Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 02:50 am BST

PDB ID	:	5IX1
Title	:	Crystal structure of mouse Morc3 ATPase-CW cassette in complex with AMPPNP and H3K4me3 peptide
Authors	:	Li, S.; Du, J.; Patel, D.J.
Deposited on	:	2016-03-23
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.231
Clashscore		26
Ramachandran outliers		0.2%
Sidechain outliers		13.4%
RSRZ outliers		4.4%

Worse → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
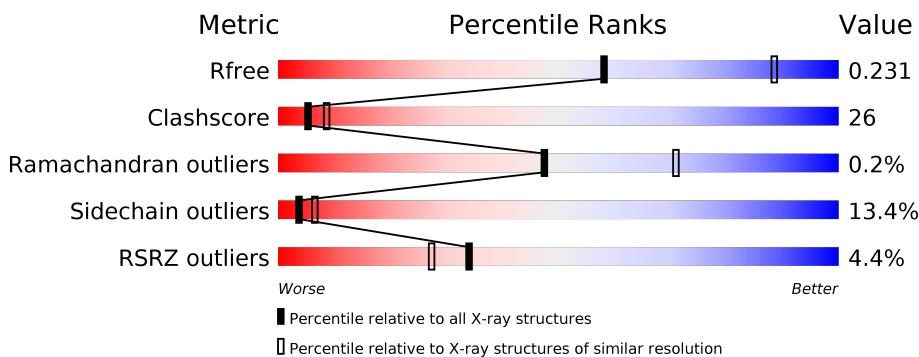
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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 <=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	A	451	5% / 53% / 32% / 7% / 8%
1	B	451	3% / 52% / 33% / 7% · 7%
2	P	15	13% / 33% / 13% / 40%
2	Q	15	7% / 20% / 33% / 13% / 33%
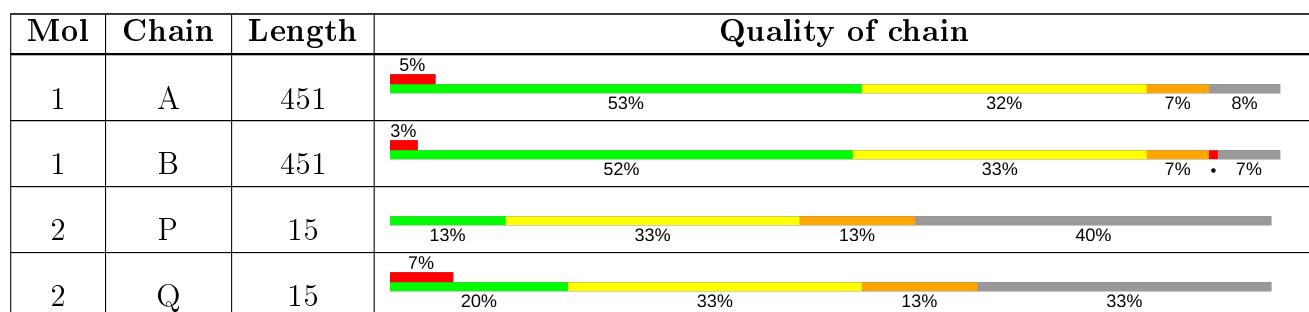
2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7042 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MORC family CW-type zinc finger protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total 3355	C 2139	N 576	O 617	S 23	0	0	0
1	B	419	Total 3396	C 2164	N 587	O 622	S 23	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	SER	-	expression tag	UNP F7BJB9
B	6	SER	-	expression tag	UNP F7BJB9

- Molecule 2 is a protein called Peptide from Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	9	Total 76	C 46	N 18	O 12	0	0	0
2	Q	10	Total 82	C 49	N 19	O 14	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).
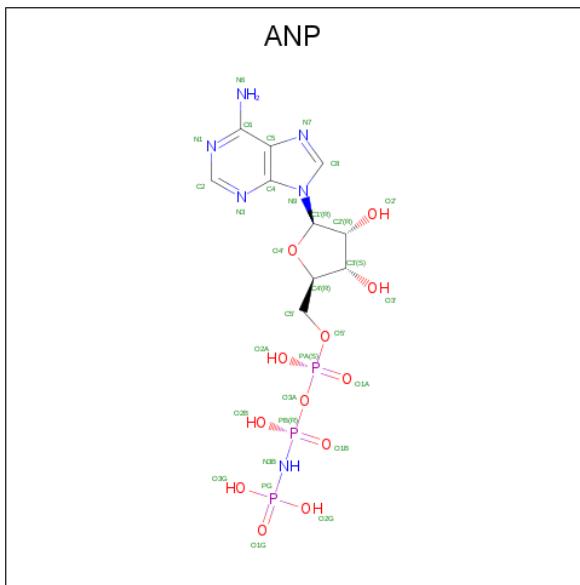
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3		0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3		0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total 43	O 43	0	0
6	B	24	Total 24	O 24	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 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: MORC family CW-type zinc finger protein 3
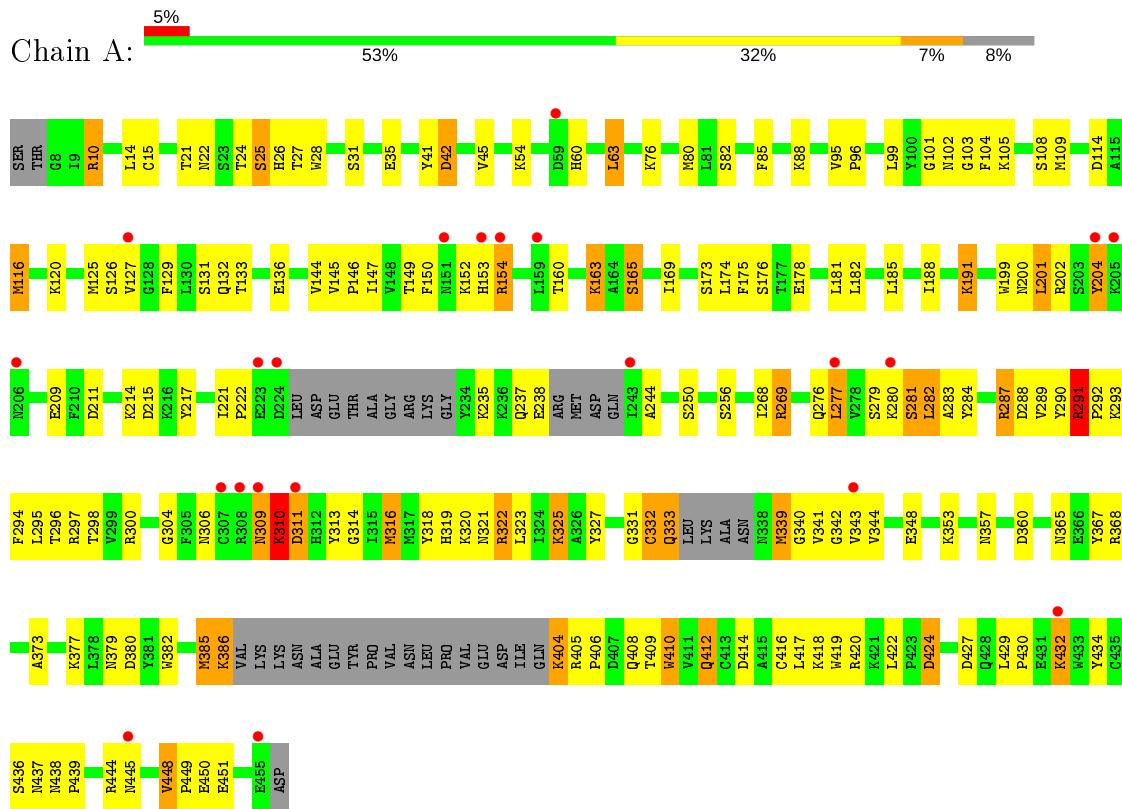
- Molecule 1: MORC family CW-type zinc finger protein 3

• Molecule 2: Peptide from Histone H3.1

Chain P:

• Molecule 2: Peptide from Histone H3.1

Chain Q:
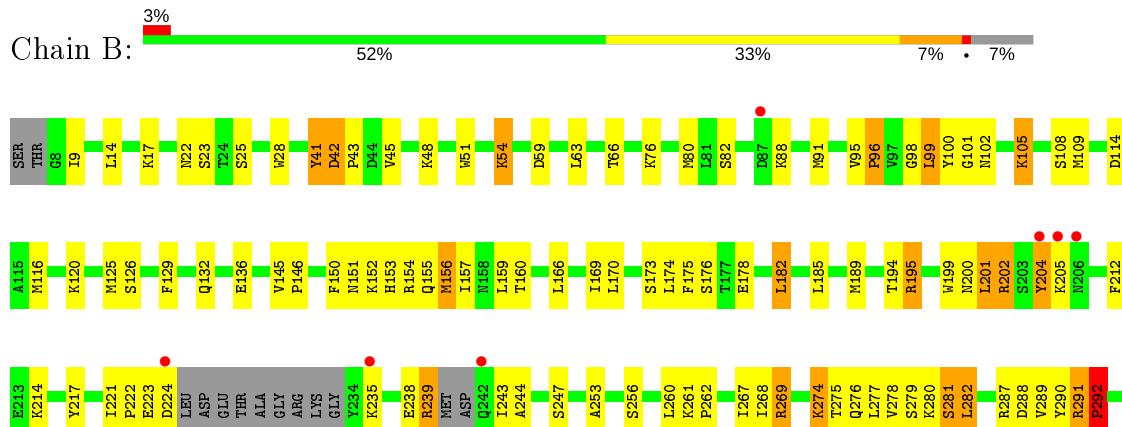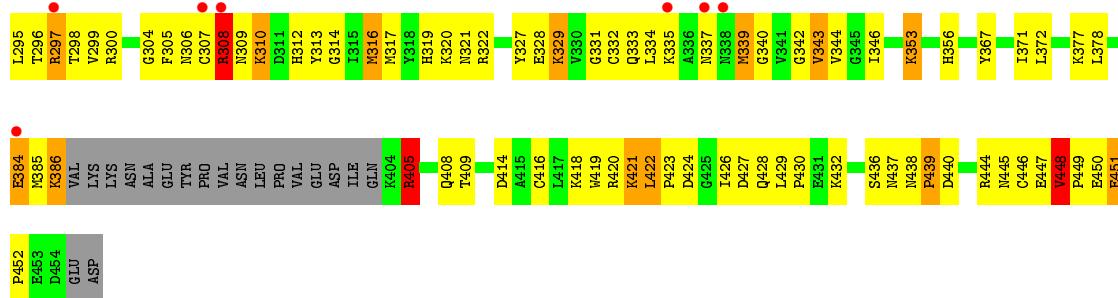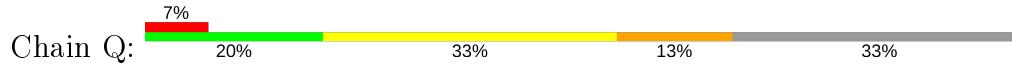
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	111.35Å 149.08Å 173.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.60 19.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.76-2.60) 99.9 (19.76-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.59Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.218 , 0.230 0.227 , 0.231	Depositor DCC
R_{free} test set	2242 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	59.1	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.2	EDS
L-test for twinning[2]	$< |L| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1290e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M3L, ANP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.03	3/3428 (0.1%)	0.78	13/4622 (0.3%)
1	B	1.04	8/3470 (0.2%)	0.78	17/4679 (0.4%)
2	P	0.72	0/63	0.69	0/82
2	Q	0.79	0/69	0.70	0/90
All	All	1.03	11/7030 (0.2%)	0.78	30/9473 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	449	PRO	N-CD	5.45	1.55	1.47
1	A	449	PRO	N-CD	5.44	1.55	1.47
1	B	292	PRO	N-CD	5.21	1.55	1.47
1	B	430	PRO	N-CD	5.18	1.55	1.47
1	B	452	PRO	N-CD	5.13	1.55	1.47
1	A	96	PRO	N-CD	5.06	1.54	1.47
1	A	430	PRO	N-CD	5.05	1.54	1.47
1	B	423	PRO	N-CD	5.04	1.54	1.47
1	B	222	PRO	N-CD	5.03	1.54	1.47
1	B	439	PRO	N-CD	5.03	1.54	1.47
1	B	96	PRO	N-CD	5.01	1.54	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	353	LYS	C-N-CD	6.17	141.36	128.40
1	A	291	ARG	C-N-CD	6.16	141.34	128.40
1	B	353	LYS	C-N-CD	5.94	140.88	128.40
1	B	244	ALA	C-N-CD	5.94	140.87	128.40
1	B	405	ARG	C-N-CD	5.94	140.87	128.40
1	A	15	CYS	C-N-CD	5.85	140.69	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	ARG	N-CA-C	-5.82	95.29	111.00
1	B	261	LYS	C-N-CD	5.79	140.56	128.40
1	B	28	TRP	C-N-CD	5.78	140.55	128.40
1	B	440	ASP	C-N-CD	5.77	140.51	128.40
1	A	244	ALA	C-N-CD	5.76	140.50	128.40
1	B	42	ASP	C-N-CD	5.75	140.47	128.40
1	A	451	GLU	C-N-CD	5.74	140.44	128.40
1	A	438	ASN	C-N-CD	5.73	140.43	128.40
1	A	95	VAL	C-N-CD	5.73	140.43	128.40
1	A	42	ASP	C-N-CD	5.72	140.41	128.40
1	A	429	LEU	C-N-CD	5.71	140.39	128.40
1	B	422	LEU	C-N-CD	5.69	140.35	128.40
1	B	438	ASN	C-N-CD	5.69	140.35	128.40
1	A	221	ILE	C-N-CD	5.68	140.33	128.40
1	B	429	LEU	C-N-CD	5.67	140.30	128.40
1	B	95	VAL	C-N-CD	5.64	140.24	128.40
1	A	145	VAL	C-N-CD	5.62	140.20	128.40
1	B	291	ARG	C-N-CD	5.61	140.19	128.40
1	B	221	ILE	C-N-CD	5.61	140.18	128.40
1	A	28	TRP	C-N-CD	5.58	140.12	128.40
1	B	451	GLU	C-N-CD	5.55	140.06	128.40
1	B	448	VAL	C-N-CD	5.49	139.92	128.40
1	B	145	VAL	C-N-CD	5.39	139.72	128.40
1	A	448	VAL	C-N-CD	5.33	139.59	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3355	0	3335	181	0
1	B	3396	0	3386	178	0
2	P	76	0	92	18	0
2	Q	82	0	97	13	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	31	0	13	5	0
4	B	31	0	13	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	43	0	0	4	0
6	B	24	0	0	8	0
All	All	7042	0	6936	367	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 26.

All (367) 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:B:169:ILE:O	1:B:173:SER:HB3	1.53	1.06
1:B:343:VAL:HG11	1:B:378:LEU:HD11	1.32	1.05
1:B:414:ASP:OD2	1:B:432:LYS:HE2	1.58	1.04
1:B:343:VAL:CG1	1:B:378:LEU:HD11	1.86	1.04
1:A:412:GLN:OE1	2:P:2:ARG:HD3	1.58	1.03
1:A:22:ASN:ND2	1:A:102:ASN:HD21	1.57	1.02
1:A:22:ASN:HD21	1:A:102:ASN:ND2	1.59	0.98
1:B:297:ARG:HH21	1:B:297:ARG:HG3	1.26	0.97
1:B:151:ASN:ND2	1:B:155:GLN:HB2	1.80	0.96
1:B:239:ARG:HH11	1:B:239:ARG:HG2	1.31	0.93
1:B:277:LEU:HD23	1:B:278:VAL:N	1.82	0.93
1:A:322:ARG:HH11	1:A:322:ARG:HG2	1.29	0.93
1:B:310:LYS:HE2	1:B:310:LYS:HA	1.49	0.93
1:A:22:ASN:HD21	1:A:102:ASN:HD21	0.95	0.91
1:B:151:ASN:HD21	1:B:155:GLN:HB2	1.31	0.91
1:B:416:CYS:SG	1:B:418:LYS:HG3	2.11	0.91
1:A:26:HIS:HD2	1:A:31:SER:OG	1.55	0.90
1:A:169:ILE:O	1:A:173:SER:HB3	1.72	0.90
1:B:445:ASN:O	1:B:448:VAL:HG12	1.74	0.88
1:B:178:GLU:O	1:B:182:LEU:HD23	1.74	0.87
1:A:35:GLU:HG3	6:A:604:HOH:O	1.76	0.85
1:B:279:SER:OG	1:B:280:LYS:HD3	1.75	0.85
1:B:169:ILE:O	1:B:173:SER:CB	2.23	0.85
1:B:277:LEU:HD23	1:B:279:SER:H	1.41	0.85
1:A:178:GLU:O	1:A:182:LEU:HD12	1.78	0.84
1:B:419:TRP:CD1	2:Q:4:M3L:HM32	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HD2	1:A:163:LYS:O	1.79	0.82
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.45	0.81
1:B:166:LEU:O	1:B:166:LEU:HD12	1.81	0.81
1:B:98:GLY:HA3	6:B:609:HOH:O	1.78	0.81
1:A:420:ARG:NH2	1:A:448:VAL:HB	1.96	0.81
1:A:445:ASN:HB3	1:A:448:VAL:HG23	1.64	0.80
1:A:290:TYR:CZ	1:A:292:PRO:HG3	2.17	0.80
1:B:277:LEU:CD2	1:B:279:SER:H	1.93	0.80
1:A:310:LYS:HG3	1:A:311:ASP:H	1.48	0.78
1:B:436:SER:HA	1:B:444:ARG:O	1.82	0.78
1:B:385:MET:HE2	1:B:385:MET:HA	1.65	0.78
1:B:343:VAL:HG11	1:B:378:LEU:CD1	2.10	0.78
1:A:419:TRP:CD1	2:P:4:M3L:HM32	2.17	0.78
1:A:291:ARG:HG3	1:A:298:THR:HG22	1.66	0.78
1:A:386:LYS:HD3	1:A:386:LYS:C	2.04	0.77
1:B:308:ARG:O	1:B:310:LYS:HE3	1.85	0.76
1:B:269:ARG:HG3	1:B:269:ARG:HH11	1.48	0.76
1:A:191:LYS:NZ	1:A:191:LYS:H	1.82	0.75
1:A:310:LYS:HD2	1:A:311:ASP:OD2	1.86	0.75
1:B:239:ARG:NH1	1:B:239:ARG:HG2	1.99	0.75
1:A:26:HIS:CD2	1:A:31:SER:OG	2.39	0.75
1:A:202:ARG:HH21	1:A:202:ARG:HG2	1.53	0.74
1:A:269:ARG:HH11	1:A:269:ARG:HG3	1.53	0.73
1:A:277:LEU:HD12	1:A:277:LEU:N	2.03	0.73
1:A:116:MET:CE	1:A:169:ILE:HD13	2.18	0.73
1:B:439:PRO:O	1:B:444:ARG:NH2	2.22	0.73
1:A:116:MET:HE2	1:A:169:ILE:HD13	1.70	0.72
1:A:287:ARG:HG3	1:A:287:ARG:NH1	2.04	0.72
1:A:269:ARG:NH1	1:A:269:ARG:HG3	2.03	0.72
1:A:333:GLN:N	1:A:333:GLN:HE21	1.89	0.71
1:A:169:ILE:O	1:A:173:SER:CB	2.37	0.71
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.55	0.71
1:B:202:ARG:NH1	1:B:202:ARG:HG3	2.00	0.71
1:B:297:ARG:NH2	1:B:297:ARG:HG3	2.01	0.71
1:B:424:ASP:CG	2:Q:8:ARG:HH12	1.94	0.71
1:B:269:ARG:HG3	1:B:269:ARG:NH1	2.04	0.70
1:B:384:GLU:C	1:B:385:MET:HE3	2.11	0.70
1:B:424:ASP:OD2	2:Q:8:ARG:NH1	2.23	0.70
1:A:332:CYS:SG	1:A:379:ASN:OD1	2.49	0.70
1:B:54:LYS:HD2	1:B:54:LYS:C	2.11	0.70
1:A:405:ARG:HH11	2:P:9:LYS:HG3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LYS:HE2	1:B:310:LYS:CA	2.20	0.69
1:B:132:GLN:O	1:B:136:GLU:HG3	1.92	0.69
1:A:420:ARG:HH22	1:A:448:VAL:HB	1.58	0.68
1:A:412:GLN:OE1	2:P:2:ARG:CD	2.39	0.68
1:A:129:PHE:HB3	1:A:146:PRO:HD2	1.74	0.68
1:A:331:GLY:O	1:A:333:GLN:NE2	2.27	0.68
1:B:129:PHE:HB3	1:B:146:PRO:HD2	1.76	0.67
1:A:217:TYR:CZ	2:P:8:ARG:HG2	2.28	0.67
1:B:414:ASP:OD2	1:B:432:LYS:CE	2.40	0.67
1:A:420:ARG:NH1	1:A:448:VAL:O	2.26	0.66
1:A:202:ARG:NH2	6:A:605:HOH:O	2.28	0.66
1:B:419:TRP:CZ3	2:Q:4:M3L:HG2	2.30	0.66
1:A:132:GLN:O	1:A:136:GLU:HG3	1.95	0.66
1:A:408:GLN:HG3	1:A:409:THR:N	2.09	0.66
1:A:404:LYS:N	1:A:404:LYS:HD2	2.11	0.65
1:B:408:GLN:HG3	1:B:409:THR:N	2.11	0.65
1:A:310:LYS:HG3	1:A:311:ASP:OD1	1.97	0.65
1:A:416:CYS:CB	1:A:418:LYS:HG3	2.26	0.65
1:A:147:ILE:N	1:A:165:SER:OG	2.30	0.65
1:B:269:ARG:CG	1:B:269:ARG:HH11	2.10	0.65
1:A:153:HIS:O	1:A:154:ARG:HB2	1.96	0.64
1:A:163:LYS:HD2	1:A:163:LYS:C	2.17	0.64
1:A:25:SER:OG	1:A:357:ASN:HB3	1.98	0.64
1:A:279:SER:O	1:A:280:LYS:HB3	1.95	0.64
1:A:322:ARG:HH11	1:A:322:ARG:CG	2.07	0.63
1:B:310:LYS:HD2	1:B:310:LYS:N	2.13	0.63
1:A:105:LYS:CD	1:A:105:LYS:H	2.10	0.63
1:B:116:MET:CE	1:B:169:ILE:HG23	2.27	0.63
1:B:88:LYS:HB2	6:B:611:HOH:O	1.97	0.63
1:A:82:SER:O	1:A:105:LYS:CE	2.47	0.63
1:A:290:TYR:CE2	1:A:292:PRO:HG3	2.34	0.63
1:A:310:LYS:HD2	1:A:311:ASP:CG	2.20	0.62
1:B:419:TRP:CE3	2:Q:4:M3L:HG2	2.34	0.62
1:B:151:ASN:HD21	1:B:155:GLN:CB	2.10	0.62
1:B:66:THR:OG1	1:B:195:ARG:HD2	1.99	0.62
1:B:277:LEU:C	1:B:277:LEU:HD23	2.19	0.62
1:B:202:ARG:CD	6:B:613:HOH:O	2.46	0.62
1:B:307:CYS:O	1:B:308:ARG:HB2	2.00	0.62
1:A:341:VAL:O	1:A:343:VAL:HG23	1.99	0.62
1:A:10:ARG:HG2	1:A:10:ARG:NH2	2.14	0.62
1:B:277:LEU:HD23	1:B:279:SER:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:CD1	1:A:201:LEU:HD21	2.30	0.61
1:A:45:VAL:HG22	4:A:502:ANP:C2	2.30	0.61
1:B:202:ARG:HH11	1:B:202:ARG:CG	2.11	0.61
1:B:99:LEU:HD23	1:B:99:LEU:H	1.64	0.61
1:B:343:VAL:CG1	1:B:378:LEU:CD1	2.69	0.61
1:A:416:CYS:HB2	1:A:418:LYS:H	1.65	0.61
1:A:238:GLU:O	1:A:238:GLU:HG2	1.98	0.61
1:B:340:GLY:O	1:B:343:VAL:HB	2.01	0.61
1:A:202:ARG:NH1	6:A:607:HOH:O	2.34	0.61
1:B:418:LYS:HE3	1:B:446:CYS:O	2.00	0.61
1:A:373:ALA:HB1	1:A:377:LYS:NZ	2.16	0.60
1:B:385:MET:O	1:B:386:LYS:HD3	2.01	0.60
1:B:98:GLY:CA	6:B:609:HOH:O	2.44	0.60
2:P:9:LYS:HD3	2:P:9:LYS:O	2.01	0.60
1:B:319:HIS:NE2	1:B:320:LYS:HD2	2.17	0.60
1:B:445:ASN:O	1:B:448:VAL:CG1	2.49	0.60
1:A:310:LYS:HG3	1:A:311:ASP:N	2.14	0.60
1:A:287:ARG:CG	1:A:287:ARG:HH11	2.14	0.59
1:B:82:SER:O	1:B:105:LYS:HE2	2.02	0.59
1:B:22:ASN:ND2	1:B:102:ASN:OD1	2.30	0.59
1:A:322:ARG:NH1	1:A:322:ARG:HG2	2.10	0.59
1:B:385:MET:CE	1:B:385:MET:HA	2.33	0.59
1:A:416:CYS:O	1:A:417:LEU:HB2	2.01	0.59
1:A:269:ARG:CG	1:A:269:ARG:HH11	2.14	0.59
1:B:116:MET:HE1	1:B:169:ILE:HG23	1.84	0.59
1:B:419:TRP:CG	2:Q:4:M3L:HM32	2.37	0.58
1:A:319:HIS:NE2	1:A:320:LYS:HD2	2.18	0.58
1:A:202:ARG:CG	1:A:202:ARG:HH21	2.16	0.58
1:A:152:LYS:HG3	1:A:153:HIS:CE1	2.39	0.58
1:B:308:ARG:HH11	1:B:308:ARG:CG	2.16	0.58
1:A:120:LYS:NZ	1:A:188:ILE:O	2.34	0.58
1:A:211:ASP:HB2	1:A:222:PRO:HG3	1.86	0.58
1:B:367:TYR:O	1:B:371:ILE:HG12	2.03	0.58
1:B:310:LYS:HD2	1:B:310:LYS:H	1.67	0.57
1:B:343:VAL:HG12	1:B:378:LEU:HD11	1.79	0.57
1:A:82:SER:O	1:A:105:LYS:HE3	2.04	0.57
1:A:10:ARG:HH21	1:A:10:ARG:CG	2.17	0.57
1:B:108:SER:OG	1:B:109:MET:N	2.34	0.57
1:B:152:LYS:NZ	1:B:153:HIS:CE1	2.73	0.57
1:A:282:LEU:HD12	1:A:306:ASN:HA	1.86	0.57
1:A:405:ARG:HH11	2:P:9:LYS:CG	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:PRO:O	1:A:444:ARG:NH2	2.38	0.56
1:B:313:TYR:O	1:B:329:LYS:HE3	2.04	0.56
1:B:125:MET:HG3	1:B:150:PHE:HB2	1.87	0.56
1:B:277:LEU:O	1:B:281:SER:HB2	2.05	0.56
1:A:191:LYS:HZ2	1:A:191:LYS:H	1.52	0.56
1:A:80:MET:HB2	4:A:502:ANP:O4'	2.06	0.56
1:A:325:LYS:NZ	1:A:367:TYR:OH	2.33	0.56
1:B:308:ARG:HG2	1:B:308:ARG:NH1	2.21	0.55
1:A:406:PRO:O	2:P:8:ARG:HD2	2.05	0.55
1:B:223:GLU:HG3	1:B:224:ASP:N	2.21	0.55
1:A:175:PHE:CB	1:A:181:LEU:HD23	2.37	0.55
1:A:105:LYS:HD3	1:A:105:LYS:H	1.71	0.55
1:B:152:LYS:HZ1	1:B:153:HIS:CE1	2.25	0.55
1:B:23:SER:HA	6:B:602:HOH:O	2.05	0.55
1:B:45:VAL:HG22	4:B:502:ANP:C2	2.37	0.55
1:A:63:LEU:HD13	1:A:201:LEU:HD21	1.88	0.55
1:B:99:LEU:HD23	1:B:100:TYR:H	1.70	0.55
1:B:314:GLY:O	1:B:344:VAL:HA	2.07	0.55
1:B:105:LYS:NZ	4:B:502:ANP:O1A	2.40	0.55
1:A:313:TYR:HB2	1:A:343:VAL:O	2.06	0.55
1:A:45:VAL:CG2	4:A:502:ANP:C2	2.85	0.55
1:B:337:ASN:OD1	1:B:337:ASN:N	2.37	0.54
1:B:343:VAL:O	1:B:343:VAL:HG12	2.07	0.54
1:B:385:MET:CE	1:B:385:MET:CA	2.86	0.54
2:P:6:THR:HG22	2:P:7:ALA:N	2.20	0.54
1:A:414:ASP:OD2	1:A:432:LYS:HB3	2.08	0.54
1:A:108:SER:OG	1:A:109:MET:N	2.41	0.54
1:B:262:PRO:HG2	1:B:275:THR:HG21	1.90	0.54
1:A:10:ARG:HH21	1:A:10:ARG:HG2	1.74	0.53
1:A:26:HIS:HD2	1:A:31:SER:CB	2.20	0.53
1:B:287:ARG:NH2	1:B:300:ARG:HB3	2.24	0.53
1:B:175:PHE:CD2	1:B:175:PHE:N	2.76	0.53
1:B:42:ASP:CB	1:B:88:LYS:NZ	2.72	0.53
1:A:325:LYS:HE3	1:A:360:ASP:OD1	2.09	0.53
1:A:280:LYS:HG3	1:A:280:LYS:O	2.08	0.53
1:A:382:TRP:O	1:A:386:LYS:HD2	2.09	0.53
1:A:416:CYS:HB3	1:A:418:LYS:HG3	1.90	0.53
1:A:420:ARG:NH2	1:A:448:VAL:O	2.41	0.53
2:Q:6:THR:CG2	2:Q:7:ALA:N	2.72	0.53
1:B:260:LEU:HB3	1:B:321:ASN:OD1	2.09	0.52
1:B:51:TRP:NE1	1:B:267:ILE:HD13	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:N	1:A:410:TRP:CD1	2.77	0.52
1:A:199:TRP:O	1:A:200:ASN:HB2	2.09	0.52
1:A:114:ASP:OD1	1:A:133:THR:HB	2.10	0.52
1:B:108:SER:OG	1:B:109:MET:HG2	2.08	0.52
1:A:310:LYS:CG	1:A:311:ASP:N	2.73	0.52
1:B:101:GLY:H	4:B:502:ANP:HNB1	1.58	0.52
1:B:80:MET:HG3	4:B:502:ANP:O4'	2.10	0.52
1:A:105:LYS:N	1:A:105:LYS:CD	2.73	0.52
1:A:333:GLN:NE2	1:A:333:GLN:CA	2.73	0.52
1:B:182:LEU:N	1:B:182:LEU:CD2	2.73	0.52
1:B:239:ARG:HH21	1:B:327:TYR:HD2	1.57	0.52
1:B:99:LEU:CD2	1:B:99:LEU:N	2.73	0.52
1:A:191:LYS:HZ3	1:A:191:LYS:H	1.54	0.52
1:A:282:LEU:HG	1:A:304:GLY:HA3	1.91	0.52
1:A:373:ALA:HB1	1:A:377:LYS:HZ3	1.75	0.51
1:A:104:PHE:O	1:A:108:SER:HB3	2.09	0.51
1:A:434:TYR:O	1:A:437:ASN:OD1	2.29	0.51
2:P:6:THR:CG2	2:P:7:ALA:N	2.73	0.51
1:B:421:LYS:HE2	1:B:451:GLU:OE1	2.11	0.51
1:A:10:ARG:CG	1:A:10:ARG:NH2	2.73	0.51
1:A:322:ARG:NH1	1:A:323:LEU:O	2.43	0.51
1:B:310:LYS:CD	1:B:310:LYS:N	2.73	0.51
1:A:341:VAL:C	1:A:343:VAL:HG23	2.30	0.50
1:A:125:MET:HG3	1:A:150:PHE:HB2	1.94	0.50
1:A:215:ASP:OD2	1:A:217:TYR:N	2.39	0.50
1:A:288:ASP:OD1	1:A:289:VAL:N	2.44	0.50
1:A:316:MET:HE3	1:A:327:TYR:H	1.76	0.50
1:B:99:LEU:HD23	1:B:100:TYR:N	2.26	0.50
1:B:308:ARG:NH1	1:B:308:ARG:CG	2.73	0.50
1:B:42:ASP:HB3	1:B:88:LYS:HZ3	1.77	0.50
1:B:424:ASP:CG	2:Q:8:ARG:NH1	2.60	0.50
1:A:22:ASN:HD21	1:A:102:ASN:CG	2.10	0.50
1:B:289:VAL:O	1:B:377:LYS:HE3	2.12	0.49
1:A:144:VAL:HG22	1:B:9:ILE:HG22	1.94	0.49
1:A:283:ALA:O	1:A:284:TYR:HB2	2.12	0.49
1:A:416:CYS:HB2	1:A:418:LYS:HG3	1.93	0.49
1:B:25:SER:HB3	1:B:356:HIS:ND1	2.27	0.49
1:B:331:GLY:O	1:B:334:LEU:N	2.41	0.49
1:A:101:GLY:H	4:A:502:ANP:HNB1	1.60	0.49
1:B:41:TYR:C	1:B:41:TYR:CD2	2.86	0.49
1:B:419:TRP:CZ3	2:Q:4:M3L:CG	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:TYR:O	1:B:205:LYS:HB2	2.13	0.49
1:A:309:ASN:O	1:A:310:LYS:HB3	2.13	0.48
1:A:339:MET:HG3	1:A:382:TRP:CZ3	2.48	0.48
1:B:445:ASN:OD1	1:B:448:VAL:HG12	2.13	0.48
2:P:6:THR:HG22	2:P:7:ALA:O	2.13	0.48
1:B:290:TYR:HB3	1:B:299:VAL:HB	1.95	0.48
1:A:41:TYR:C	1:A:41:TYR:CD2	2.86	0.48
1:A:14:LEU:HG	1:B:14:LEU:HD11	1.96	0.48
1:B:99:LEU:CD2	1:B:99:LEU:H	2.26	0.48
1:A:217:TYR:OH	2:P:8:ARG:HG2	2.13	0.48
1:B:189:MET:HE1	1:B:426:ILE:HG23	1.95	0.48
1:A:237:GLN:O	1:A:238:GLU:HB3	2.13	0.48
1:A:420:ARG:HH22	1:A:448:VAL:CB	2.26	0.47
1:A:269:ARG:HA	1:A:269:ARG:HD2	1.64	0.47
1:A:293:LYS:HG2	1:A:294:PHE:N	2.28	0.47
1:A:341:VAL:HG22	1:A:342:GLY:N	2.28	0.47
1:B:277:LEU:HB3	1:B:280:LYS:HG2	1.97	0.47
1:B:99:LEU:HD23	1:B:99:LEU:N	2.26	0.47
1:A:277:LEU:HD12	1:A:277:LEU:H	1.79	0.47
1:A:277:LEU:O	1:A:281:SER:HB2	2.13	0.47
1:A:175:PHE:HB2	1:A:181:LEU:HD23	1.96	0.47
1:B:282:LEU:HG	1:B:304:GLY:HA3	1.96	0.47
1:A:316:MET:HE2	1:A:327:TYR:CE1	2.50	0.47
1:B:332:CYS:SG	1:B:339:MET:HB3	2.54	0.47
1:A:116:MET:HE1	1:A:169:ILE:HD13	1.97	0.47
1:A:427:ASP:N	1:A:427:ASP:OD1	2.46	0.47
1:A:114:ASP:OD1	1:A:131:SER:OG	2.29	0.46
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.81	0.46
1:B:420:ARG:NH2	1:B:448:VAL:HG13	2.30	0.46
1:B:331:GLY:O	1:B:332:CYS:C	2.51	0.46
1:B:277:LEU:CD2	1:B:279:SER:N	2.73	0.46
1:A:404:LYS:CD	1:A:404:LYS:N	2.73	0.46
1:A:412:GLN:OE1	2:P:2:ARG:CB	2.64	0.46
1:A:408:GLN:NE2	1:A:422:LEU:O	2.48	0.46
1:A:292:PRO:HD2	1:A:295:LEU:HB2	1.97	0.46
1:A:202:ARG:CG	1:A:202:ARG:NH2	2.73	0.46
1:B:166:LEU:C	1:B:166:LEU:HD12	2.32	0.46
1:B:385:MET:HE3	1:B:385:MET:N	2.31	0.46
1:A:165:SER:O	1:A:169:ILE:HG13	2.16	0.46
2:Q:9:LYS:HD3	2:Q:10:SER:C	2.36	0.46
1:A:21:THR:O	1:A:24:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:O	2:P:3:THR:HA	2.16	0.46
1:B:174:LEU:HA	1:B:174:LEU:HD12	1.81	0.46
1:A:333:GLN:NE2	1:A:333:GLN:N	2.60	0.45
1:A:385:MET:CE	1:A:385:MET:CA	2.95	0.45
1:B:331:GLY:O	1:B:333:GLN:N	2.49	0.45
1:A:149:THR:HG22	1:A:150:PHE:N	2.31	0.45
1:A:340:GLY:HA2	1:A:382:TRP:CE2	2.51	0.45
1:A:108:SER:OG	1:A:109:MET:HG2	2.16	0.45
1:B:48:LYS:HD3	1:B:48:LYS:HA	1.72	0.45
1:B:42:ASP:CB	1:B:88:LYS:HZ3	2.29	0.45
1:A:424:ASP:OD1	1:A:424:ASP:N	2.50	0.45
1:A:27:THR:N	6:A:603:HOH:O	2.26	0.45
1:B:310:LYS:CA	1:B:310:LYS:CE	2.87	0.45
1:A:204:TYR:O	1:A:204:TYR:CD1	2.70	0.45
1:A:60:HIS:ND1	1:A:174:LEU:HD11	2.32	0.44
1:B:202:ARG:HD3	6:B:613:HOH:O	2.15	0.44
1:B:54:LYS:HG3	1:B:212:PHE:CD1	2.51	0.44
1:B:416:CYS:HB3	1:B:446:CYS:HB3	2.00	0.44
1:A:318:TYR:O	1:A:348:GLU:HA	2.16	0.44
1:B:204:TYR:O	1:B:204:TYR:CD2	2.70	0.44
1:A:419:TRP:CG	2:P:4:M3L:HM32	2.51	0.44
1:A:290:TYR:CE1	1:A:292:PRO:HG3	2.50	0.44
1:B:288:ASP:OD1	1:B:289:VAL:N	2.49	0.44
1:B:76:LYS:HG3	6:B:608:HOH:O	2.16	0.44
1:B:269:ARG:HD2	1:B:269:ARG:HA	1.72	0.44
2:Q:9:LYS:CD	2:Q:9:LYS:C	2.86	0.44
1:A:173:SER:OG	1:A:174:LEU:N	2.51	0.44
1:B:317:MET:CE	1:B:328:GLU:HG2	2.47	0.44
1:B:427:ASP:OD1	1:B:427:ASP:N	2.50	0.44
2:P:8:ARG:O	2:P:9:LYS:HB2	2.17	0.44
2:Q:4:M3L:O	2:Q:5:GLN:HG2	2.18	0.44
1:B:156:MET:C	1:B:157:ILE:CG2	2.86	0.44
1:B:316:MET:HG3	1:B:346:ILE:HG13	1.99	0.43
1:B:173:SER:OG	1:B:175:PHE:HD2	2.02	0.43
1:A:287:ARG:NH2	1:A:300:ARG:HB3	2.33	0.43
1:A:116:MET:HE2	1:A:127:VAL:CG1	2.48	0.43
1:B:274:LYS:HB2	1:B:274:LYS:HE3	1.56	0.43
1:B:239:ARG:HD3	1:B:239:ARG:HA	1.70	0.43
1:A:125:MET:HE2	1:A:125:MET:HB3	1.90	0.43
1:B:151:ASN:CG	1:B:155:GLN:HB2	2.37	0.43
1:B:291:ARG:HG3	1:B:298:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLY:O	1:A:344:VAL:HA	2.19	0.42
1:A:322:ARG:CG	1:A:322:ARG:NH1	2.73	0.42
1:B:116:MET:HE3	1:B:169:ILE:HG23	2.00	0.42
1:A:116:MET:CE	1:A:127:VAL:HG12	2.50	0.42
1:A:82:SER:HB3	1:A:85:PHE:CE2	2.53	0.42
1:B:306:ASN:N	1:B:342:GLY:O	2.43	0.42
1:A:293:LYS:CG	1:A:294:PHE:N	2.83	0.42
2:Q:6:THR:HG22	2:Q:7:ALA:N	2.33	0.42
1:B:156:MET:C	1:B:157:ILE:HG23	2.39	0.42
1:B:17:LYS:HE3	1:B:17:LYS:HB2	1.68	0.42
1:B:319:HIS:CD2	1:B:320:LYS:HD2	2.55	0.42
1:A:320:LYS:O	1:A:321:ASN:HB3	2.20	0.42
1:B:416:CYS:SG	1:B:418:LYS:CG	2.97	0.42
2:P:4:M3L:HD2	2:P:4:M3L:HM33	1.78	0.42
1:B:420:ARG:NH2	1:B:448:VAL:O	2.43	0.41
1:A:146:PRO:HA	1:B:9:ILE:HG23	2.01	0.41
1:A:292:PRO:HB3	1:A:294:PHE:CE2	2.54	0.41
1:B:297:ARG:NH2	1:B:297:ARG:CG	2.73	0.41
1:B:306:ASN:ND2	1:B:312:HIS:O	2.45	0.41
1:B:54:LYS:CD	1:B:54:LYS:C	2.85	0.41
1:A:268:ILE:O	1:A:269:ARG:HB2	2.20	0.41
1:B:217:TYR:HD2	1:B:405:ARG:NH1	2.18	0.41
1:A:310:LYS:CD	1:A:311:ASP:CG	2.87	0.41
1:A:365:ASN:HA	1:A:368:ARG:NH1	2.35	0.41
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.84	0.41
1:B:253:ALA:O	1:B:256:SER:OG	2.27	0.41
1:B:419:TRP:HB2	1:B:450:GLU:OE1	2.21	0.41
1:A:209:GLU:O	1:A:222:PRO:HD3	2.21	0.41
1:A:333:GLN:HA	1:A:333:GLN:NE2	2.35	0.41
1:B:80:MET:O	1:B:105:LYS:HE3	2.20	0.41
1:B:63:LEU:HG	1:B:201:LEU:HD21	2.01	0.41
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.84	0.41
1:A:35:GLU:HG2	1:A:103:GLY:O	2.20	0.41
1:A:416:CYS:HB2	1:A:418:LYS:CG	2.51	0.41
1:B:307:CYS:SG	1:B:307:CYS:O	2.78	0.41
1:A:42:ASP:OD2	1:A:88:LYS:NZ	2.46	0.41
1:B:182:LEU:N	1:B:182:LEU:HD22	2.36	0.41
1:B:156:MET:O	1:B:157:ILE:HG22	2.21	0.41
1:B:43:PRO:HD2	1:B:96:PRO:HB3	2.02	0.41
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.82	0.40
1:B:268:ILE:O	1:B:269:ARG:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HG22	4:A:502:ANP:H2	2.03	0.40
1:B:194:THR:OG1	6:B:601:HOH:O	2.22	0.40
1:B:199:TRP:O	1:B:200:ASN:HB2	2.21	0.40
1:B:278:VAL:HG13	1:B:282:LEU:HD22	2.04	0.40
1:B:292:PRO:CG	1:B:295:LEU:HD12	2.51	0.40
1:B:384:GLU:C	1:B:385:MET:CE	2.86	0.40
1:A:191:LYS:N	1:A:191:LYS:HZ3	2.17	0.40
1:B:384:GLU:HA	1:B:384:GLU:OE1	2.22	0.40
1:B:120:LYS:HG2	1:B:125:MET:HE2	2.04	0.40
1:B:166:LEU:HD12	1:B:170:LEU:HG	2.02	0.40
1:A:385:MET:HE2	1:A:385:MET:HA	2.04	0.40
1:A:405:ARG:HD3	2:P:8:ARG:HB3	2.04	0.40
1:B:153:HIS:O	1:B:154:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/451 (90%)	393 (97%)	10 (2%)	1 (0%)	47	71
1	B	411/451 (91%)	406 (99%)	4 (1%)	1 (0%)	47	71
2	P	6/15 (40%)	6 (100%)	0	0	100	100
2	Q	7/15 (47%)	7 (100%)	0	0	100	100
All	All	828/932 (89%)	812 (98%)	14 (2%)	2 (0%)	47	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	LYS
1	B	308	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/403 (92%)	324 (87%)	47 (13%)	4	8
1	B	375/403 (93%)	324 (86%)	51 (14%)	3	6
2	P	6/9 (67%)	4 (67%)	2 (33%)	0	0
2	Q	7/9 (78%)	5 (71%)	2 (29%)	0	0
All	All	759/824 (92%)	657 (87%)	102 (13%)	4	6

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	25	SER
1	A	54	LYS
1	A	63	LEU
1	A	76	LYS
1	A	116	MET
1	A	126	SER
1	A	154	ARG
1	A	160	THR
1	A	163	LYS
1	A	165	SER
1	A	176	SER
1	A	191	LYS
1	A	201	LEU
1	A	204	TYR
1	A	214	LYS
1	A	235	LYS
1	A	250	SER
1	A	256	SER
1	A	269	ARG
1	A	276	GLN
1	A	277	LEU
1	A	281	SER
1	A	282	LEU

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Mol	Chain	Res	Type
1	A	287	ARG
1	A	291	ARG
1	A	296	THR
1	A	297	ARG
1	A	309	ASN
1	A	310	LYS
1	A	311	ASP
1	A	316	MET
1	A	322	ARG
1	A	325	LYS
1	A	332	CYS
1	A	333	GLN
1	A	339	MET
1	A	380	ASP
1	A	385	MET
1	A	386	LYS
1	A	404	LYS
1	A	410	TRP
1	A	412	GLN
1	A	424	ASP
1	A	432	LYS
1	A	436	SER
1	A	450	GLU
1	B	41	TYR
1	B	54	LYS
1	B	59	ASP
1	B	91	MET
1	B	99	LEU
1	B	105	LYS
1	B	114	ASP
1	B	126	SER
1	B	156	MET
1	B	159	LEU
1	B	160	THR
1	B	176	SER
1	B	182	LEU
1	B	195	ARG
1	B	201	LEU
1	B	202	ARG
1	B	204	TYR
1	B	214	LYS
1	B	235	LYS

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Mol	Chain	Res	Type
1	B	238	GLU
1	B	239	ARG
1	B	243	ILE
1	B	247	SER
1	B	269	ARG
1	B	274	LYS
1	B	276	GLN
1	B	281	SER
1	B	282	LEU
1	B	292	PRO
1	B	296	THR
1	B	297	ARG
1	B	305	PHE
1	B	308	ARG
1	B	309	ASN
1	B	310	LYS
1	B	316	MET
1	B	322	ARG
1	B	329	LYS
1	B	335	LYS
1	B	339	MET
1	B	343	VAL
1	B	353	LYS
1	B	372	LEU
1	B	384	GLU
1	B	386	LYS
1	B	405	ARG
1	B	421	LYS
1	B	428	GLN
1	B	437	ASN
1	B	447	GLU
1	B	448	VAL
2	P	2	ARG
2	P	9	LYS
2	Q	9	LYS
2	Q	10	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	26	HIS

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Mol	Chain	Res	Type
1	A	237	GLN
1	A	306	ASN
1	A	312	HIS
1	A	333	GLN
1	A	408	GLN
1	B	22	ASN
1	B	102	ASN
1	B	153	HIS
1	B	265	GLN
1	B	408	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#|Z| > 2$
2	M3L	Q	4	2	10,11,12	1.23	0	9,14,16	0.95	1 (11%)
2	M3L	P	4	2	10,11,12	1.23	1 (10%)	9,14,16	0.72	0

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
2	M3L	Q	4	2	-	1/9/10/12	-
2	M3L	P	4	2	-	2/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	4	M3L	CB-CA	-2.05	1.50	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	4	M3L	CD-CG-CB	-2.22	105.77	113.62

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	4	M3L	CG-CD-CE-NZ
2	P	4	M3L	CA-CB-CG-CD
2	Q	4	M3L	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	4	M3L	6	0
2	P	4	M3L	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	B	502	5	29,33,33	1.84	7 (24%)	31,52,52	1.60	8 (25%)
4	ANP	A	502	5	29,33,33	1.91	8 (27%)	31,52,52	2.14	9 (29%)

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	B	502	5	-	5/14/38/38	0/3/3/3
4	ANP	A	502	5	-	5/14/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ANP	PG-O3G	-4.19	1.45	1.56
4	B	502	ANP	PG-O2G	-3.95	1.46	1.56
4	A	502	ANP	PB-O2B	-3.90	1.46	1.56
4	B	502	ANP	PG-O3G	-3.59	1.47	1.56
4	A	502	ANP	PG-O2G	-3.51	1.47	1.56
4	B	502	ANP	PB-O2B	-3.29	1.47	1.56
4	B	502	ANP	PB-N3B	3.24	1.71	1.63
4	A	502	ANP	PB-O3A	-3.23	1.55	1.59
4	A	502	ANP	PB-N3B	3.19	1.71	1.63
4	B	502	ANP	PB-O3A	-2.88	1.55	1.59
4	A	502	ANP	C2'-C1'	-2.84	1.49	1.53
4	A	502	ANP	PG-N3B	2.78	1.70	1.63
4	B	502	ANP	PG-N3B	2.72	1.70	1.63
4	B	502	ANP	C2'-C1'	-2.72	1.49	1.53
4	A	502	ANP	PA-O2A	-2.05	1.45	1.55

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	ANP	O1G-PG-N3B	-5.85	103.16	111.77
4	A	502	ANP	O3G-PG-O2G	3.95	118.15	107.64
4	A	502	ANP	O1B-PB-N3B	-3.93	105.99	111.77
4	A	502	ANP	O2B-PB-O1B	3.54	117.34	109.92
4	A	502	ANP	PA-O3A-PB	-3.46	120.44	132.62
4	B	502	ANP	PA-O3A-PB	-3.29	121.02	132.62
4	A	502	ANP	C3'-C2'-C1'	3.15	105.72	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	502	ANP	O2B-PB-O1B	2.89	115.98	109.92
4	B	502	ANP	C3'-C2'-C1'	2.80	105.20	100.98
4	B	502	ANP	O2B-PB-O3A	2.80	113.98	104.64
4	A	502	ANP	N3-C2-N1	-2.77	124.35	128.68
4	A	502	ANP	C4-C5-N7	-2.70	106.58	109.40
4	B	502	ANP	O1G-PG-N3B	-2.65	107.87	111.77
4	B	502	ANP	C4-C5-N7	-2.64	106.65	109.40
4	B	502	ANP	N3-C2-N1	-2.63	124.57	128.68
4	B	502	ANP	O3G-PG-O2G	2.22	113.54	107.64
4	A	502	ANP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	ANP	PB-N3B-PG-O1G
4	B	502	ANP	PA-O3A-PB-O1B
4	B	502	ANP	PA-O3A-PB-O2B
4	A	502	ANP	PG-N3B-PB-O1B
4	A	502	ANP	PA-O3A-PB-O1B
4	A	502	ANP	PA-O3A-PB-O2B
4	A	502	ANP	O4'-C4'-C5'-O5'
4	A	502	ANP	C3'-C4'-C5'-O5'
4	B	502	ANP	C3'-C4'-C5'-O5'
4	B	502	ANP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	ANP	4	0
4	A	502	ANP	5	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 then 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.

Ligand ANP B 502

Bond lengths   Bond angles

Torsions   Rings

Ligand ANP A 502

Bond lengths

Bond angles

Torsions

Rings
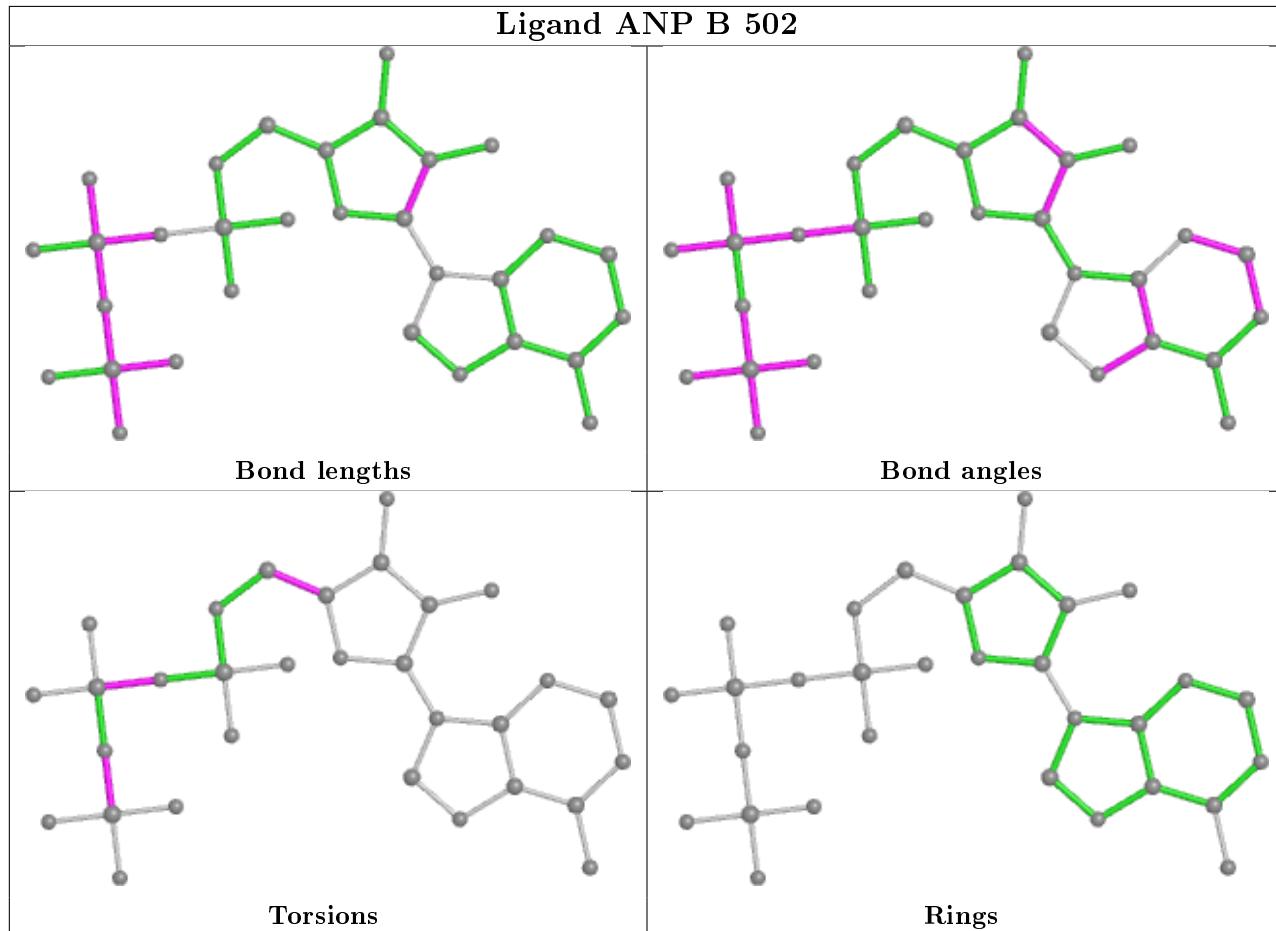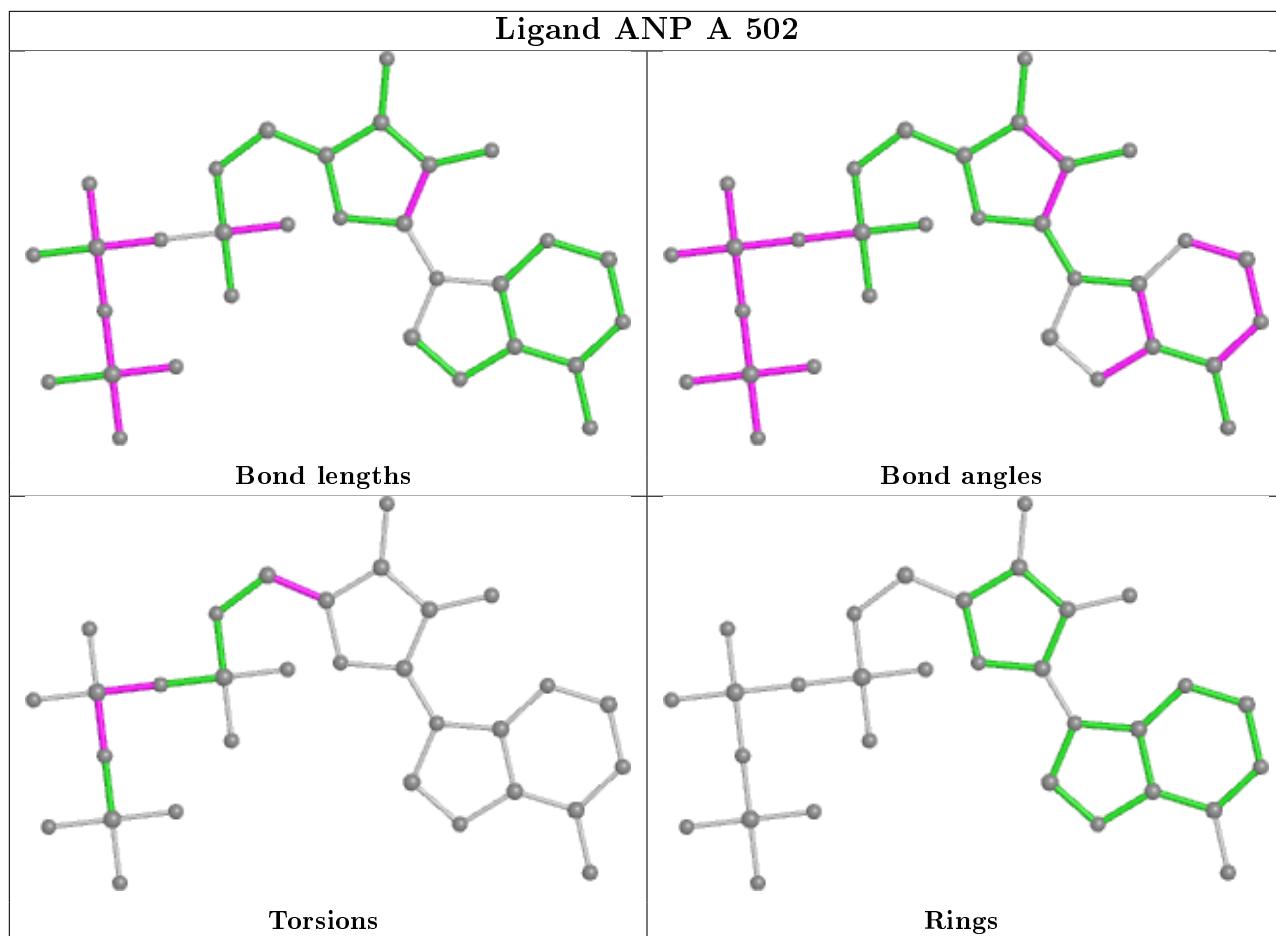
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	A	414/451 (91%)	0.04	22 (5%)	26	20	51, 73, 102, 120	0
1	B	419/451 (92%)	-0.01	14 (3%)	46	39	51, 73, 103, 131	0
2	P	8/15 (53%)	-0.29	0	100	100	80, 91, 96, 102	0
2	Q	9/15 (60%)	0.27	1 (11%)	5	3	88, 91, 103, 105	0
All	All	850/932 (91%)	0.02	37 (4%)	34	27	51, 74, 103, 131	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	ASN	5.8
1	A	308	ARG	5.2
1	B	206	ASN	5.0
1	A	204	TYR	4.7
1	B	204	TYR	4.2
1	A	243	ILE	4.1
1	B	205	LYS	3.9
1	A	223	GLU	3.5
1	B	308	ARG	3.4
1	A	206	ASN	3.3
1	A	159	LEU	3.3
1	A	205	LYS	3.2
1	A	309	ASN	3.2
1	A	311	ASP	3.1
1	B	335	LYS	3.1
1	A	224	ASP	3.1
1	B	338	ASN	3.1
1	A	127	VAL	3.0
1	B	384	GLU	3.0
1	B	307	CYS	2.9
1	A	307	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	297	ARG	2.8
1	A	343	VAL	2.7
1	B	235	LYS	2.7
1	A	280	LYS	2.6
1	B	242	GLN	2.5
1	A	277	LEU	2.5
1	A	154	ARG	2.4
1	A	445	ASN	2.4
1	A	455	GLU	2.3
1	A	153	HIS	2.3
1	A	151	ASN	2.3
1	A	59	ASP	2.3
1	A	432	LYS	2.2
1	B	224	ASP	2.2
1	B	87	ASP	2.1
2	Q	10	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
2	M3L	Q	4	12/13	0.94	0.18	88,92,98,99	0
2	M3L	P	4	12/13	0.95	0.16	84,88,91,92	0

## 6.3 Carbohydrates (i)

There are no carbohydrates 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(Å^2)	Q<0.9
4	ANP	A	502	31/31	0.90	0.20	49,66,111,112	0
5	MG	A	503	1/1	0.92	0.10	60,60,60,60	0
5	MG	B	503	1/1	0.93	0.16	57,57,57,57	0
3	ZN	B	501	1/1	0.94	0.12	87,87,87,87	0
4	ANP	B	502	31/31	0.96	0.17	44,58,68,69	0
3	ZN	A	501	1/1	0.97	0.17	97,97,97,97	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 502:

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

Electron density around ANP B 502:

$2mF_o$-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 (i)

There are no such residues in this entry.