



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:04 PM UTC

PDB ID : 5IX2 / pdb_00005ix2
Title : Crystal structure of mouse Morc3 ATPase-CW cassette in complex with
AMPPNP and unmodified H3 peptide
Authors : Li, S.; Du, J.; Patel, D.J.
Deposited on : 2016-03-23
Resolution : 2.90 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

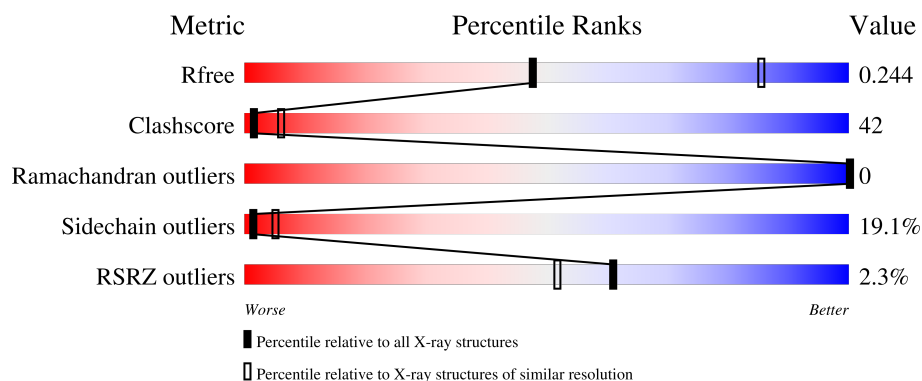
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	A	451	2% 39% 39% 16% 7%
1	B	451	2% 42% 39% 11% 6%
2	P	32	9% 19% 69%
2	Q	32	3% 12% 9% 9% 69%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ANP	A	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7049 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	420	Total	C	N	O	S	0	0	0
			3404	2169	588	624	23			
1	B	422	Total	C	N	O	S	0	0	0
			3421	2181	592	625	23			

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

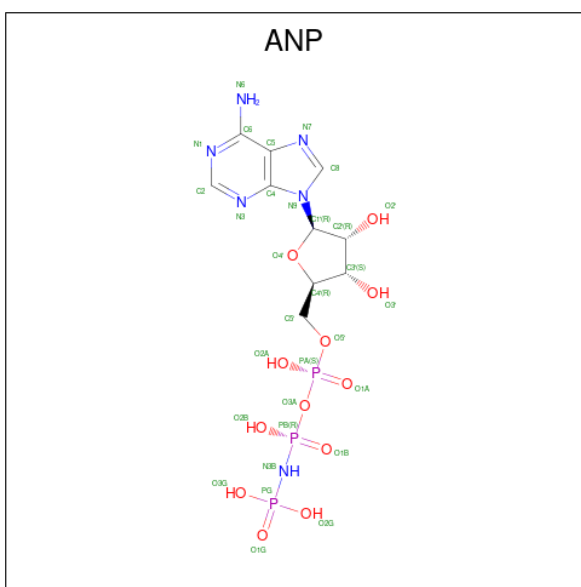
- Molecule 2 is a protein called peptide from Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	0	0	0
			79	46	19	14			
2	Q	10	Total	C	N	O	0	0	0
			79	46	19	14			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

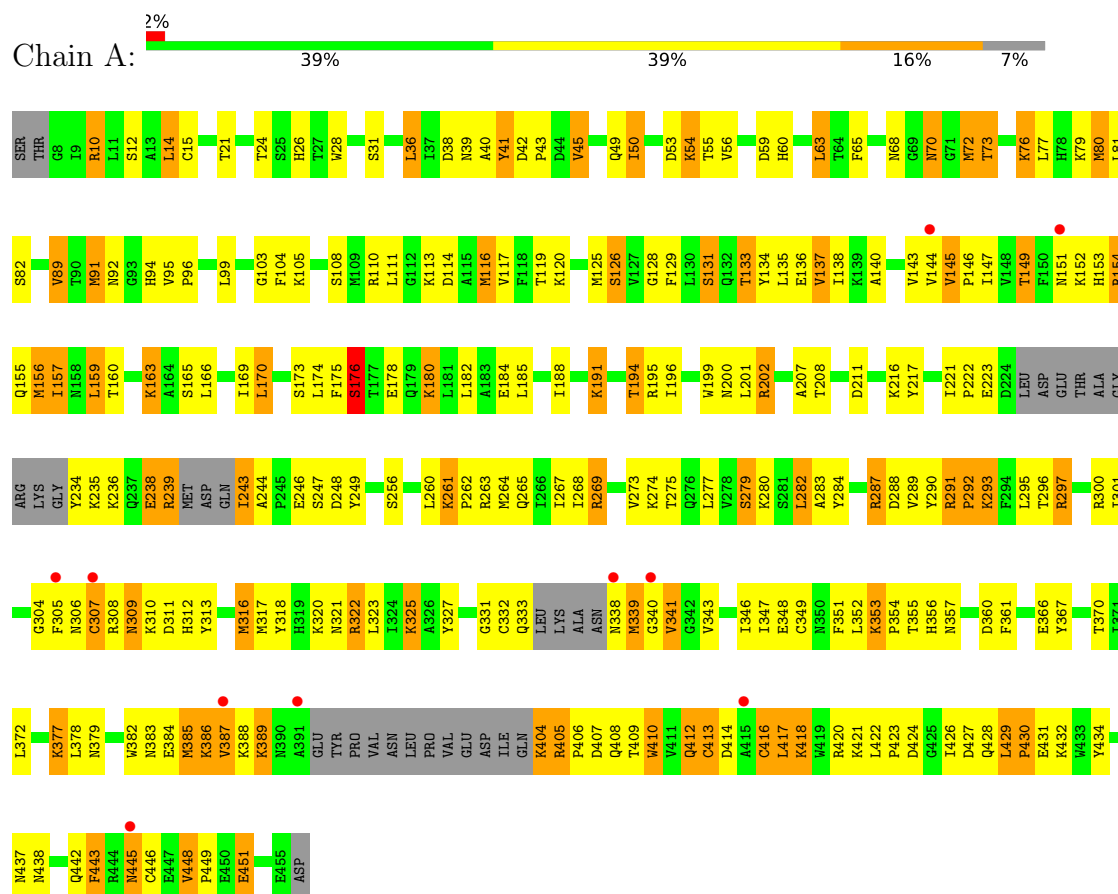
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

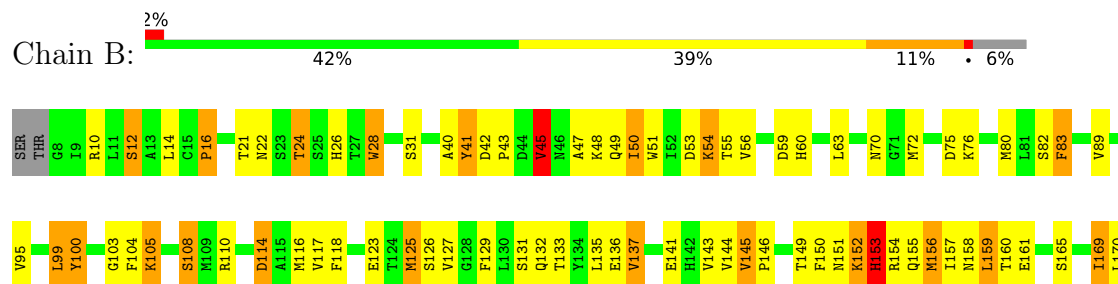
3 Residue-property plots

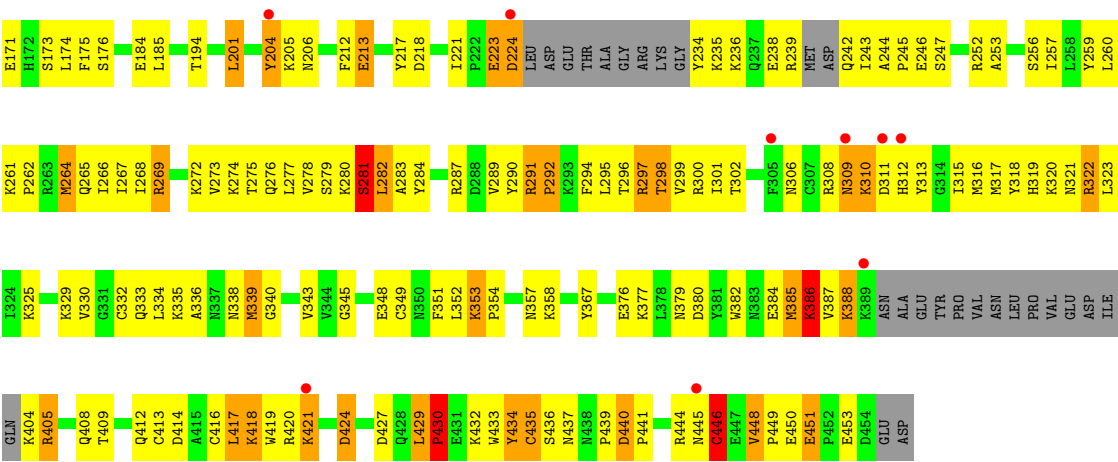
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: MORC family CW-type zinc finger protein 3

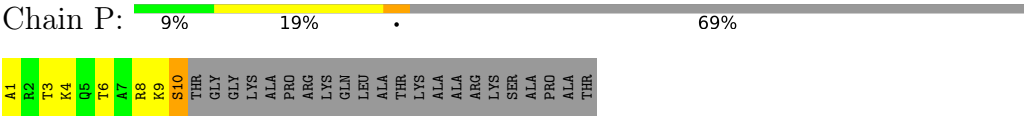


• Molecule 1: MORC family CW-type zinc finger protein 3

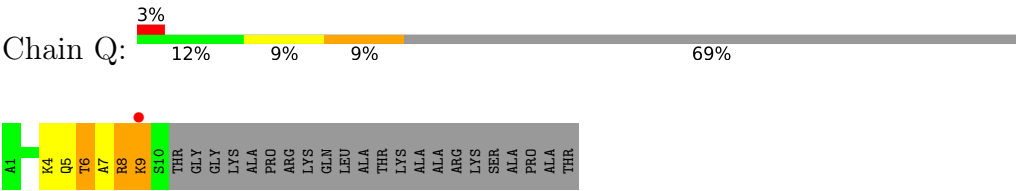




● Molecule 2: peptide from Histone H3.1



● Molecule 2: peptide from Histone H3.1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.20Å 147.54Å 173.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.75 – 2.90 19.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.75-2.90) 99.5 (19.75-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.88Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.236 0.233 , 0.244	Depositor DCC
R_{free} test set	1629 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtrriage
Anisotropy	0.677	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7049	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.98 % 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 1.6311e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A	1.52	14/3477 (0.4%)	1.22	43/4686 (0.9%)
1	B	1.56	22/3495 (0.6%)	1.24	39/4711 (0.8%)
2	P	1.19	0/78	1.14	0/101
2	Q	1.33	0/78	1.12	1/101 (1.0%)
All	All	1.53	36/7128 (0.5%)	1.23	83/9599 (0.9%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	ASP	N-CA	8.36	1.53	1.46
1	B	310	LYS	CA-C	6.91	1.62	1.52
1	B	309	ASN	CA-C	6.39	1.60	1.52
1	B	311	ASP	CA-C	6.21	1.59	1.52
1	A	405	ARG	C-N	6.04	1.40	1.33
1	B	405	ARG	C-N	5.93	1.40	1.33
1	B	291	ARG	C-N	5.85	1.40	1.33
1	A	353	LYS	C-N	5.72	1.40	1.33
1	A	244	ALA	C-N	5.65	1.40	1.33
1	B	244	ALA	C-N	5.60	1.40	1.33
1	A	291	ARG	C-N	5.51	1.40	1.33
1	B	429	LEU	C-N	5.50	1.40	1.33
1	A	429	LEU	C-N	5.48	1.40	1.33
1	A	15	CYS	C-N	5.42	1.40	1.33
1	B	430	PRO	N-CD	5.40	1.55	1.47
1	B	145	VAL	C-N	5.37	1.40	1.33
1	B	42	ASP	C-N	5.36	1.40	1.33
1	B	16	PRO	N-CD	5.33	1.55	1.47
1	B	449	PRO	N-CD	5.33	1.55	1.47
1	A	430	PRO	N-CD	5.32	1.55	1.47
1	A	145	VAL	C-N	5.32	1.40	1.33
1	B	451	GLU	C-N	5.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	PRO	N-CD	5.30	1.55	1.47
1	A	449	PRO	N-CD	5.30	1.55	1.47
1	A	451	GLU	C-N	5.26	1.40	1.33
1	B	353	LYS	C-N	5.25	1.40	1.33
1	B	440	ASP	C-N	5.24	1.40	1.34
1	B	95	VAL	C-N	5.23	1.40	1.33
1	A	28	TRP	C-N	5.21	1.40	1.33
1	B	221	ILE	C-N	5.21	1.40	1.33
1	A	42	ASP	C-N	5.16	1.40	1.33
1	A	95	VAL	C-N	5.08	1.40	1.33
1	B	439	PRO	N-CD	5.07	1.54	1.47
1	B	43	PRO	N-CD	5.06	1.54	1.47
1	B	28	TRP	C-N	5.03	1.40	1.33
1	A	96	PRO	N-CD	5.02	1.54	1.47

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	HIS	N-CA-C	-13.12	89.18	109.52
1	B	213	GLU	N-CA-C	8.24	120.35	111.36
1	A	73	THR	N-CA-C	-8.17	100.36	110.41
1	B	70	ASN	N-CA-C	7.64	120.49	111.71
1	A	387	VAL	N-CA-C	7.57	118.35	110.62
1	B	291	ARG	CA-C-N	-7.12	113.33	120.31
1	B	291	ARG	C-N-CA	-7.12	113.33	120.31
1	A	429	LEU	CA-C-N	-7.10	113.49	120.52
1	A	429	LEU	C-N-CA	-7.10	113.49	120.52
1	B	429	LEU	CA-C-N	-7.09	113.50	120.52
1	B	429	LEU	C-N-CA	-7.09	113.50	120.52
1	A	244	ALA	CA-C-N	-7.00	113.10	120.03
1	A	244	ALA	C-N-CA	-7.00	113.10	120.03
1	A	111	LEU	N-CA-C	6.97	118.67	111.14
1	B	309	ASN	N-CA-C	6.87	118.45	110.97
1	A	95	VAL	CA-C-N	-6.85	112.91	119.76
1	A	95	VAL	C-N-CA	-6.85	112.91	119.76
1	B	446	CYS	CA-CB-SG	-6.80	98.77	114.40
1	B	244	ALA	CA-C-N	-6.74	113.36	120.03
1	B	244	ALA	C-N-CA	-6.74	113.36	120.03
1	A	339	MET	N-CA-C	6.73	118.62	111.28
1	A	448	VAL	CA-C-N	-6.46	113.13	119.78
1	A	448	VAL	C-N-CA	-6.46	113.13	119.78
1	B	405	ARG	CA-C-N	-6.44	113.65	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	ARG	C-N-CA	-6.44	113.65	120.03
1	A	261	LYS	CA-C-N	-6.42	113.17	119.78
1	A	261	LYS	C-N-CA	-6.42	113.17	119.78
1	A	291	ARG	CA-C-N	-6.40	113.69	120.03
1	A	291	ARG	C-N-CA	-6.40	113.69	120.03
1	A	221	ILE	CA-C-N	-6.35	113.41	119.76
1	A	221	ILE	C-N-CA	-6.35	113.41	119.76
1	A	451	GLU	CA-C-N	-6.27	113.30	119.76
1	A	451	GLU	C-N-CA	-6.27	113.30	119.76
1	B	95	VAL	CA-C-N	-6.26	113.50	119.76
1	B	95	VAL	C-N-CA	-6.26	113.50	119.76
1	A	405	ARG	CA-C-N	-6.25	113.85	120.03
1	A	405	ARG	C-N-CA	-6.25	113.85	120.03
1	A	176	SER	N-CA-C	6.13	117.96	111.28
2	Q	8	ARG	N-CA-C	-6.10	99.24	109.07
1	A	353	LYS	CA-C-N	-6.09	114.00	120.03
1	A	353	LYS	C-N-CA	-6.09	114.00	120.03
1	B	261	LYS	CA-C-N	-6.08	113.50	119.76
1	B	261	LYS	C-N-CA	-6.08	113.50	119.76
1	B	221	ILE	CA-C-N	-6.07	113.72	119.85
1	B	221	ILE	C-N-CA	-6.07	113.72	119.85
1	B	103	GLY	N-CA-C	6.05	119.99	112.73
1	B	145	VAL	CA-C-N	-6.02	113.74	119.76
1	B	145	VAL	C-N-CA	-6.02	113.74	119.76
1	B	451	GLU	CA-C-N	-6.01	113.78	119.85
1	B	451	GLU	C-N-CA	-6.01	113.78	119.85
1	B	171	GLU	N-CA-C	5.92	117.82	111.36
1	A	157	ILE	N-CA-C	5.92	118.88	113.20
1	B	42	ASP	CA-C-N	-5.91	113.53	119.56
1	B	42	ASP	C-N-CA	-5.91	113.53	119.56
1	A	416	CYS	CA-CB-SG	5.87	127.89	114.40
1	B	353	LYS	CA-C-N	-5.86	113.93	119.85
1	B	353	LYS	C-N-CA	-5.86	113.93	119.85
1	B	448	VAL	CA-C-N	-5.76	113.85	119.78
1	B	448	VAL	C-N-CA	-5.76	113.85	119.78
1	A	42	ASP	CA-C-N	-5.72	113.72	119.56
1	A	42	ASP	C-N-CA	-5.72	113.72	119.56
1	A	145	VAL	CA-C-N	-5.66	114.10	119.76
1	A	145	VAL	C-N-CA	-5.66	114.10	119.76
1	A	341	VAL	N-CA-C	5.58	116.39	108.42
1	A	15	CYS	CA-C-N	-5.53	113.20	119.28
1	A	15	CYS	C-N-CA	-5.53	113.20	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	CYS	CB-CA-C	-5.50	100.41	109.65
1	B	281	SER	N-CA-C	5.43	117.28	111.36
1	B	45	VAL	N-CA-C	5.42	115.62	110.53
1	B	149	THR	N-CA-C	5.33	117.50	109.23
1	A	137	VAL	N-CA-C	5.25	116.02	110.72
1	A	309	ASN	N-CA-C	5.22	116.97	111.28
1	B	311	ASP	N-CA-C	5.21	122.10	113.50
1	B	441	PRO	CA-N-CD	-5.13	104.82	112.00
1	B	386	LYS	N-CA-C	-5.12	105.70	111.28
1	A	238	GLU	N-CA-C	5.11	116.84	111.28
1	A	28	TRP	CA-C-N	-5.09	113.68	119.28
1	A	28	TRP	C-N-CA	-5.09	113.68	119.28
1	B	100	TYR	N-CA-C	5.09	117.57	111.71
1	A	292	PRO	CA-N-CD	-5.08	104.89	112.00
1	A	103	GLY	N-CA-C	5.04	118.97	112.83
1	A	354	PRO	CA-N-CD	-5.02	104.98	112.00
1	B	137	VAL	N-CA-C	5.01	115.78	110.72

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	A	3404	0	3391	328	0
1	B	3421	0	3422	268	0
2	P	79	0	91	15	0
2	Q	79	0	91	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	13	20	0
4	B	31	0	13	7	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	7049	0	7021	597	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 42.

All (597) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:MET:HE2	4:A:502:ANP:N3	1.36	1.39
1:B:287:ARG:NH2	1:B:300:ARG:HB3	1.44	1.32
1:B:245:PRO:HA	1:B:312:HIS:NE2	1.55	1.22
1:B:435:CYS:HB2	1:B:446:CYS:SG	1.83	1.19
1:A:410:TRP:HE1	2:P:6:THR:HG22	1.06	1.14
1:A:50:ILE:HB	1:A:264:MET:CE	1.82	1.10
1:A:131:SER:O	1:A:135:LEU:HD12	1.52	1.09
1:B:266:ILE:O	1:B:273:VAL:HG23	1.53	1.07
1:B:245:PRO:HA	1:B:312:HIS:HE2	0.89	1.06
1:B:416:CYS:SG	1:B:418:LYS:HG3	1.94	1.06
1:A:156:MET:CE	1:A:166:LEU:HD13	1.86	1.04
1:A:414:ASP:OD2	1:A:432:LYS:HD3	1.58	1.04
1:A:72:MET:HE2	4:A:502:ANP:C2	1.87	1.04
1:B:80:MET:HG3	4:B:502:ANP:O4'	1.60	1.01
1:B:159:LEU:HD22	1:B:159:LEU:H	1.19	1.01
1:B:287:ARG:NH2	1:B:300:ARG:CB	2.23	1.00
1:A:63:LEU:CD1	1:A:201:LEU:HD21	1.92	1.00
1:A:414:ASP:OD2	1:A:432:LYS:HB3	1.60	1.00
1:A:50:ILE:HB	1:A:264:MET:HE3	1.42	0.99
1:A:43:PRO:HB3	1:A:94:HIS:ND1	1.76	0.99
1:B:421:LYS:HG2	1:B:451:GLU:OE1	1.62	0.99
1:A:322:ARG:HG2	1:A:322:ARG:HH11	1.24	0.99
1:A:72:MET:HE2	4:A:502:ANP:C4	1.90	0.99
1:A:191:LYS:H	1:A:191:LYS:HD2	1.21	0.98
1:A:202:ARG:HH21	1:A:202:ARG:HG3	1.27	0.98
1:A:382:TRP:O	1:A:386:LYS:HB3	1.64	0.98
1:B:287:ARG:HH21	1:B:300:ARG:HB3	0.97	0.97
1:B:245:PRO:CA	1:B:312:HIS:HE2	1.77	0.97
1:A:306:ASN:O	1:A:310:LYS:HG2	1.64	0.95
1:B:245:PRO:CA	1:B:312:HIS:NE2	2.29	0.95
1:A:114:ASP:OD1	1:A:131:SER:HB2	1.65	0.94
1:B:277:LEU:HD23	1:B:278:VAL:N	1.81	0.94
1:A:293:LYS:H	1:A:293:LYS:HD2	1.31	0.94
1:A:45:VAL:HG21	4:A:502:ANP:N1	1.83	0.93
1:A:239:ARG:H	1:A:239:ARG:HD2	1.32	0.93
1:A:282:LEU:HD12	1:A:305:PHE:O	1.69	0.93
1:A:410:TRP:HE1	2:P:6:THR:CG2	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:CYS:CB	1:B:446:CYS:SG	2.57	0.92
1:A:72:MET:CE	4:A:502:ANP:N3	2.30	0.92
1:A:94:HIS:CD2	1:A:263:ARG:CD	2.53	0.92
1:B:336:ALA:HB3	1:B:338:ASN:OD1	1.70	0.91
1:A:45:VAL:CG2	4:A:502:ANP:C2	2.47	0.91
1:B:384:GLU:HB2	1:B:385:MET:SD	2.11	0.91
1:A:156:MET:HE2	1:A:166:LEU:HD13	1.52	0.90
1:A:316:MET:HE1	1:A:327:TYR:CE1	2.07	0.89
1:A:72:MET:CE	4:A:502:ANP:C2	2.50	0.88
1:A:416:CYS:CB	1:A:418:LYS:HG3	2.02	0.88
1:A:355:THR:HG22	1:A:356:HIS:N	1.87	0.88
1:A:385:MET:N	1:A:385:MET:HE2	1.89	0.88
1:B:125:MET:HE2	1:B:150:PHE:HB2	1.54	0.88
1:A:306:ASN:O	1:A:310:LYS:CG	2.22	0.88
1:B:289:VAL:O	1:B:377:LYS:HE2	1.74	0.88
1:A:414:ASP:OD2	1:A:432:LYS:CB	2.22	0.87
1:A:178:GLU:O	1:A:182:LEU:HD12	1.73	0.87
1:B:322:ARG:HH22	1:B:358:LYS:CB	1.87	0.87
1:A:445:ASN:HB3	1:A:448:VAL:HG23	1.57	0.87
1:B:322:ARG:HH22	1:B:358:LYS:HB3	1.35	0.87
1:B:336:ALA:CB	1:B:338:ASN:OD1	2.22	0.86
1:B:245:PRO:HB3	1:B:312:HIS:CD2	2.11	0.86
1:A:414:ASP:OD2	1:A:432:LYS:CD	2.23	0.86
1:B:408:GLN:HG3	1:B:409:THR:N	1.89	0.86
1:A:40:ALA:HA	1:A:45:VAL:HG11	1.55	0.85
1:B:40:ALA:HA	1:B:45:VAL:HG11	1.57	0.85
1:A:382:TRP:O	1:A:386:LYS:CB	2.24	0.85
1:A:410:TRP:NE1	2:P:6:THR:HG22	1.91	0.85
1:A:63:LEU:HD12	1:A:201:LEU:HD21	1.56	0.85
1:B:40:ALA:O	1:B:45:VAL:HG12	1.75	0.84
1:A:40:ALA:O	1:A:45:VAL:HG12	1.78	0.84
1:A:94:HIS:HD2	1:A:263:ARG:NE	1.74	0.84
1:A:60:HIS:ND1	1:A:174:LEU:HD11	1.91	0.84
1:B:445:ASN:O	1:B:448:VAL:HG12	1.77	0.84
1:A:80:MET:HE2	1:A:117:VAL:HG21	1.59	0.83
1:B:280:LYS:HD2	1:B:308:ARG:NH2	1.92	0.83
1:A:45:VAL:HG23	4:A:502:ANP:C2	2.08	0.83
1:B:110:ARG:HH11	1:B:110:ARG:HG3	1.41	0.83
1:A:445:ASN:O	1:A:448:VAL:HG23	1.80	0.82
1:A:131:SER:O	1:A:135:LEU:CD1	2.29	0.81
1:A:443:PHE:CZ	1:A:451:GLU:OE1	2.33	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LYS:HD2	1:B:308:ARG:HH21	1.46	0.81
1:A:239:ARG:HD2	1:A:239:ARG:N	1.90	0.81
1:B:278:VAL:HA	1:B:281:SER:HB2	1.60	0.81
1:A:50:ILE:CB	1:A:264:MET:CE	2.59	0.81
1:A:246:GLU:HA	1:A:249:TYR:CE2	2.16	0.81
1:B:157:ILE:HA	1:B:159:LEU:CD1	2.11	0.81
1:A:45:VAL:CG2	4:A:502:ANP:N1	2.44	0.80
1:A:423:PRO:HG2	1:A:426:ILE:HD11	1.60	0.80
1:A:445:ASN:HB3	1:A:448:VAL:CG2	2.12	0.80
1:A:126:SER:HB3	1:A:149:THR:HG23	1.63	0.80
1:A:416:CYS:HB2	1:A:418:LYS:H	1.45	0.80
1:A:94:HIS:CD2	1:A:263:ARG:HD2	2.16	0.80
1:B:322:ARG:NH2	1:B:358:LYS:HD2	1.96	0.79
1:A:293:LYS:H	1:A:293:LYS:CD	1.97	0.78
1:B:217:TYR:CD2	1:B:405:ARG:NH1	2.52	0.78
1:A:416:CYS:HB3	1:A:418:LYS:CG	2.13	0.78
1:A:191:LYS:H	1:A:191:LYS:CD	1.94	0.77
1:A:50:ILE:CB	1:A:264:MET:HE3	2.14	0.77
1:B:277:LEU:H	1:B:280:LYS:HE2	1.49	0.77
1:B:412:GLN:HB2	1:B:419:TRP:CZ3	2.19	0.77
1:A:416:CYS:CB	1:A:418:LYS:CG	2.61	0.77
1:B:129:PHE:HB3	1:B:146:PRO:HD2	1.64	0.77
1:A:306:ASN:ND2	1:A:310:LYS:H	1.83	0.77
1:B:217:TYR:CE1	2:Q:8:ARG:HD3	2.19	0.77
1:B:330:VAL:O	1:B:333:GLN:HG3	1.84	0.77
1:A:416:CYS:SG	1:A:418:LYS:HG3	2.25	0.77
1:A:165:SER:O	1:A:169:ILE:HG13	1.85	0.76
1:B:132:GLN:O	1:B:136:GLU:HG3	1.84	0.76
1:A:269:ARG:HG3	1:A:269:ARG:HH11	1.49	0.76
1:A:287:ARG:NH1	1:A:300:ARG:HB3	1.99	0.76
1:A:202:ARG:HG3	1:A:202:ARG:NH2	1.95	0.76
1:A:239:ARG:HH21	1:A:239:ARG:HG3	1.49	0.76
1:A:325:LYS:HE3	1:A:360:ASP:OD1	1.85	0.76
1:B:416:CYS:SG	1:B:418:LYS:CG	2.74	0.75
1:A:355:THR:HG22	1:A:356:HIS:H	1.50	0.75
1:B:287:ARG:HH22	1:B:300:ARG:CB	1.97	0.75
1:A:429:LEU:HD12	1:A:429:LEU:N	2.01	0.75
1:A:445:ASN:CB	1:A:448:VAL:CG2	2.65	0.75
1:B:385:MET:HE3	1:B:385:MET:HA	1.69	0.75
1:A:114:ASP:OD1	1:A:131:SER:CB	2.35	0.74
1:B:40:ALA:O	1:B:45:VAL:CG1	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:MET:O	1:A:382:TRP:CH2	2.40	0.74
1:B:217:TYR:HB2	1:B:405:ARG:HH12	1.52	0.74
1:B:266:ILE:O	1:B:273:VAL:CG2	2.35	0.74
1:A:261:LYS:H	1:A:321:ASN:HD21	1.35	0.74
1:A:355:THR:CG2	1:A:356:HIS:N	2.51	0.74
1:B:45:VAL:HG21	4:B:502:ANP:N1	2.03	0.74
1:B:110:ARG:HG3	1:B:110:ARG:NH1	2.02	0.74
1:A:72:MET:CE	4:A:502:ANP:C4	2.66	0.74
1:B:277:LEU:HD23	1:B:278:VAL:H	1.50	0.74
1:A:129:PHE:HB3	1:A:146:PRO:HD2	1.69	0.73
1:A:153:HIS:O	1:A:154:ARG:HG3	1.87	0.73
1:B:429:LEU:N	1:B:429:LEU:HD12	2.02	0.73
1:A:385:MET:HE2	1:A:385:MET:CA	2.15	0.73
1:A:290:TYR:CZ	1:A:292:PRO:HG3	2.23	0.73
1:A:156:MET:HE2	1:A:166:LEU:CD1	2.17	0.73
1:A:143:VAL:HG12	1:B:12:SER:HB2	1.70	0.73
1:B:322:ARG:HH11	1:B:322:ARG:HG2	1.54	0.72
1:B:125:MET:HE2	1:B:150:PHE:CB	2.19	0.72
1:A:170:LEU:HD23	1:A:176:SER:O	1.87	0.72
1:A:166:LEU:CD2	1:A:170:LEU:HD13	2.19	0.72
1:A:416:CYS:HB3	1:A:418:LYS:HG3	1.67	0.72
1:B:408:GLN:HG3	1:B:409:THR:H	1.52	0.72
1:A:355:THR:CG2	1:A:356:HIS:H	2.02	0.71
1:A:378:LEU:C	1:A:378:LEU:HD23	2.15	0.71
1:A:155:GLN:O	1:A:157:ILE:HG23	1.90	0.71
1:A:50:ILE:HB	1:A:264:MET:HE1	1.67	0.71
1:A:295:LEU:HD22	1:A:297:ARG:HD2	1.71	0.71
1:A:166:LEU:HD23	1:A:170:LEU:HD13	1.71	0.71
1:A:408:GLN:HG3	1:A:409:THR:N	2.04	0.70
1:A:50:ILE:CG2	1:A:264:MET:CE	2.70	0.70
1:A:159:LEU:O	1:A:163:LYS:HG2	1.92	0.70
1:A:382:TRP:O	1:A:386:LYS:N	2.24	0.70
1:A:389:LYS:HD3	1:A:389:LYS:C	2.16	0.70
1:B:54:LYS:HD2	1:B:54:LYS:C	2.16	0.70
1:A:288:ASP:OD1	1:A:289:VAL:N	2.25	0.70
1:A:418:LYS:CE	1:A:446:CYS:O	2.40	0.70
1:A:268:ILE:HD12	1:A:273:VAL:CG2	2.22	0.69
1:A:217:TYR:CZ	2:P:8:ARG:HG2	2.27	0.69
1:A:413:CYS:SG	1:A:416:CYS:N	2.65	0.69
1:B:157:ILE:C	1:B:159:LEU:HD13	2.18	0.69
1:B:283:ALA:O	1:B:284:TYR:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:HIS:HD2	1:A:263:ARG:CD	1.99	0.68
1:A:290:TYR:CE2	1:A:292:PRO:HG3	2.28	0.68
1:A:169:ILE:O	1:A:173:SER:CB	2.41	0.68
1:A:191:LYS:HD2	1:A:191:LYS:N	2.03	0.68
1:A:269:ARG:HG3	1:A:269:ARG:NH1	2.04	0.68
1:B:252:ARG:NH1	1:B:272:LYS:O	2.27	0.68
1:A:445:ASN:CB	1:A:448:VAL:HG23	2.24	0.68
1:B:419:TRP:CG	2:Q:4:LYS:HZ1	2.10	0.68
1:B:313:TYR:O	1:B:329:LYS:NZ	2.27	0.68
1:B:151:ASN:OD1	1:B:155:GLN:HB2	1.94	0.67
1:B:26:HIS:HB2	1:B:110:ARG:HD3	1.76	0.67
1:B:278:VAL:O	1:B:282:LEU:N	2.26	0.67
1:B:385:MET:SD	1:B:385:MET:N	2.66	0.67
1:B:340:GLY:O	1:B:343:VAL:HG23	1.93	0.67
1:B:49:GLN:HG3	1:B:265:GLN:CB	2.25	0.67
1:B:414:ASP:OD2	1:B:432:LYS:CD	2.42	0.67
1:B:152:LYS:C	1:B:153:HIS:HD1	2.03	0.67
1:B:414:ASP:OD2	1:B:432:LYS:HD3	1.95	0.67
1:A:40:ALA:O	1:A:45:VAL:CG1	2.42	0.67
1:A:114:ASP:OD1	1:A:133:THR:HB	1.95	0.67
1:A:313:TYR:HB2	1:A:343:VAL:O	1.94	0.67
1:B:116:MET:HE1	1:B:169:ILE:HD13	1.77	0.66
1:B:49:GLN:HG3	1:B:265:GLN:HB3	1.78	0.66
1:A:239:ARG:HG3	1:A:239:ARG:NH2	2.05	0.66
1:B:245:PRO:CB	1:B:312:HIS:NE2	2.57	0.66
1:A:14:LEU:CD2	1:B:14:LEU:HG	2.25	0.66
1:A:309:ASN:OD1	1:A:311:ASP:HB2	1.96	0.66
1:B:322:ARG:HH11	1:B:322:ARG:CG	2.09	0.66
1:B:322:ARG:HG2	1:B:322:ARG:NH1	2.09	0.66
1:B:429:LEU:HD12	1:B:429:LEU:H	1.60	0.66
1:B:45:VAL:HG23	4:B:502:ANP:C2	2.26	0.65
1:B:416:CYS:O	1:B:417:LEU:HB2	1.97	0.65
1:B:169:ILE:O	1:B:173:SER:HB3	1.96	0.65
1:B:278:VAL:CA	1:B:281:SER:HB2	2.26	0.65
1:A:169:ILE:O	1:A:173:SER:HB3	1.96	0.65
1:B:421:LYS:HE2	1:B:421:LYS:O	1.96	0.65
1:A:120:LYS:NZ	1:A:188:ILE:O	2.30	0.64
1:A:311:ASP:C	1:A:312:HIS:ND1	2.55	0.64
1:A:414:ASP:OD2	1:A:432:LYS:CG	2.45	0.64
1:B:114:ASP:OD2	1:B:114:ASP:N	2.28	0.64
1:B:382:TRP:O	1:B:386:LYS:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:CG2	1:A:264:MET:HE2	2.27	0.64
1:B:269:ARG:HG3	1:B:269:ARG:NH1	2.12	0.64
1:A:144:VAL:HG23	1:B:10:ARG:O	1.97	0.64
1:A:385:MET:O	1:A:386:LYS:C	2.40	0.64
1:A:443:PHE:CE1	1:A:451:GLU:OE1	2.50	0.64
1:B:45:VAL:CG2	4:B:502:ANP:N1	2.60	0.64
1:A:287:ARG:NH1	1:A:300:ARG:CB	2.59	0.64
1:A:63:LEU:HD13	1:A:201:LEU:HD21	1.78	0.64
1:B:421:LYS:NZ	1:B:440:ASP:OD2	2.31	0.64
1:A:269:ARG:HH11	1:A:269:ARG:CG	2.11	0.64
1:B:157:ILE:HA	1:B:159:LEU:HD11	1.80	0.63
2:Q:6:THR:HG23	2:Q:7:ALA:N	2.13	0.63
1:A:239:ARG:HH21	1:A:239:ARG:CG	2.10	0.63
1:B:413:CYS:SG	1:B:435:CYS:N	2.72	0.63
1:A:105:LYS:H	1:A:105:LYS:HD2	1.62	0.63
1:B:80:MET:O	1:B:105:LYS:HE2	1.98	0.63
1:B:269:ARG:HG3	1:B:269:ARG:HH11	1.64	0.63
1:A:322:ARG:HG2	1:A:322:ARG:NH1	2.04	0.63
1:A:379:ASN:O	1:A:383:ASN:ND2	2.32	0.63
1:B:145:VAL:HG23	1:B:145:VAL:O	1.99	0.63
1:A:316:MET:HE1	1:A:327:TYR:CD1	2.34	0.62
1:A:318:TYR:CE2	1:A:323:LEU:HB2	2.35	0.62
1:A:116:MET:HG3	1:A:128:GLY:O	1.98	0.62
1:A:94:HIS:NE2	1:A:263:ARG:HD2	2.14	0.62
1:B:213:GLU:N	1:B:213:GLU:OE1	2.32	0.62
1:B:436:SER:HA	1:B:444:ARG:O	2.00	0.62
1:A:80:MET:HB2	4:A:502:ANP:O4'	1.99	0.62
2:Q:6:THR:CG2	2:Q:7:ALA:N	2.63	0.62
1:B:388:LYS:O	1:B:388:LYS:NZ	2.28	0.62
1:A:49:GLN:HG3	1:A:265:GLN:HB3	1.82	0.61
1:A:279:SER:O	1:A:280:LYS:HB2	1.99	0.61
1:B:280:LYS:CD	1:B:308:ARG:NH2	2.62	0.61
1:A:131:SER:OG	1:A:134:TYR:CB	2.48	0.61
1:A:293:LYS:HD2	1:A:293:LYS:N	2.11	0.61
1:B:277:LEU:O	1:B:281:SER:HB2	2.01	0.61
1:B:159:LEU:H	1:B:159:LEU:CD2	1.92	0.61
1:A:385:MET:O	1:A:387:VAL:N	2.33	0.61
1:B:322:ARG:NH2	1:B:358:LYS:HB3	2.12	0.61
1:B:269:ARG:HH11	1:B:269:ARG:CG	2.13	0.61
1:B:99:LEU:HD23	1:B:100:TYR:H	1.65	0.60
1:A:94:HIS:CD2	1:A:263:ARG:NE	2.61	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HH21	1:B:358:LYS:HD2	1.66	0.60
1:B:47:ALA:O	1:B:264:MET:HG2	2.00	0.60
1:B:419:TRP:CD1	2:Q:4:LYS:HZ1	2.19	0.60
1:B:151:ASN:CG	1:B:155:GLN:HB2	2.26	0.60
1:A:126:SER:CB	1:A:149:THR:HG23	2.32	0.60
1:B:99:LEU:HD23	1:B:100:TYR:N	2.16	0.60
1:A:105:LYS:H	1:A:105:LYS:CD	2.14	0.60
1:A:10:ARG:NH2	1:A:10:ARG:HG2	2.16	0.60
1:B:245:PRO:HB3	1:B:312:HIS:NE2	2.17	0.60
4:A:502:ANP:H5'1	4:A:502:ANP:H8	1.84	0.59
1:B:278:VAL:O	1:B:281:SER:N	2.35	0.59
1:A:131:SER:OG	1:A:134:TYR:HB3	2.02	0.59
1:A:405:ARG:NH1	2:P:10:SER:HA	2.16	0.59
1:A:295:LEU:HD22	1:A:297:ARG:CD	2.32	0.59
1:B:99:LEU:HD23	1:B:99:LEU:H	1.68	0.59
1:A:265:GLN:HG2	1:A:267:ILE:HD11	1.85	0.59
1:A:338:ASN:CG	1:A:339:MET:H	2.09	0.59
1:B:223:GLU:HG3	1:B:224:ASP:N	2.18	0.59
1:A:321:ASN:O	1:A:321:ASN:ND2	2.36	0.59
1:B:205:LYS:O	1:B:206:ASN:HB2	2.03	0.59
1:B:280:LYS:CD	1:B:308:ARG:HH21	2.15	0.59
1:A:287:ARG:CZ	1:A:300:ARG:HB3	2.32	0.59
1:A:416:CYS:HB3	1:A:418:LYS:HG2	1.84	0.58
1:B:104:PHE:O	1:B:108:SER:OG	2.21	0.58
1:B:278:VAL:HG13	1:B:282:LEU:HD22	1.85	0.58
1:B:47:ALA:O	1:B:264:MET:CG	2.51	0.58
1:B:336:ALA:HB1	1:B:338:ASN:OD1	2.03	0.58
1:A:43:PRO:CB	1:A:94:HIS:ND1	2.61	0.58
1:A:427:ASP:N	1:A:427:ASP:OD1	2.35	0.58
1:B:424:ASP:N	1:B:424:ASP:OD1	2.37	0.58
1:B:292:PRO:HG2	1:B:295:LEU:HB2	1.83	0.58
1:A:10:ARG:HH21	1:A:10:ARG:CG	2.17	0.57
1:A:322:ARG:NH1	1:A:323:LEU:O	2.37	0.57
1:A:404:LYS:HD2	1:A:404:LYS:N	2.19	0.57
1:A:428:GLN:C	1:A:429:LEU:HD12	2.30	0.57
1:B:152:LYS:O	1:B:152:LYS:HG3	2.03	0.57
1:A:423:PRO:O	1:A:426:ILE:HD12	2.05	0.57
1:B:427:ASP:OD1	1:B:427:ASP:N	2.35	0.57
1:A:418:LYS:HE2	1:A:446:CYS:O	2.04	0.57
1:B:217:TYR:O	1:B:252:ARG:NH2	2.22	0.57
1:B:338:ASN:OD1	1:B:338:ASN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:CYS:HB2	1:A:418:LYS:CG	2.34	0.57
1:B:60:HIS:ND1	1:B:174:LEU:HD11	2.19	0.57
1:B:309:ASN:ND2	1:B:312:HIS:ND1	2.53	0.57
1:B:83:PHE:CD1	1:B:83:PHE:N	2.73	0.56
1:B:278:VAL:CG1	1:B:282:LEU:HD22	2.35	0.56
1:B:277:LEU:H	1:B:280:LYS:CE	2.16	0.56
1:B:277:LEU:CD2	1:B:279:SER:H	2.17	0.56
1:B:434:TYR:N	1:B:434:TYR:CD2	2.73	0.56
1:A:405:ARG:HH11	2:P:10:SER:HA	1.70	0.56
1:A:410:TRP:CD1	1:A:410:TRP:N	2.73	0.56
1:B:175:PHE:CD2	1:B:175:PHE:N	2.72	0.56
1:A:49:GLN:HB2	1:A:68:ASN:HD21	1.71	0.56
1:A:145:VAL:O	1:A:145:VAL:HG23	2.04	0.56
1:A:412:GLN:OE1	1:A:417:LEU:O	2.23	0.56
1:B:420:ARG:NE	1:B:435:CYS:SG	2.73	0.56
1:B:28:TRP:O	1:B:31:SER:OG	2.24	0.56
1:A:99:LEU:H	4:A:502:ANP:HNB1	1.54	0.56
1:B:21:THR:O	1:B:24:THR:OG1	2.23	0.56
1:A:331:GLY:O	1:A:333:GLN:NE2	2.39	0.56
1:A:207:ALA:O	1:A:208:THR:C	2.47	0.55
1:A:268:ILE:HD12	1:A:273:VAL:HG21	1.88	0.55
1:B:295:LEU:HD22	1:B:297:ARG:HG2	1.88	0.55
1:A:366:GLU:O	1:A:370:THR:OG1	2.21	0.55
1:A:80:MET:SD	4:A:502:ANP:C8	2.94	0.55
1:B:289:VAL:O	1:B:377:LYS:CE	2.52	0.55
1:A:306:ASN:HD22	1:A:310:LYS:HA	1.71	0.55
1:A:410:TRP:NE1	2:P:6:THR:CG2	2.60	0.55
1:B:421:LYS:HE2	1:B:421:LYS:C	2.31	0.55
1:B:45:VAL:CG2	4:B:502:ANP:C2	2.84	0.55
1:B:55:THR:OG1	1:B:56:VAL:N	2.37	0.55
1:A:175:PHE:HB3	1:A:180:LYS:HB3	1.88	0.55
1:A:202:ARG:HH21	1:A:202:ARG:CG	2.11	0.55
1:B:309:ASN:HD22	1:B:312:HIS:HB2	1.71	0.55
1:A:199:TRP:O	1:A:200:ASN:HB2	2.07	0.55
1:A:306:ASN:HD22	1:A:310:LYS:H	1.54	0.55
1:B:159:LEU:HD13	1:B:159:LEU:N	2.21	0.55
1:A:236:LYS:HG3	1:A:248:ASP:OD2	2.07	0.55
1:A:445:ASN:HB2	1:A:448:VAL:CG2	2.37	0.55
1:A:155:GLN:O	1:A:157:ILE:CG2	2.55	0.54
1:A:243:ILE:HD13	1:A:243:ILE:N	2.21	0.54
1:A:416:CYS:CB	1:A:418:LYS:HG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:PHE:N	1:A:443:PHE:CD2	2.73	0.54
1:A:12:SER:HB2	1:B:143:VAL:HG12	1.90	0.54
1:A:283:ALA:O	1:A:284:TYR:HB2	2.07	0.54
1:A:153:HIS:C	1:A:154:ARG:HG3	2.33	0.54
1:B:41:TYR:C	1:B:41:TYR:CD2	2.85	0.54
1:A:14:LEU:HD21	1:B:14:LEU:HG	1.89	0.54
1:B:322:ARG:NH2	1:B:358:LYS:CB	2.66	0.54
1:A:41:TYR:C	1:A:41:TYR:CD2	2.85	0.54
1:A:442:GLN:C	1:A:443:PHE:CD2	2.86	0.54
1:B:217:TYR:HD2	1:B:405:ARG:NH1	2.04	0.54
1:A:36:LEU:HD23	1:A:65:PHE:CE1	2.42	0.54
1:A:408:GLN:N	2:P:6:THR:O	2.40	0.54
1:B:99:LEU:H	1:B:99:LEU:CD2	2.21	0.54
1:A:385:MET:CA	1:A:385:MET:CE	2.85	0.54
1:A:131:SER:OG	1:A:134:TYR:N	2.32	0.54
1:B:245:PRO:HA	1:B:312:HIS:CE1	2.37	0.54
1:B:357:ASN:O	1:B:358:LYS:HB2	2.06	0.54
1:A:318:TYR:HA	1:A:322:ARG:O	2.08	0.54
1:B:351:PHE:CD1	1:B:352:LEU:HD23	2.43	0.54
1:B:433:TRP:C	1:B:434:TYR:CD2	2.86	0.54
1:B:156:MET:C	1:B:157:ILE:HG23	2.33	0.53
1:B:276:GLN:HA	1:B:280:LYS:NZ	2.22	0.53
1:A:296:THR:HG23	1:A:297:ARG:HG3	1.90	0.53
1:B:291:ARG:HG3	1:B:298:THR:HG22	1.90	0.53
1:B:434:TYR:O	1:B:437:ASN:OD1	2.26	0.53
1:B:384:GLU:O	1:B:385:MET:HE3	2.08	0.53
1:A:262:PRO:HG2	1:A:275:THR:HG21	1.90	0.53
1:B:157:ILE:CA	1:B:159:LEU:CD1	2.86	0.52
1:B:433:TRP:C	1:B:433:TRP:CE3	2.87	0.52
1:A:234:TYR:CD1	1:A:234:TYR:C	2.86	0.52
1:A:236:LYS:HG3	1:A:248:ASP:CG	2.33	0.52
1:B:157:ILE:CA	1:B:159:LEU:HD13	2.38	0.52
1:B:309:ASN:ND2	1:B:312:HIS:HB2	2.24	0.52
1:A:117:VAL:HG22	1:A:196:ILE:HG12	1.91	0.52
1:B:332:CYS:SG	1:B:379:ASN:OD1	2.67	0.52
1:B:276:GLN:HA	1:B:280:LYS:HZ3	1.75	0.52
1:A:105:LYS:HD2	1:A:105:LYS:N	2.24	0.52
1:A:10:ARG:NH2	1:A:10:ARG:CG	2.72	0.52
1:A:389:LYS:HE2	1:A:389:LYS:O	2.09	0.52
1:A:404:LYS:N	1:A:404:LYS:CD	2.73	0.52
1:B:404:LYS:N	1:B:404:LYS:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:TRP:CZ3	1:B:434:TYR:C	2.88	0.52
1:B:157:ILE:HA	1:B:159:LEU:HD13	1.90	0.51
1:A:21:THR:O	1:A:24:THR:HG23	2.10	0.51
1:A:418:LYS:HE3	1:A:446:CYS:O	2.09	0.51
1:B:99:LEU:CD2	1:B:99:LEU:N	2.73	0.51
1:A:45:VAL:CG2	4:A:502:ANP:H2	2.40	0.51
1:A:72:MET:HG2	1:A:76:LYS:HB3	1.92	0.51
1:B:384:GLU:C	1:B:385:MET:SD	2.94	0.51
1:A:36:LEU:HD23	1:A:65:PHE:CZ	2.46	0.51
1:A:306:ASN:O	1:A:310:LYS:CE	2.60	0.50
1:A:290:TYR:CE2	1:A:292:PRO:CG	2.92	0.50
1:A:289:VAL:HG12	1:A:290:TYR:N	2.27	0.50
1:A:322:ARG:HH11	1:A:322:ARG:CG	2.06	0.50
1:B:41:TYR:CD1	1:B:259:TYR:CE1	3.00	0.50
1:B:116:MET:HE1	1:B:169:ILE:HG23	1.93	0.50
1:B:133:THR:O	1:B:137:VAL:HG23	2.11	0.50
1:B:50:ILE:HG23	1:B:50:ILE:O	2.11	0.49
1:B:49:GLN:HG3	1:B:265:GLN:HB2	1.93	0.49
1:B:440:ASP:O	1:B:444:ARG:HG3	2.12	0.49
1:A:260:LEU:C	1:A:261:LYS:HD3	2.36	0.49
1:B:384:GLU:C	1:B:385:MET:CE	2.85	0.49
1:A:49:GLN:HB2	1:A:68:ASN:ND2	2.28	0.49
1:A:153:HIS:C	1:A:154:ARG:CG	2.85	0.49
1:A:317:MET:HE1	1:A:325:LYS:HZ2	1.77	0.49
1:B:433:TRP:CE3	1:B:434:TYR:N	2.81	0.49
2:Q:4:LYS:O	2:Q:5:GLN:HG3	2.13	0.49
1:B:144:VAL:O	1:B:144:VAL:HG23	2.12	0.49
1:B:329:LYS:C	1:B:330:VAL:HG13	2.38	0.49
1:A:70:ASN:OD1	1:A:70:ASN:N	2.44	0.49
1:A:216:LYS:O	1:A:269:ARG:HG3	2.13	0.49
1:A:45:VAL:HG21	4:A:502:ANP:C2	2.29	0.49
1:A:63:LEU:CD1	1:A:201:LEU:CD2	2.81	0.49
1:B:321:ASN:N	1:B:348:GLU:OE1	2.45	0.49
1:B:384:GLU:CB	1:B:385:MET:SD	2.94	0.49
1:B:156:MET:C	1:B:157:ILE:CG2	2.86	0.48
1:A:389:LYS:C	1:A:389:LYS:CD	2.85	0.48
1:B:277:LEU:HD23	1:B:279:SER:H	1.78	0.48
2:Q:9:LYS:HD2	2:Q:9:LYS:HA	1.56	0.48
1:A:382:TRP:O	1:A:386:LYS:CA	2.60	0.48
1:B:242:GLN:NE2	1:B:242:GLN:N	2.60	0.48
1:B:419:TRP:CE2	2:Q:4:LYS:HE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:TYR:C	1:B:234:TYR:CD2	2.92	0.48
1:A:99:LEU:N	4:A:502:ANP:HNB1	2.12	0.48
1:A:104:PHE:O	1:A:108:SER:OG	2.25	0.48
1:A:144:VAL:HG13	1:A:144:VAL:O	2.13	0.48
1:B:262:PRO:HG2	1:B:275:THR:HG21	1.96	0.48
1:B:306:ASN:OD1	1:B:309:ASN:HB2	2.14	0.48
1:B:322:ARG:HG3	1:B:323:LEU:N	2.27	0.48
1:A:325:LYS:NZ	1:A:367:TYR:OH	2.31	0.48
1:B:54:LYS:HG3	1:B:212:PHE:CD1	2.49	0.48
1:A:306:ASN:O	1:A:310:LYS:HG3	2.13	0.48
1:B:412:GLN:HB2	1:B:419:TRP:CH2	2.49	0.48
1:A:414:ASP:HB2	1:A:434:TYR:CE2	2.49	0.48
1:A:116:MET:HG3	1:A:117:VAL:N	2.28	0.48
1:A:339:MET:O	1:A:382:TRP:CZ2	2.67	0.48
1:A:306:ASN:O	1:A:310:LYS:HE2	2.14	0.47
1:A:420:ARG:NH1	1:A:448:VAL:O	2.45	0.47
1:B:54:LYS:C	1:B:54:LYS:CD	2.85	0.47
1:B:173:SER:OG	1:B:175:PHE:HD2	1.96	0.47
1:A:10:ARG:HG2	1:A:10:ARG:HH21	1.79	0.47
1:A:119:THR:HB	1:A:194:THR:HG23	1.96	0.47
1:B:48:LYS:HA	1:B:48:LYS:HD3	1.73	0.47
1:B:319:HIS:CD2	1:B:320:LYS:HD2	2.50	0.47
1:A:412:GLN:OE1	1:A:417:LEU:HG	2.14	0.47
1:A:295:LEU:HD11	1:A:351:PHE:CD2	2.49	0.47
1:A:12:SER:OG	1:B:82:SER:HA	2.14	0.47
1:A:211:ASP:HB2	1:A:222:PRO:HG3	1.97	0.47
1:A:346:ILE:N	1:A:346:ILE:HD12	2.30	0.47
1:A:420:ARG:NH2	1:A:448:VAL:O	2.46	0.47
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.74	0.47
1:B:152:LYS:C	1:B:153:HIS:ND1	2.73	0.47
1:B:290:TYR:HB3	1:B:299:VAL:HB	1.96	0.47
1:B:429:LEU:N	1:B:429:LEU:CD1	2.73	0.47
1:A:94:HIS:HE2	1:A:263:ARG:HD2	1.78	0.47
1:A:39:ASN:ND2	4:A:502:ANP:O1A	2.48	0.47
1:A:312:HIS:ND1	1:A:312:HIS:N	2.63	0.47
1:B:418:LYS:HE3	1:B:446:CYS:O	2.14	0.47
1:A:306:ASN:HD22	1:A:310:LYS:N	2.12	0.47
1:A:318:TYR:O	1:A:348:GLU:HA	2.15	0.47
1:A:105:LYS:CD	1:A:105:LYS:N	2.78	0.46
1:A:443:PHE:N	1:A:443:PHE:HD2	2.12	0.46
1:A:338:ASN:CG	1:A:339:MET:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:ND2	1:B:155:GLN:HB2	2.30	0.46
1:B:292:PRO:HB2	1:B:294:PHE:CE2	2.50	0.46
1:B:256:SER:OG	1:B:257:ILE:HG23	2.15	0.46
1:A:429:LEU:N	1:A:429:LEU:CD1	2.73	0.46
1:A:217:TYR:OH	2:P:8:ARG:HG2	2.15	0.46
1:A:260:LEU:HB3	1:A:321:ASN:ND2	2.31	0.46
1:A:351:PHE:O	1:A:353:LYS:NZ	2.49	0.46
1:A:114:ASP:OD2	1:A:200:ASN:ND2	2.36	0.46
1:B:419:TRP:N	1:B:450:GLU:OE2	2.36	0.46
1:B:367:TYR:C	1:B:367:TYR:CD2	2.94	0.46
1:A:50:ILE:HG21	1:A:264:MET:HE2	1.97	0.46
1:A:438:ASN:ND2	1:A:443:PHE:O	2.30	0.46
1:B:173:SER:OG	1:B:174:LEU:N	2.48	0.46
1:B:387:VAL:HG23	1:B:388:LYS:N	2.31	0.46
1:A:81:LEU:O	1:B:12:SER:OG	2.32	0.45
1:A:306:ASN:HD22	1:A:310:LYS:CA	2.29	0.45
1:A:340:GLY:C	1:A:341:VAL:HG13	2.41	0.45
1:B:218:ASP:O	1:B:269:ARG:NH1	2.49	0.45
1:B:301:ILE:HG22	1:B:302:THR:N	2.30	0.45
1:A:45:VAL:HG23	4:A:502:ANP:H2	1.92	0.45
1:A:94:HIS:CD2	1:A:263:ARG:HD3	2.47	0.45
1:B:80:MET:CG	4:B:502:ANP:O4'	2.47	0.45
1:B:404:LYS:N	1:B:404:LYS:HD2	2.30	0.45
1:B:429:LEU:H	1:B:429:LEU:CD1	2.27	0.45
1:A:147:ILE:N	1:A:165:SER:OG	2.46	0.45
1:A:173:SER:OG	1:A:174:LEU:N	2.50	0.45
1:A:429:LEU:HB3	1:A:430:PRO:HD2	1.98	0.45
1:A:269:ARG:HD2	1:A:269:ARG:HA	1.62	0.45
1:A:340:GLY:C	1:A:341:VAL:CG1	2.90	0.45
1:A:110:ARG:HD2	1:A:110:ARG:O	2.17	0.45
1:A:113:LYS:HB2	1:A:200:ASN:HB3	1.98	0.45
1:A:175:PHE:CD2	1:A:175:PHE:N	2.85	0.45
1:B:72:MET:HB3	1:B:76:LYS:HB3	1.99	0.45
1:B:421:LYS:CG	1:B:451:GLU:OE1	2.50	0.45
1:A:26:HIS:CD2	1:A:31:SER:OG	2.70	0.45
1:A:410:TRP:CZ2	2:P:6:THR:HG21	2.51	0.45
1:B:287:ARG:NH2	1:B:300:ARG:HD2	2.32	0.45
1:B:174:LEU:HD12	1:B:174:LEU:HA	1.76	0.45
1:B:260:LEU:HB3	1:B:321:ASN:OD1	2.17	0.45
1:A:94:HIS:HD2	1:A:263:ARG:CZ	2.29	0.44
1:A:434:TYR:O	1:A:437:ASN:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:OD2	1:A:322:ARG:NE	2.48	0.44
1:A:133:THR:O	1:A:137:VAL:HG23	2.17	0.44
1:B:118:PHE:CD2	1:B:118:PHE:N	2.86	0.44
1:A:82:SER:O	1:A:105:LYS:CE	2.65	0.44
1:A:166:LEU:CD2	1:A:170:LEU:CD1	2.94	0.44
1:A:295:LEU:HD22	1:A:297:ARG:NE	2.33	0.44
1:A:432:LYS:HA	2:P:1:ALA:HB2	2.00	0.44
1:B:204:TYR:CD2	1:B:204:TYR:O	2.70	0.44
1:B:239:ARG:C	1:B:242:GLN:OE1	2.61	0.44
1:B:420:ARG:NH2	1:B:435:CYS:SG	2.85	0.44
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.87	0.44
1:A:322:ARG:NH1	1:A:322:ARG:CG	2.72	0.44
1:B:217:TYR:CB	1:B:405:ARG:HH12	2.28	0.44
1:B:264:MET:HE3	1:B:264:MET:HB3	1.77	0.44
1:B:377:LYS:O	1:B:380:ASP:HB2	2.18	0.44
1:A:54:LYS:C	1:A:54:LYS:CD	2.91	0.44
1:A:268:ILE:O	1:A:269:ARG:HB2	2.18	0.44
1:A:282:LEU:HG	1:A:304:GLY:HA3	2.00	0.44
1:B:158:ASN:N	1:B:159:LEU:HD13	2.33	0.44
1:B:339:MET:HB2	1:B:339:MET:HE3	1.70	0.44
1:B:175:PHE:CE1	1:B:184:GLU:HG3	2.52	0.43
1:A:289:VAL:O	1:A:377:LYS:HE2	2.18	0.43
1:A:406:PRO:O	2:P:8:ARG:HD2	2.18	0.43
1:A:407:ASP:HB3	2:P:6:THR:O	2.19	0.43
1:A:424:ASP:OD1	1:A:424:ASP:N	2.48	0.43
1:B:287:ARG:HE	1:B:287:ARG:HB3	1.53	0.43
1:B:316:MET:N	1:B:345:GLY:O	2.39	0.43
1:B:418:LYS:CE	1:B:446:CYS:O	2.65	0.43
1:A:26:HIS:CD2	1:A:357:ASN:HB2	2.53	0.43
1:A:77:LEU:HD23	1:A:147:ILE:HD13	2.00	0.43
1:A:185:LEU:HA	1:A:185:LEU:HD23	1.75	0.43
1:B:117:VAL:O	1:B:127:VAL:HA	2.18	0.43
1:B:129:PHE:CE1	1:B:131:SER:HB2	2.53	0.43
1:B:159:LEU:HD22	1:B:159:LEU:N	2.04	0.43
1:B:157:ILE:O	1:B:158:ASN:HB2	2.18	0.43
1:B:160:THR:OG1	1:B:161:GLU:N	2.52	0.43
1:A:120:LYS:HE3	1:A:185:LEU:O	2.17	0.43
1:B:118:PHE:O	1:B:194:THR:HG23	2.19	0.43
1:B:246:GLU:HB3	1:B:253:ALA:CB	2.49	0.43
1:B:165:SER:O	1:B:169:ILE:HG13	2.19	0.43
1:B:278:VAL:HA	1:B:281:SER:CB	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:O	1:A:165:SER:CB	2.67	0.43
1:B:153:HIS:C	1:B:155:GLN:H	2.27	0.43
1:A:82:SER:O	1:A:105:LYS:HE2	2.19	0.43
1:A:169:ILE:O	1:A:173:SER:HB2	2.17	0.43
1:A:79:LYS:HA	1:A:82:SER:HB2	2.01	0.43
1:B:153:HIS:ND1	1:B:153:HIS:N	2.65	0.43
1:B:252:ARG:HG3	1:B:273:VAL:HG13	2.01	0.43
1:A:442:GLN:C	1:A:443:PHE:HD2	2.25	0.42
1:B:268:ILE:O	1:B:269:ARG:HB2	2.19	0.42
1:A:116:MET:HG3	1:A:117:VAL:H	1.84	0.42
1:B:152:LYS:HG3	1:B:153:HIS:CE1	2.55	0.42
1:B:269:ARG:HA	1:B:269:ARG:HD2	1.63	0.42
1:B:277:LEU:HD23	1:B:277:LEU:C	2.39	0.42
1:B:317:MET:HE3	1:B:325:LYS:HD3	2.01	0.42
1:A:385:MET:C	1:A:387:VAL:N	2.75	0.42
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.86	0.42
4:B:502:ANP:O2B	4:B:502:ANP:O1A	2.38	0.42
1:A:320:LYS:O	1:A:321:ASN:HB3	2.20	0.42
1:B:329:LYS:N	1:B:329:LYS:HD3	2.34	0.42
1:B:420:ARG:NH2	1:B:448:VAL:HG13	2.35	0.42
1:A:114:ASP:CG	1:A:131:SER:HB2	2.39	0.42
1:A:410:TRP:O	2:P:3:THR:HA	2.19	0.42
1:A:239:ARG:N	1:A:239:ARG:CD	2.73	0.42
1:A:289:VAL:O	1:A:377:LYS:CE	2.68	0.42
1:A:40:ALA:CA	1:A:45:VAL:HG11	2.39	0.41
1:A:135:LEU:HD23	1:A:140:ALA:HB3	2.02	0.41
1:A:316:MET:CE	1:A:327:TYR:CD1	3.02	0.41
1:B:319:HIS:NE2	1:B:320:LYS:HD2	2.35	0.41
1:A:134:TYR:CE1	1:A:138:ILE:HD13	2.55	0.41
1:A:445:ASN:C	1:A:448:VAL:HG23	2.42	0.41
1:B:315:ILE:HG22	1:B:316:MET:N	2.34	0.41
1:B:175:PHE:HE1	1:B:184:GLU:HG3	1.84	0.41
1:A:116:MET:HE2	1:A:116:MET:HB2	1.72	0.41
1:A:184:GLU:OE2	1:A:184:GLU:HA	2.20	0.41
1:A:389:LYS:HD3	1:A:389:LYS:O	2.19	0.41
1:A:307:CYS:O	1:A:308:ARG:HB3	2.21	0.41
1:B:320:LYS:O	1:B:321:ASN:HB3	2.20	0.41
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.84	0.41
1:A:89:VAL:HG23	1:A:91:MET:HE3	2.02	0.41
1:A:125:MET:HB3	1:A:125:MET:HE2	1.76	0.41
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:TYR:OH	1:B:354:PRO:O	2.28	0.41
1:B:135:LEU:HA	1:B:135:LEU:HD23	1.82	0.41
1:B:153:HIS:C	1:B:155:GLN:N	2.79	0.41
1:B:318:TYR:HA	1:B:322:ARG:O	2.20	0.41
1:A:114:ASP:CB	1:A:131:SER:HB2	2.51	0.41
1:A:410:TRP:HZ2	2:P:6:THR:HG21	1.86	0.41
2:Q:6:THR:HG23	2:Q:7:ALA:H	1.86	0.41
1:A:301:ILE:HG12	1:A:347:ILE:HD12	2.02	0.40
1:B:201:LEU:N	1:B:201:LEU:CD1	2.83	0.40
1:A:72:MET:HE3	4:A:502:ANP:C2	2.45	0.40
1:B:83:PHE:HD1	1:B:83:PHE:H	1.69	0.40
2:Q:4:LYS:HG2	2:Q:5:GLN:H	1.85	0.40
1:A:81:LEU:HB3	1:A:145:VAL:HG11	2.02	0.40
1:A:94:HIS:CD2	1:A:263:ARG:CZ	3.03	0.40
1:A:307:CYS:HA	1:A:310:LYS:HE3	2.02	0.40
1:A:352:LEU:HB3	1:A:361:PHE:CD1	2.56	0.40
1:B:116:MET:CE	1:B:169:ILE:HG23	2.51	0.40
1:B:150:PHE:HA	1:B:155:GLN:O	2.21	0.40
1:B:291:ARG:HG3	1:B:298:THR:CG2	2.50	0.40
1:B:351:PHE:CD1	1:B:352:LEU:CD2	3.03	0.40
1:A:55:THR:OG1	1:A:56:VAL:N	2.54	0.40
1:B:278:VAL:C	1:B:281:SER:H	2.28	0.40
1:B:429:LEU:HB3	1:B:430:PRO:HD2	2.03	0.40
1:A:431:GLU:O	1:A:432:LYS:HG3	2.22	0.40
1:A:438:ASN:ND2	1:A:443:PHE:HB2	2.36	0.40
1:B:51:TRP:NE1	1:B:267:ILE:HD13	2.36	0.40
1:B:322:ARG:HH22	1:B:358:LYS:HB2	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/451 (91%)	402 (98%)	8 (2%)	0	100	100
1	B	414/451 (92%)	406 (98%)	8 (2%)	0	100	100
2	P	8/32 (25%)	8 (100%)	0	0	100	100
2	Q	8/32 (25%)	7 (88%)	1 (12%)	0	100	100
All	All	840/966 (87%)	823 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/403 (93%)	299 (80%)	77 (20%)	1	4
1	B	378/403 (94%)	313 (83%)	65 (17%)	2	7
2	P	8/22 (36%)	5 (62%)	3 (38%)	0	0
2	Q	8/22 (36%)	6 (75%)	2 (25%)	0	2
All	All	770/850 (91%)	623 (81%)	147 (19%)	1	5

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	14	LEU
1	A	36	LEU
1	A	41	TYR
1	A	45	VAL
1	A	50	ILE
1	A	53	ASP
1	A	54	LYS
1	A	59	ASP
1	A	63	LEU
1	A	70	ASN
1	A	72	MET
1	A	73	THR

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Mol	Chain	Res	Type
1	A	76	LYS
1	A	80	MET
1	A	89	VAL
1	A	91	MET
1	A	92	ASN
1	A	116	MET
1	A	126	SER
1	A	131	SER
1	A	133	THR
1	A	136	GLU
1	A	149	THR
1	A	151	ASN
1	A	152	LYS
1	A	154	ARG
1	A	156	MET
1	A	159	LEU
1	A	160	THR
1	A	163	LYS
1	A	170	LEU
1	A	176	SER
1	A	180	LYS
1	A	191	LYS
1	A	194	THR
1	A	195	ARG
1	A	202	ARG
1	A	223	GLU
1	A	235	LYS
1	A	238	GLU
1	A	239	ARG
1	A	243	ILE
1	A	247	SER
1	A	256	SER
1	A	269	ARG
1	A	274	LYS
1	A	277	LEU
1	A	279	SER
1	A	282	LEU
1	A	287	ARG
1	A	291	ARG
1	A	293	LYS
1	A	297	ARG
1	A	307	CYS

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Mol	Chain	Res	Type
1	A	316	MET
1	A	322	ARG
1	A	325	LYS
1	A	332	CYS
1	A	349	CYS
1	A	372	LEU
1	A	377	LYS
1	A	384	GLU
1	A	385	MET
1	A	386	LYS
1	A	388	LYS
1	A	389	LYS
1	A	404	LYS
1	A	410	TRP
1	A	412	GLN
1	A	413	CYS
1	A	417	LEU
1	A	418	LYS
1	A	421	LYS
1	A	422	LEU
1	A	443	PHE
1	A	445	ASN
1	B	12	SER
1	B	16	PRO
1	B	22	ASN
1	B	24	THR
1	B	41	TYR
1	B	45	VAL
1	B	50	ILE
1	B	53	ASP
1	B	54	LYS
1	B	59	ASP
1	B	63	LEU
1	B	75	ASP
1	B	83	PHE
1	B	89	VAL
1	B	99	LEU
1	B	105	LYS
1	B	108	SER
1	B	114	ASP
1	B	123	GLU
1	B	125	MET

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Mol	Chain	Res	Type
1	B	126	SER
1	B	141	GLU
1	B	152	LYS
1	B	153	HIS
1	B	154	ARG
1	B	156	MET
1	B	159	LEU
1	B	169	ILE
1	B	176	SER
1	B	201	LEU
1	B	204	TYR
1	B	223	GLU
1	B	224	ASP
1	B	235	LYS
1	B	236	LYS
1	B	238	GLU
1	B	243	ILE
1	B	247	SER
1	B	264	MET
1	B	269	ARG
1	B	274	LYS
1	B	281	SER
1	B	282	LEU
1	B	296	THR
1	B	297	ARG
1	B	298	THR
1	B	310	LYS
1	B	322	ARG
1	B	335	LYS
1	B	339	MET
1	B	349	CYS
1	B	353	LYS
1	B	376	GLU
1	B	385	MET
1	B	386	LYS
1	B	388	LYS
1	B	417	LEU
1	B	418	LYS
1	B	421	LYS
1	B	424	ASP
1	B	430	PRO
1	B	434	TYR

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Mol	Chain	Res	Type
1	B	435	CYS
1	B	446	CYS
1	B	453	GLU
2	P	4	LYS
2	P	9	LYS
2	P	10	SER
2	Q	6	THR
2	Q	9	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	151	ASN
1	A	172	HIS
1	A	306	ASN
1	A	321	ASN
1	A	408	GLN
1	A	442	GLN
1	A	445	ASN
1	B	22	ASN
1	B	102	ASN
1	B	142	HIS
1	B	306	ASN
1	B	309	ASN
1	B	337	ASN
1	B	408	GLN

5.3.3 RNA [i](#)

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

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	A	502	5	33,33,33	2.17	14 (42%)	45,52,52	2.51	16 (35%)
4	ANP	B	502	5	33,33,33	1.03	5 (15%)	45,52,52	1.09	4 (8%)

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	502	5	-	5/18/38/38	0/3/3/3
4	ANP	B	502	5	-	3/18/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ANP	PA-O3A	-4.54	1.54	1.59
4	A	502	ANP	PG-O3G	-4.04	1.46	1.56
4	A	502	ANP	PB-O2B	-3.95	1.46	1.56
4	A	502	ANP	C5-C4	3.37	1.45	1.39
4	A	502	ANP	C5-N7	-3.35	1.33	1.39
4	A	502	ANP	PB-N3B	3.13	1.71	1.63
4	A	502	ANP	PG-O2G	-3.08	1.48	1.56
4	A	502	ANP	C8-N9	-3.01	1.32	1.37
4	A	502	ANP	C4-N9	-2.93	1.31	1.37
4	A	502	ANP	PB-O3A	-2.66	1.55	1.59
4	B	502	ANP	PG-N3B	2.63	1.70	1.63
4	A	502	ANP	PG-N3B	2.62	1.70	1.63
4	B	502	ANP	PA-O3A	-2.39	1.56	1.59
4	A	502	ANP	C2'-C3'	-2.33	1.47	1.53
4	B	502	ANP	PB-N3B	2.17	1.69	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	ANP	PB-O1B	2.10	1.49	1.46
4	A	502	ANP	O4'-C4'	-2.08	1.40	1.45
4	A	502	ANP	PA-O2A	-2.08	1.45	1.55
4	B	502	ANP	PG-O1G	2.06	1.49	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	ANP	O1B-PB-N3B	-6.57	102.10	111.77
4	A	502	ANP	O2B-PB-O1B	5.99	122.72	109.87
4	A	502	ANP	C5-C4-N3	-5.71	118.86	126.72
4	A	502	ANP	O1G-PG-N3B	-5.46	103.73	111.77
4	A	502	ANP	N3-C4-N9	4.59	134.98	127.17
4	A	502	ANP	C2-N3-C4	3.45	120.26	111.83
4	A	502	ANP	C4-C5-N7	-3.25	106.87	110.58
4	A	502	ANP	O2G-PG-O3G	3.19	116.17	107.59
4	A	502	ANP	N3-C2-N1	-3.06	123.95	128.58
4	A	502	ANP	O2A-PA-O3A	2.98	115.33	107.27
4	A	502	ANP	O3'-C3'-C2'	-2.97	102.30	111.82
4	B	502	ANP	O2A-PA-O3A	2.89	115.08	107.27
4	B	502	ANP	O1G-PG-N3B	-2.72	107.77	111.77
4	A	502	ANP	C4-N9-C8	2.71	108.58	105.74
4	A	502	ANP	O2'-C2'-C3'	-2.70	103.15	111.82
4	B	502	ANP	O3G-PG-O1G	-2.60	106.94	113.45
4	B	502	ANP	O1B-PB-N3B	-2.52	108.06	111.77
4	A	502	ANP	C2'-C1'-N9	-2.34	107.50	113.30
4	A	502	ANP	C5-N7-C8	2.20	106.91	103.45
4	A	502	ANP	C3'-C2'-C1'	2.11	105.45	101.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

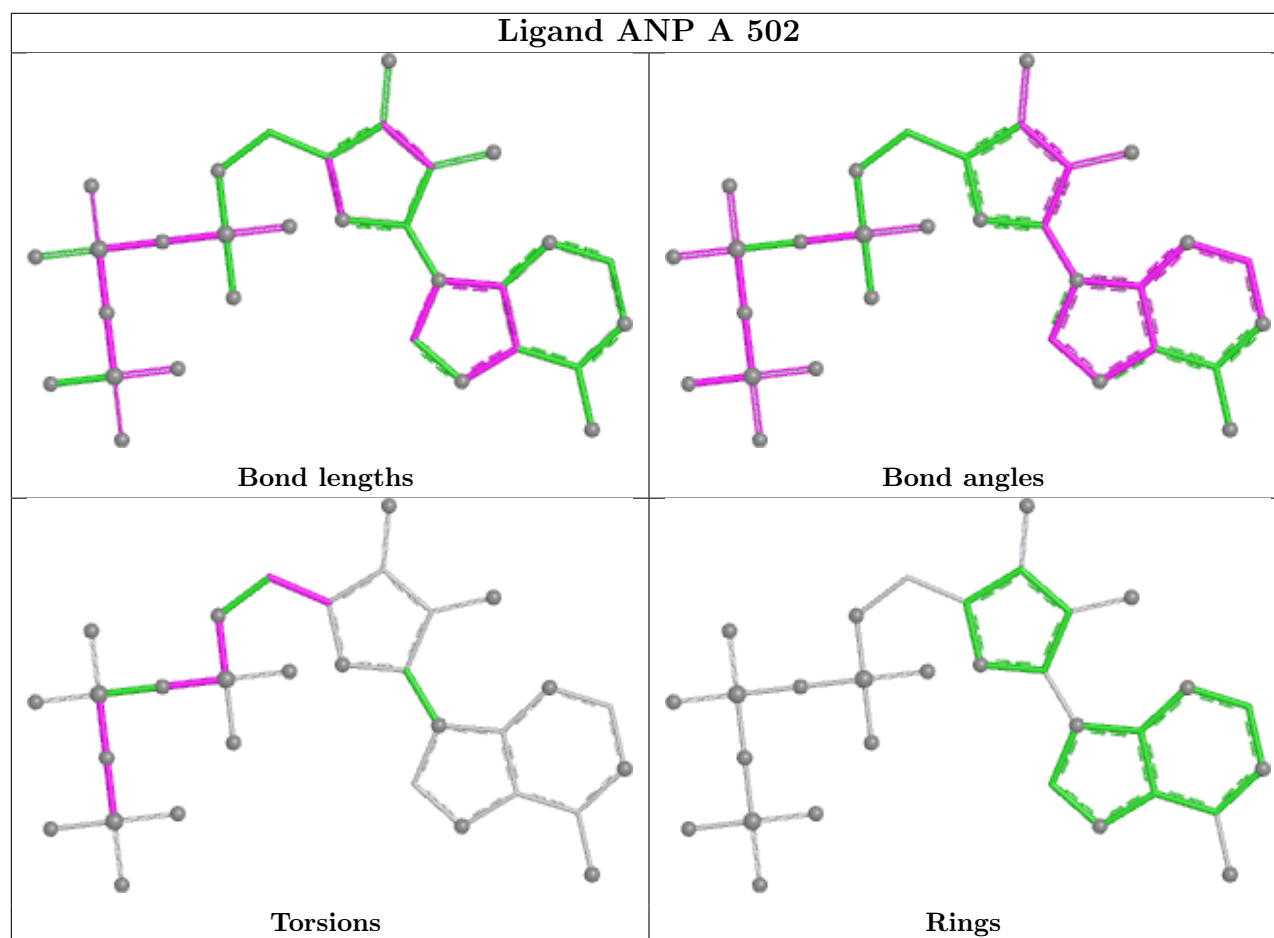
Mol	Chain	Res	Type	Atoms
4	A	502	ANP	PB-N3B-PG-O1G
4	A	502	ANP	PG-N3B-PB-O1B
4	A	502	ANP	C5'-O5'-PA-O1A
4	B	502	ANP	PA-O3A-PB-O2B
4	B	502	ANP	O4'-C4'-C5'-O5'
4	B	502	ANP	C3'-C4'-C5'-O5'
4	A	502	ANP	PB-O3A-PA-O5'
4	A	502	ANP	O4'-C4'-C5'-O5'

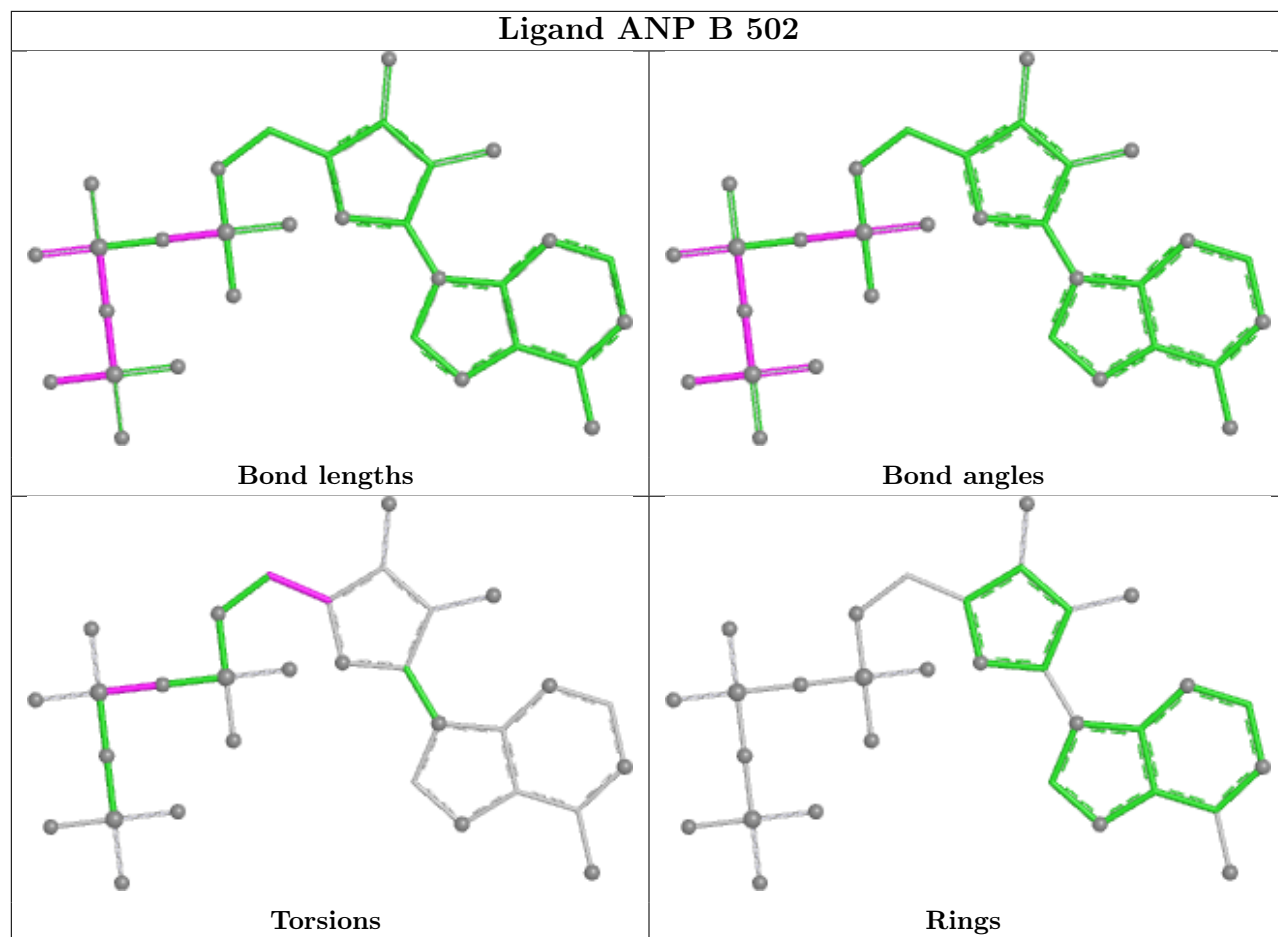
There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	ANP	20	0
4	B	502	ANP	7	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	A	420/451 (93%)	0.05	10 (2%) 59 50	53, 76, 112, 141	0
1	B	422/451 (93%)	0.02	9 (2%) 63 54	52, 76, 113, 142	0
2	P	10/32 (31%)	0.34	0 100 100	86, 98, 107, 116	0
2	Q	10/32 (31%)	0.81	1 (10%) 12 10	89, 99, 115, 117	0
All	All	862/966 (89%)	0.05	20 (2%) 61 52	52, 77, 113, 142	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	224	ASP	5.6
1	A	415	ALA	3.5
1	A	340	GLY	3.4
1	B	311	ASP	3.1
1	B	204	TYR	3.1
1	B	312	HIS	3.1
1	A	391	ALA	2.8
1	A	338	ASN	2.7
1	B	389	LYS	2.6
1	A	307	CYS	2.4
1	A	305	PHE	2.3
1	B	445	ASN	2.3
1	A	387	VAL	2.3
1	A	144	VAL	2.3
1	A	151	ASN	2.2
1	A	445	ASN	2.2
1	B	421	LYS	2.2
1	B	305	PHE	2.1
2	Q	9	LYS	2.0
1	B	309	ASN	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](#)

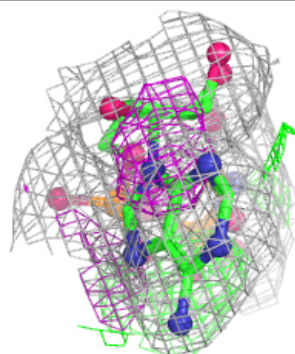
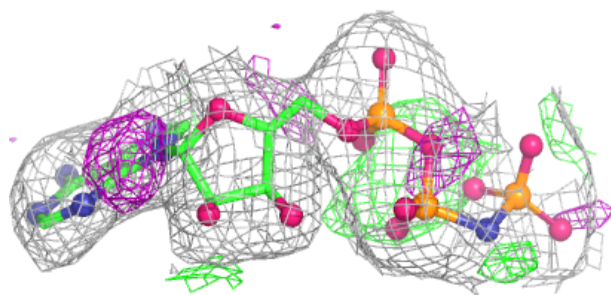
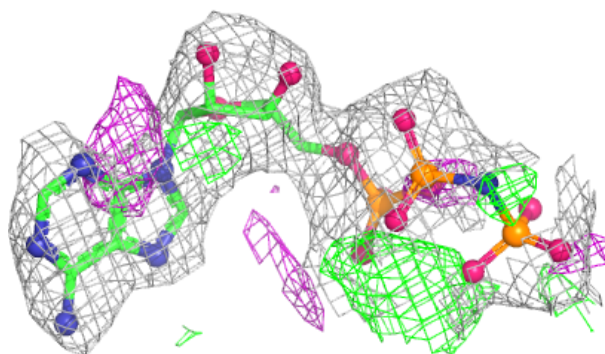
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	MG	B	503	1/1	0.57	0.23	61,61,61,61	0
5	MG	A	503	1/1	0.78	0.15	56,56,56,56	0
3	ZN	A	501	1/1	0.85	0.13	92,92,92,92	0
4	ANP	A	502	31/31	0.91	0.11	38,67,74,134	0
3	ZN	B	501	1/1	0.93	0.07	84,84,84,84	0
4	ANP	B	502	31/31	0.93	0.11	31,57,70,71	0

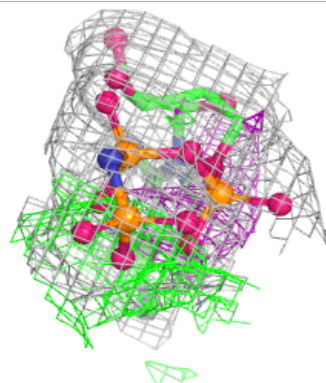
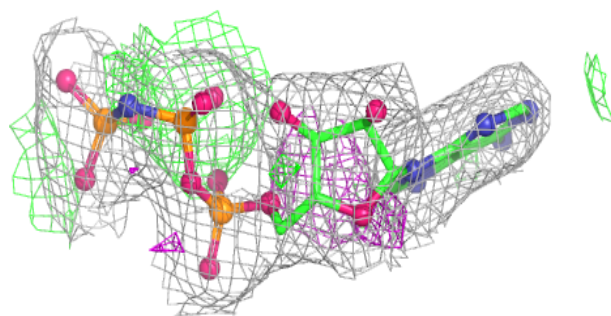
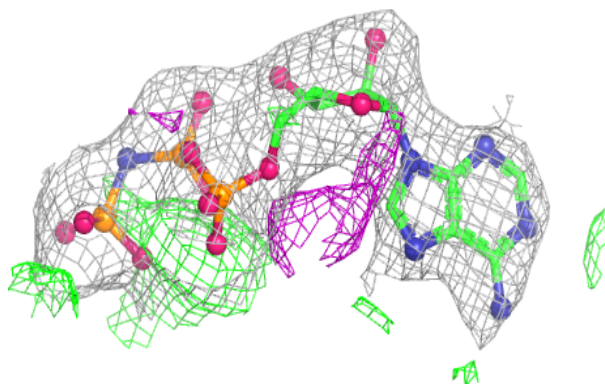
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 502:

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

**Electron density around ANP B 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.