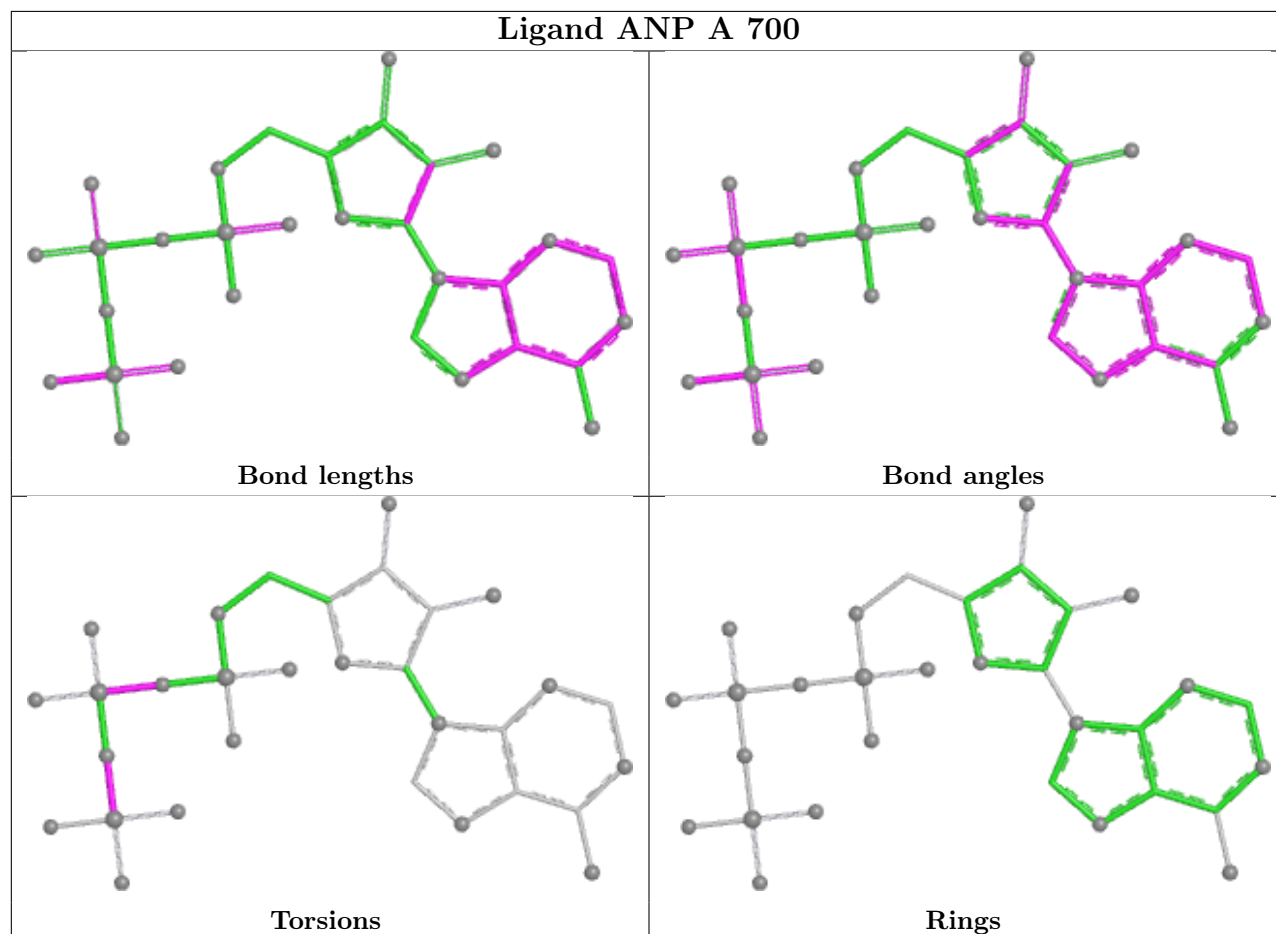
There are no ring outliers.

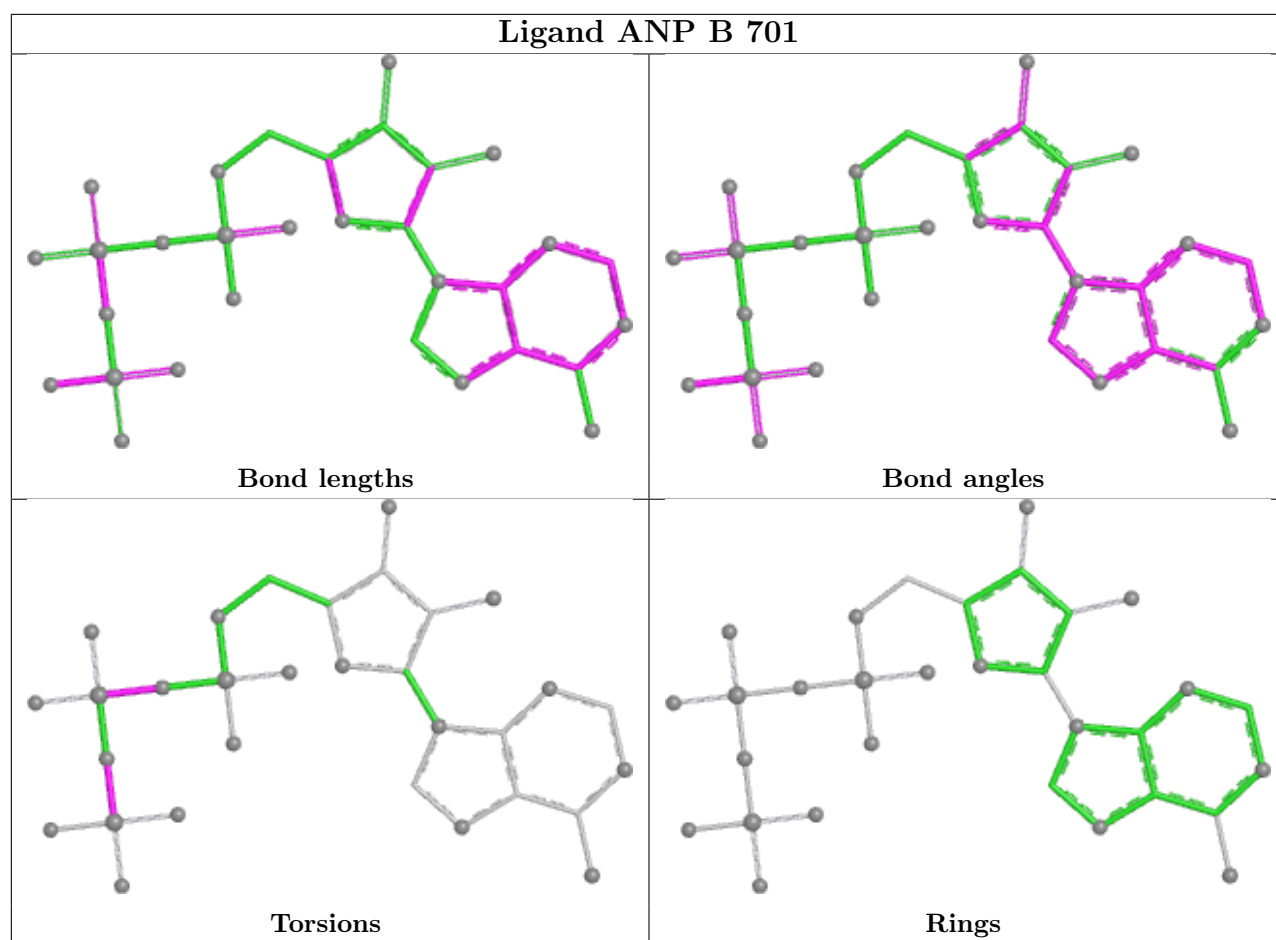
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	ANP	3	0
4	B	701	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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(Å ²)	Q<0.9
1	C	25/26 (96%)	0.85	3 (12%) 9 7	51, 117, 165, 171	0
1	D	25/26 (96%)	0.90	3 (12%) 9 7	59, 117, 150, 153	0
2	A	646/680 (95%)	0.27	29 (4%) 38 32	31, 73, 126, 140	1 (0%)
2	B	632/680 (92%)	0.18	28 (4%) 39 33	36, 68, 122, 179	1 (0%)
All	All	1328/1412 (94%)	0.25	63 (4%) 36 30	31, 72, 126, 179	2 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	163	GLY	5.8
2	A	164	ASN	5.2
2	B	658	ARG	4.8
2	B	535	LEU	4.1
2	A	234	ARG	3.8
2	A	160	GLN	3.7
2	B	304	LEU	3.7
2	B	234	ARG	3.6
2	B	379	GLY	3.6
2	A	134	GLU	3.6
2	B	519	PHE	3.5
2	A	497	GLU	3.5
2	B	537	HIS	3.5
2	A	442	ARG	3.5
2	B	654	VAL	3.5
2	A	499	GLY	3.3
2	B	538	ALA	3.3
2	B	134	GLU	3.3
2	B	528	LEU	3.2
2	A	451	ALA	3.1
2	B	531	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	520	SER	3.1
2	A	544	GLU	3.1
2	A	662	PRO	2.9
2	B	137	TRP	2.9
2	B	481	THR	2.8
2	B	159	ILE	2.8
2	B	651	SER	2.8
2	A	455	ALA	2.8
2	A	437	LEU	2.8
2	A	465	ILE	2.7
2	A	549	THR	2.7
2	B	549	THR	2.7
2	A	1	MET	2.6
2	A	166	VAL	2.6
2	B	650	VAL	2.6
1	C	22	DG	2.6
2	A	80	THR	2.5
2	B	125	ARG	2.5
1	D	2	DC	2.5
2	A	144	TRP	2.4
2	A	435	LEU	2.3
2	B	548	ASP	2.3
2	A	464	LEU	2.3
2	B	657	GLN	2.3
2	B	166	VAL	2.3
2	A	82	GLN	2.2
2	A	506	ILE	2.2
1	D	21	DT	2.2
2	A	551	GLN	2.2
2	A	444	LEU	2.1
1	C	16	DC	2.1
2	B	530	PRO	2.1
2	B	532	GLN	2.1
2	A	529	MET	2.1
2	B	5	TYR	2.1
2	B	458	LEU	2.1
2	A	137	TRP	2.1
2	A	481	THR	2.0
2	A	141	GLN	2.0
1	C	20	DT	2.0
1	D	6	DC	2.0
2	A	377	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

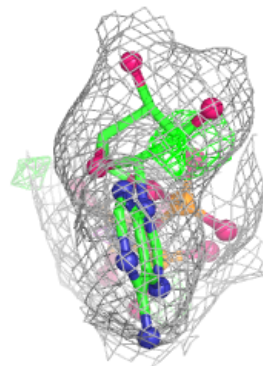
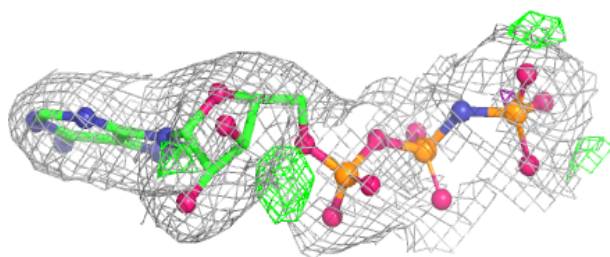
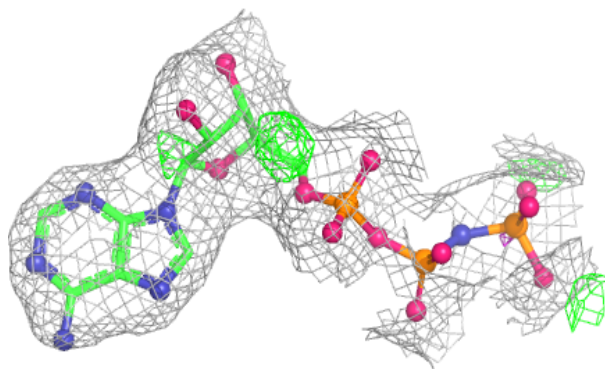
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ANP	A	700	31/31	0.96	0.07	43,48,56,58	0
4	ANP	B	701	31/31	0.97	0.07	45,52,58,61	0
3	MG	A	1001	1/1	1.00	0.02	45,45,45,45	0
3	MG	B	1002	1/1	1.00	0.03	40,40,40,40	0

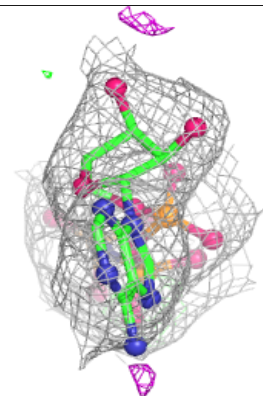
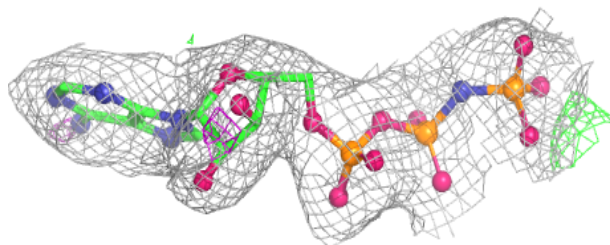
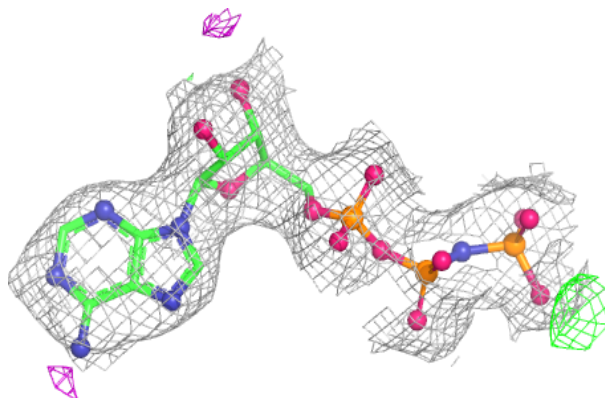
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ANP A 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ANP B 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.