Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 06:54 pm BST

PDB ID	:	1W5T
Title	:	Structure of the Aeropyrum Pernix ORC2 protein (ADPNP-ADP complexes)
Authors	:	Singleton, M.R.; Morales, R.; Grainge, I.; Cook, N.; Isupov, M.N.; Wigley, D.B.
Deposited on	:	2004-08-09
Resolution	:	2.40 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:

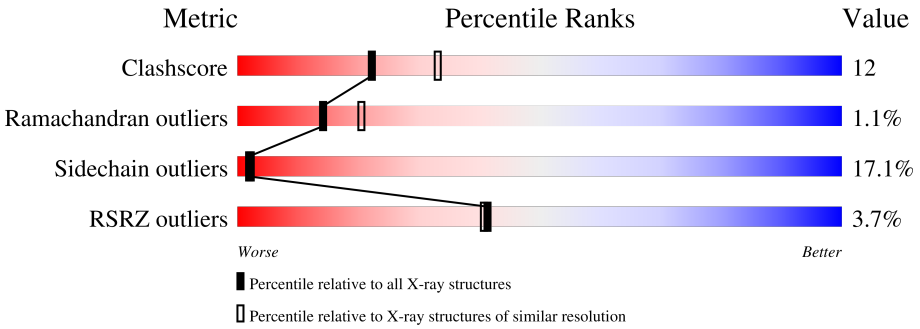
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	412	68% 21% 7%
1	B	412	3% 66% 23% 7%
1	C	412	7% 57% 29% 8%

2 Entry composition

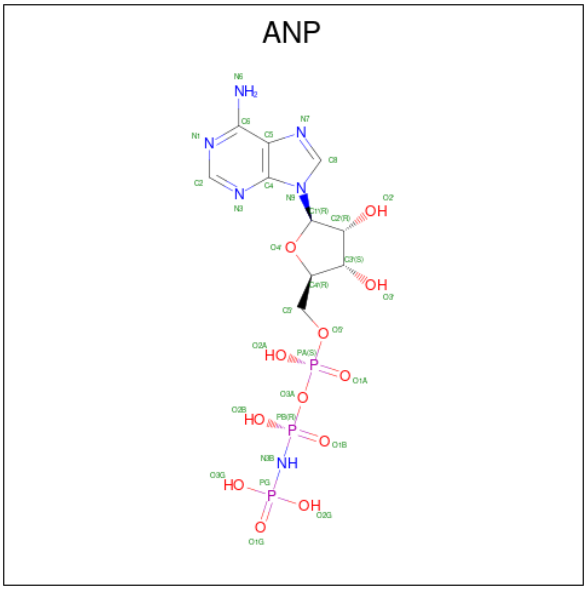
There are 5 unique types of molecules in this entry. The entry contains 9573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ORC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	1
			3109	1976	549	574	10			
1	B	397	Total	C	N	O	S	0	0	1
			3123	1984	551	578	10			
1	C	394	Total	C	N	O	S	0	0	2
			3099	1970	548	571	10			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

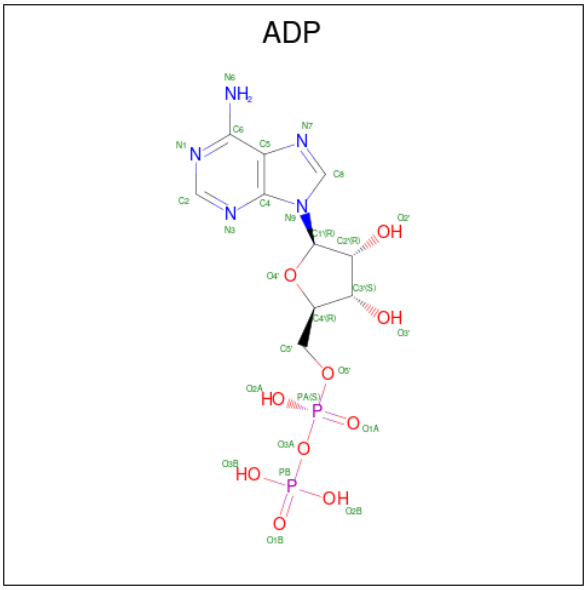


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 5 is water.

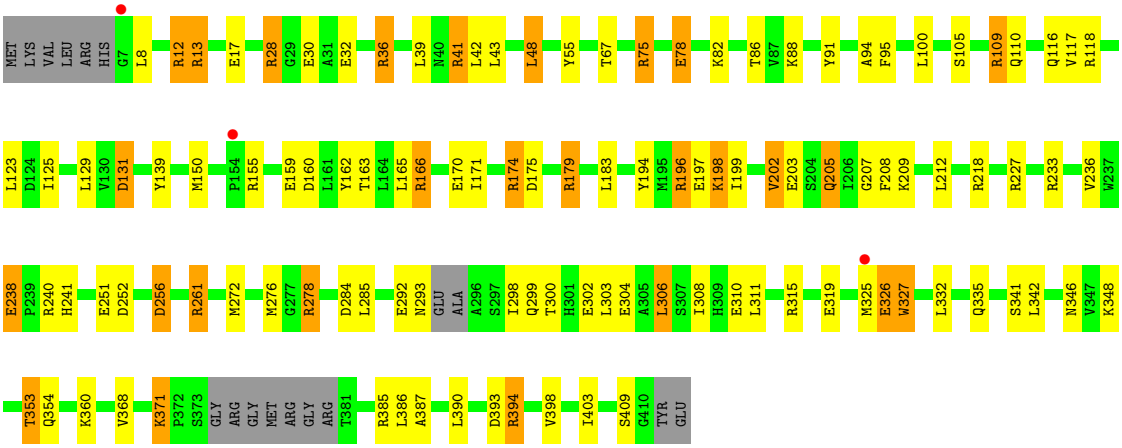
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	63	Total O 63 63	0	0
5	B	40	Total O 40 40	0	0
5	C	47	Total O 47 47	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

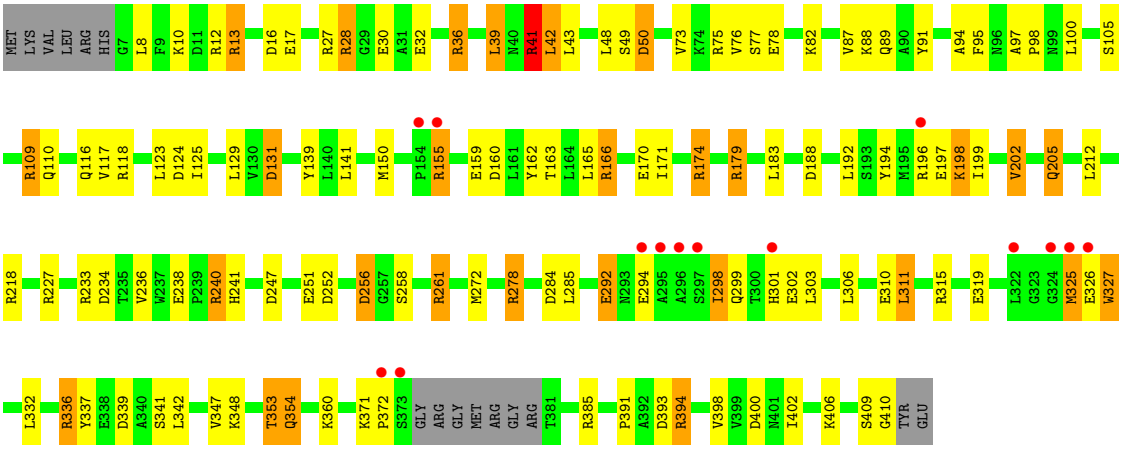
• Molecule 1: ORC2

Chain A:



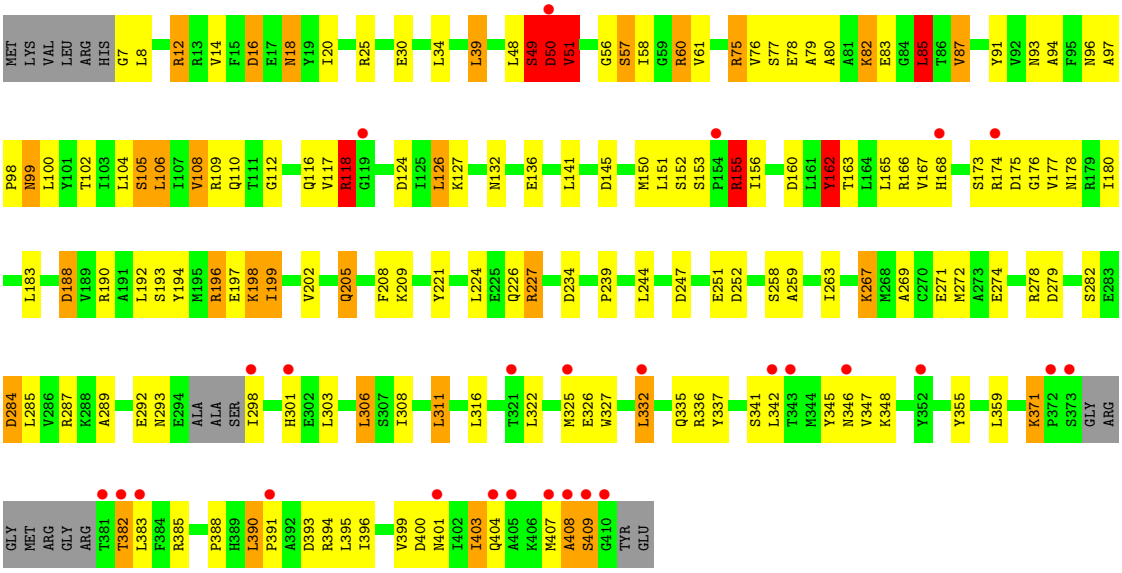
• Molecule 1: ORC2

Chain B:



• Molecule 1: ORC2

Chain C:


MET LYS VAL LEU ARG HIS G7 L8 R12 R13 V14 F15 D16 E17 N18 Y19 I20 R25 E30 L34 L39 L48 S49 D50 V51 G56 S57 I58 G59 R60 V61 R75 V76 S77 E78 A79 A80 A81 K82 E83 G84 L85 T86 V87 Y91 V92 N93 A94 F95 N96 A97
P98 N99 L100 Y101 T102 I103 L104 S105 L106 I107 V108 R109 Q110 T111 G112 Q116 V117 R118 G119 D124 I125 L126 K127 N132 E136 L141 D145 M150 L151 S152 S153 P154 R155 I156 D160 L161 V162 T163 L164 L165 R166 V167 H168 S173 R174 D175 G176 V177 N178 R179 I180
L183 D188 V189 R190 A191 L192 S193 Y194 M195 R196 E197 K198 I199 V202 Q205 F208 K209 Y221 L224 E225 Q226 R227 D234 P239 L244 D247 E251 D252 S258 A259 I263 K267 M268 A269 C270 E271 M272 A273 E274 R278 D279 S282 E283
D284 L285 V286 R287 K288 A289 E292 N293 E294 ALA ALA SER I298 H301 E302 L303 L306 S307 I308 L311 L316 T321 L322 M325 E326 W327 L332 Q335 R336 Y337 S341 L342 T343 M344 Y345 N346 V347 K348 Y352 Y355 L359 K371 P372 S373 GLY ARG
GLY MET ARG GLY ARG T381 T382 L383 F384 R385 P388 H389 L390 P391 A392 D393 R394 L395 I396 V399 D400 N401 I402 I403 Q404 A405 K406 M407 A408 S409 G410 TYR GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	61.49Å 61.49Å 267.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.40) 90.7 (19.90-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.211 , 0.279 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.065 for h,-h-k,-l 0.066 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9573	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ADP, 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	0.76	0/3159	1.12	31/4272 (0.7%)
1	B	0.78	0/3174	1.17	43/4294 (1.0%)
1	C	0.79	5/3149 (0.2%)	0.98	14/4259 (0.3%)
All	All	0.78	5/9482 (0.1%)	1.09	88/12825 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	TYR	CB-CG	6.55	1.61	1.51
1	C	162	TYR	CD1-CE1	6.30	1.48	1.39
1	C	162	TYR	CD2-CE2	5.74	1.48	1.39
1	C	162	TYR	CE1-CZ	5.70	1.46	1.38
1	C	409	SER	C-N	-5.02	1.24	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109	ARG	NE-CZ-NH1	12.99	126.79	120.30
1	B	41	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	B	179	ARG	NE-CZ-NH1	-11.58	114.51	120.30
1	B	179	ARG	NE-CZ-NH2	10.37	125.48	120.30
1	A	12	ARG	NE-CZ-NH1	-9.90	115.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	28	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	A	174	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	240	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	B	41	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	B	240	ARG	NE-CZ-NH1	-9.39	115.61	120.30
1	A	13	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	12	ARG	NE-CZ-NH2	9.26	124.93	120.30
1	A	13	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	A	240	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	B	261	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	C	293	ASN	O-C-N	-8.87	108.51	122.70
1	B	12	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	28	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	A	409	SER	O-C-N	-8.79	108.26	123.20
1	B	109	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	261	ARG	NE-CZ-NH1	-8.59	116.01	120.30
1	A	28	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	A	261	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	179	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	409	SER	O-C-N	-8.00	109.60	123.20
1	A	109	ARG	NE-CZ-NH2	7.99	124.30	120.30
1	C	393	ASP	CB-CG-OD2	7.90	125.41	118.30
1	B	240	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	B	284	ASP	CB-CG-OD2	7.85	125.37	118.30
1	A	233	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	B	12	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	284	ASP	CB-CG-OD2	7.59	125.14	118.30
1	B	174	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	A	174	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	278	ARG	NE-CZ-NH1	-7.47	116.57	120.30
1	A	28	ARG	NE-CZ-NH1	-7.29	116.65	120.30
1	B	174	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	A	41	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	B	75	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	C	284	ASP	CB-CG-OD2	7.06	124.65	118.30
1	B	278	ARG	NE-CZ-NH2	6.99	123.79	120.30
1	A	75	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	233	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	234	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	16	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	252	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	252	ASP	CB-CG-OD2	6.59	124.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	196	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	75	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	233	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	B	13	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	179	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	188	ASP	CB-CG-OD2	6.26	123.94	118.30
1	B	339	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	175	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	252	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	233	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	B	131	ASP	CB-CG-OD2	6.05	123.75	118.30
1	C	50	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	179	ARG	CD-NE-CZ	5.94	131.92	123.60
1	B	261	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	393	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	109	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	A	41	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	C	85	LEU	CA-CB-CG	5.77	128.58	115.30
1	B	109	ARG	CD-NE-CZ	5.73	131.62	123.60
1	C	124	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	27	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	13	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	400	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	393	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	247	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	409	SER	CA-C-N	5.47	127.15	116.20
1	B	50	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	75	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	C	196	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	234	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	400	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	311	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	278	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	42	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	124	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	278	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	C	188	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	106	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	247	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	131	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	409	SER	CA-C-N	5.01	126.23	116.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	155	ARG	Peptide
1	C	48	LEU	Peptide
1	C	49	SER	Peptide

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	3109	0	3185	57	0
1	B	3123	0	3197	59	0
1	C	3099	0	3176	112	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	C	27	0	12	1	0
5	A	63	0	0	7	0
5	B	40	0	0	6	0
5	C	47	0	0	22	0
All	All	9573	0	9596	222	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 12.

All (222) 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:C:153:SER:OG	1:C:155:ARG:HG3	1.57	1.02
1:C:166:ARG:CG	1:C:205:GLN:HE22	1.73	0.99
1:C:162:TYR:CD2	1:C:202:VAL:CG1	2.48	0.96
1:B:91:TYR:H	1:B:110:GLN:HE22	1.10	0.95
1:A:55:TYR:OH	1:C:209:LYS:HE3	1.67	0.95
1:C:162:TYR:CD2	1:C:202:VAL:HG13	2.01	0.94
1:C:162:TYR:CE2	1:C:202:VAL:HG13	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:TYR:CZ	1:C:199:ILE:HG22	2.06	0.91
1:C:224:LEU:HD23	5:C:2036:HOH:O	1.69	0.91
1:C:75:ARG:HD2	5:C:2012:HOH:O	1.70	0.90
1:C:168:HIS:CD2	1:C:178:ASN:HB3	2.08	0.89
1:C:166:ARG:HG3	1:C:205:GLN:HE22	1.36	0.89
1:C:105:SER:HB3	1:C:117:VAL:HG11	1.53	0.88
1:C:263:ILE:HG12	5:C:2036:HOH:O	1.74	0.86
1:C:166:ARG:HG3	1:C:205:GLN:NE2	1.91	0.84
1:B:238:GLU:H	1:B:241:HIS:HD2	1.23	0.84
1:A:91:TYR:H	1:A:110:GLN:HE22	1.28	0.81
1:C:91:TYR:H	1:C:110:GLN:HE22	1.28	0.81
1:B:179:ARG:HD2	5:B:2020:HOH:O	1.82	0.78
1:B:91:TYR:H	1:B:110:GLN:NE2	1.82	0.76
1:C:199:ILE:HB	1:C:202:VAL:HG22	1.65	0.76
1:A:116:GLN:HE21	1:A:118:ARG:H	1.33	0.76
1:B:354:GLN:HE21	1:B:354:GLN:HA	1.51	0.76
1:C:77:SER:HA	1:C:87:VAL:HG13	1.71	0.73
1:A:166:ARG:HE	1:A:205:GLN:NE2	1.87	0.73
1:B:123:LEU:HD12	1:B:171:ILE:HD11	1.70	0.73
1:C:118:ARG:HA	1:C:118:ARG:HE	1.53	0.73
1:C:162:TYR:HD2	1:C:202:VAL:CG1	2.02	0.72
1:A:199:ILE:HB	1:A:202:VAL:HG13	1.71	0.72
1:A:385:ARG:HG3	1:A:386:LEU:O	1.91	0.71
1:C:83:GLU:HB3	5:C:2017:HOH:O	1.89	0.71
1:B:41:ARG:HD2	1:B:50:ASP:OD1	1.91	0.71
1:A:196:ARG:NH2	1:C:193:SER:OG	2.22	0.71
1:B:116:GLN:HE21	1:B:118:ARG:H	1.38	0.71
1:C:18:ASN:HB3	5:C:2006:HOH:O	1.91	0.69
1:A:105:SER:HB3	1:A:117:VAL:HG21	1.74	0.69
1:B:238:GLU:H	1:B:241:HIS:CD2	2.09	0.68
1:A:100:LEU:HD22	1:A:160:ASP:HB3	1.76	0.67
1:A:166:ARG:HE	1:A:205:GLN:HE22	1.42	0.67
1:C:166:ARG:HG2	1:C:205:GLN:HE22	1.60	0.67
1:B:48:LEU:HD12	1:B:139:TYR:HB3	1.77	0.67
1:B:199:ILE:HB	1:B:202:VAL:HG13	1.77	0.66
1:B:109:ARG:NH2	5:B:2012:HOH:O	2.28	0.66
1:C:8:LEU:HG	1:C:274:GLU:HG3	1.77	0.66
1:B:166:ARG:HE	1:B:205:GLN:NE2	1.94	0.66
1:A:91:TYR:H	1:A:110:GLN:NE2	1.92	0.65
1:A:159:GLU:OE2	5:A:2033:HOH:O	2.15	0.65
1:C:162:TYR:HD2	1:C:202:VAL:HG12	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ARG:CG	1:C:205:GLN:NE2	2.51	0.65
1:C:272:MET:HE1	1:C:289:ALA:HB2	1.78	0.65
1:C:355:TYR:CE2	1:C:359:LEU:HD11	2.32	0.64
1:C:269:ALA:HA	1:C:272:MET:CE	2.28	0.64
1:A:117:VAL:HG23	1:A:125:ILE:CD1	2.27	0.64
1:B:298:ILE:HA	5:B:2031:HOH:O	1.97	0.63
1:C:145:ASP:HB3	5:C:2020:HOH:O	1.99	0.63
1:B:117:VAL:HG23	1:B:125:ILE:HD13	1.81	0.62
1:C:371:LYS:O	1:C:382:THR:OG1	2.18	0.62
1:C:118:ARG:HE	1:C:118:ARG:CA	2.11	0.62
1:A:48:LEU:HD12	1:A:139:TYR:HB3	1.82	0.62
1:C:284:ASP:HB3	5:C:2042:HOH:O	1.98	0.62
1:C:282:SER:HB3	5:C:2042:HOH:O	1.99	0.62
1:B:89:GLN:HB3	5:B:2009:HOH:O	2.03	0.59
1:A:55:TYR:HH	1:C:209:LYS:HE3	1.68	0.58
1:C:150:MET:HA	1:C:156:ILE:HD13	1.84	0.58
1:C:99:ASN:ND2	5:C:2022:HOH:O	2.36	0.58
1:A:123:LEU:HD12	1:A:171:ILE:HD11	1.84	0.58
1:A:117:VAL:HG23	1:A:125:ILE:HD13	1.84	0.58
1:B:272:MET:HB3	1:B:285:LEU:HD22	1.87	0.57
1:C:80:ALA:HB1	1:C:85:LEU:HB2	1.87	0.57
1:C:199:ILE:HD13	1:C:202:VAL:HG21	1.87	0.57
1:C:39:LEU:HD13	1:C:76:VAL:HG13	1.86	0.57
1:B:94:ALA:HB1	1:B:150:MET:HG3	1.87	0.57
1:B:117:VAL:HG23	1:B:125:ILE:CD1	2.35	0.56
1:A:196:ARG:HH22	1:C:190:ARG:HA	1.68	0.56
1:A:300:THR:O	1:A:304:GLU:HG3	2.06	0.56
1:B:100:LEU:HD22	1:B:160:ASP:HB3	1.88	0.56
1:C:94:ALA:HB2	1:C:150:MET:CE	2.35	0.56
1:A:238:GLU:H	1:A:241:HIS:HD2	1.54	0.56
1:C:244:LEU:HD11	1:C:287:ARG:NH1	2.21	0.55
1:B:8:LEU:HD23	1:B:236:VAL:HG13	1.89	0.55
1:C:155:ARG:HH21	1:C:156:ILE:HD12	1.72	0.55
1:B:105:SER:HB3	1:B:117:VAL:HG21	1.89	0.55
1:B:198:LYS:HG3	1:B:199:ILE:HG23	1.89	0.55
1:C:7:GLY:CA	5:C:2001:HOH:O	2.55	0.55
1:A:159:GLU:HB3	5:A:2033:HOH:O	2.06	0.54
1:C:50:ASP:C	1:C:51:VAL:HG23	2.27	0.54
1:C:269:ALA:HA	1:C:272:MET:HE3	1.89	0.54
1:C:94:ALA:HB2	1:C:150:MET:HE3	1.89	0.54
1:A:8:LEU:HD23	1:A:236:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:OH	5:C:2020:HOH:O	2.18	0.53
1:A:116:GLN:NE2	1:A:118:ARG:H	2.04	0.53
1:C:39:LEU:HD21	1:C:79:ALA:HB3	1.90	0.53
1:C:91:TYR:H	1:C:110:GLN:NE2	2.01	0.53
1:C:332:LEU:O	1:C:335:GLN:HB2	2.09	0.53
1:A:308:ILE:HG23	1:A:403:ILE:HG23	1.91	0.53
1:B:194:TYR:OH	1:B:198:LYS:HD3	2.09	0.53
1:C:282:SER:CB	5:C:2042:HOH:O	2.55	0.53
1:B:326:GLU:O	1:B:327:TRP:HB2	2.09	0.52
1:B:325:MET:HE1	1:B:336:ARG:HH22	1.75	0.52
1:C:306:LEU:HD23	1:C:311:LEU:HD13	1.90	0.52
1:C:259:ALA:O	1:C:263:ILE:HG13	2.10	0.52
1:A:387:ALA:HB3	1:A:390:LEU:HG	1.91	0.52
1:B:162:TYR:CE1	1:B:166:ARG:HD3	2.44	0.52
1:B:327:TRP:CZ3	1:B:385:ARG:HG2	2.45	0.52
1:B:298:ILE:HD11	1:B:303:LEU:HD11	1.91	0.51
1:A:196:ARG:CD	5:A:2041:HOH:O	2.58	0.51
1:A:198:LYS:HG3	1:A:199:ILE:HG23	1.93	0.51
1:C:153:SER:HG	1:C:155:ARG:HG3	1.71	0.51
1:A:390:LEU:HD21	5:A:2061:HOH:O	2.11	0.50
1:C:98:PRO:O	1:C:156:ILE:HD11	2.12	0.50
1:C:14:VAL:HG13	1:C:227:ARG:HD2	1.93	0.49
1:C:12:ARG:NH2	1:C:274:GLU:OE2	2.46	0.49
1:C:199:ILE:HD13	1:C:202:VAL:CG2	2.42	0.49
1:A:94:ALA:HB1	1:A:150:MET:HG3	1.95	0.49
1:C:98:PRO:O	1:C:156:ILE:CG1	2.61	0.49
1:C:116:GLN:HE21	1:C:118:ARG:HB2	1.77	0.48
1:A:303:LEU:O	1:A:306:LEU:HB2	2.13	0.48
1:C:93:ASN:HB2	5:C:2020:HOH:O	2.12	0.48
1:A:194:TYR:OH	1:A:198:LYS:HD3	2.14	0.48
1:C:56:GLY:HA3	5:C:2029:HOH:O	2.12	0.48
1:C:16:ASP:N	1:C:16:ASP:OD1	2.46	0.48
1:C:399:VAL:O	1:C:403:ILE:HB	2.13	0.47
1:B:91:TYR:N	1:B:110:GLN:HE22	1.93	0.47
1:C:198:LYS:HB3	1:C:199:ILE:HG13	1.96	0.47
1:B:298:ILE:HD11	1:B:303:LEU:CD1	2.44	0.47
1:B:353:THR:HG22	5:B:2036:HOH:O	2.14	0.47
1:C:112:GLY:HA2	5:C:2023:HOH:O	2.14	0.47
1:A:28:ARG:O	1:A:32:GLU:HG2	2.15	0.47
1:C:188:ASP:OD1	1:C:190:ARG:HB2	2.15	0.47
1:A:256:ASP:OD1	1:A:261:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLN:HA	1:B:354:GLN:NE2	2.25	0.47
1:C:316:LEU:HD11	1:C:337:TYR:HA	1.96	0.47
1:B:292:GLU:O	1:B:294:GLU:N	2.48	0.47
1:B:238:GLU:N	1:B:241:HIS:HD2	2.03	0.46
1:C:104:LEU:HD21	1:C:126:LEU:HD13	1.97	0.46
1:A:326:GLU:O	1:A:327:TRP:HB2	2.14	0.46
1:B:28:ARG:O	1:B:32:GLU:HG2	2.15	0.46
1:B:155:ARG:NH2	5:B:2016:HOH:O	2.48	0.46
1:C:14:VAL:CG1	1:C:227:ARG:HD2	2.46	0.46
1:C:345:TYR:O	1:C:407:MET:SD	2.73	0.46
1:A:36:ARG:HD3	1:A:36:ARG:HA	1.71	0.46
1:C:108:VAL:O	1:C:109:ARG:C	2.54	0.46
1:A:315:ARG:NH2	1:A:319:GLU:OE2	2.47	0.46
1:C:7:GLY:N	5:C:2001:HOH:O	2.48	0.46
1:A:238:GLU:H	1:A:241:HIS:CD2	2.34	0.46
1:C:303:LEU:HA	1:C:306:LEU:HD22	1.98	0.46
1:B:117:VAL:CG2	1:B:125:ILE:HD13	2.44	0.46
1:A:159:GLU:O	1:A:162:TYR:HB3	2.15	0.45
1:A:353:THR:HG22	1:A:354:GLN:N	2.31	0.45
1:C:151:LEU:C	1:C:153:SER:H	2.19	0.45
1:B:36:ARG:HD3	1:B:36:ARG:HA	1.79	0.45
1:A:105:SER:CB	1:A:117:VAL:HG21	2.44	0.45
1:B:327:TRP:CH2	1:B:385:ARG:HG2	2.52	0.45
1:C:93:ASN:ND2	5:C:2020:HOH:O	2.50	0.45
1:C:25:ARG:HD2	1:C:226:GLN:NE2	2.31	0.45
1:A:298:ILE:HD11	1:A:303:LEU:HD11	1.98	0.45
1:A:55:TYR:OH	1:C:209:LYS:CE	2.52	0.45
1:A:207:GLY:HA3	5:A:2014:HOH:O	2.17	0.45
1:A:208:PHE:CE1	1:C:208:PHE:HB2	2.52	0.45
1:C:224:LEU:HA	5:C:2036:HOH:O	2.17	0.45
1:A:261:ARG:NH1	1:A:293:ASN:O	2.50	0.45
1:A:394:ARG:O	1:A:398:VAL:HG23	2.17	0.45
1:C:30:GLU:O	1:C:34:LEU:HG	2.17	0.44
1:C:57:SER:HB3	1:C:60:ARG:HG3	1.99	0.44
1:A:179:ARG:NH2	5:A:2038:HOH:O	2.49	0.44
1:A:272:MET:HB3	1:A:285:LEU:HD22	2.00	0.44
1:C:78:GLU:O	1:C:82:LYS:HG2	2.17	0.44
1:C:408:ALA:HB1	5:C:2046:HOH:O	2.17	0.44
1:C:244:LEU:HD12	1:C:244:LEU:HA	1.73	0.44
1:C:99:ASN:O	1:C:102:THR:N	2.51	0.44
1:C:61:VAL:O	1:C:258:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:N	1:C:98:PRO:HD3	2.33	0.44
1:C:99:ASN:O	1:C:100:LEU:C	2.56	0.44
1:C:18:ASN:OD1	1:C:18:ASN:N	2.45	0.43
4:C:700:ADP:N1	5:C:2047:HOH:O	2.36	0.43
1:A:75:ARG:HA	1:A:78:GLU:HG3	2.01	0.43
1:C:267:LYS:O	1:C:271:GLU:HG2	2.18	0.43
1:A:162:TYR:CE1	1:A:166:ARG:HD3	2.53	0.43
1:B:371:LYS:HA	1:B:372:PRO:HD3	1.90	0.43
1:B:398:VAL:O	1:B:402:ILE:HG13	2.18	0.43
1:C:168:HIS:CG	1:C:178:ASN:HB3	2.51	0.43
1:B:123:LEU:CD1	1:B:171:ILE:HD11	2.45	0.43
1:B:97:ALA:HA	1:B:98:PRO:HD2	1.91	0.43
1:C:385:ARG:NH2	1:C:388:PRO:HD3	2.33	0.43
1:B:105:SER:CB	1:B:117:VAL:HG21	2.49	0.43
1:B:166:ARG:HE	1:B:205:GLN:HE22	1.62	0.43
1:A:276:MET:SD	1:A:285:LEU:HD21	2.58	0.42
1:C:175:ASP:C	1:C:177:VAL:H	2.23	0.42
1:C:227:ARG:HA	1:C:227:ARG:HD3	1.58	0.42
1:C:194:TYR:CZ	1:C:198:LYS:HG3	2.55	0.42
1:C:98:PRO:O	1:C:156:ILE:HG13	2.18	0.42
1:C:100:LEU:HD22	1:C:160:ASP:HB3	2.00	0.42
1:C:272:MET:HB3	1:C:285:LEU:HD22	2.02	0.42
1:A:163:THR:HG22	1:A:170:GLU:OE1	2.19	0.42
1:C:278:ARG:NH2	5:C:2042:HOH:O	2.48	0.42
1:C:326:GLU:O	1:C:327:TRP:HB2	2.20	0.42
1:A:327:TRP:CH2	1:A:371:LYS:HD2	2.55	0.41
1:B:39:LEU:HD13	1:B:76:VAL:HG13	2.02	0.41
1:B:391:PRO:HB2	1:B:394:ARG:HB2	2.01	0.41
1:A:109:ARG:NH1	1:B:410:GLY:N	2.68	0.41
1:C:162:TYR:CE1	1:C:199:ILE:HG22	2.53	0.41
1:C:192:LEU:HD13	1:C:209:LYS:HD3	2.02	0.41
1:B:337:TYR:O	1:B:341:SER:OG	2.33	0.41
1:C:390:LEU:HD22	1:C:395:LEU:HD13	2.02	0.41
1:B:192:LEU:HD23	1:B:192:LEU:HA	1.92	0.41
1:C:205:GLN:H	1:C:205:GLN:HG2	1.73	0.41
1:C:132:ASN:O	1:C:136:GLU:HG2	2.21	0.41
1:B:73:VAL:HG22	1:B:141:LEU:HG	2.03	0.41
1:C:49:SER:OG	1:C:50:ASP:N	2.54	0.41
1:C:221:TYR:OH	1:C:239:PRO:HB3	2.21	0.41
1:A:203:GLU:OE2	1:A:209:LYS:NZ	2.37	0.41
1:B:159:GLU:O	1:B:163:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:THR:HG22	1:B:170:GLU:CD	2.41	0.41
1:B:299:GLN:HB3	1:B:301:HIS:CD2	2.56	0.41
1:B:117:VAL:CG2	1:B:125:ILE:CD1	2.99	0.41
1:A:159:GLU:CD	5:A:2033:HOH:O	2.57	0.40
1:C:93:ASN:CB	5:C:2020:HOH:O	2.68	0.40
1:B:256:ASP:HB3	1:B:258:SER:H	1.86	0.40
1:C:396:ILE:O	1:C:396:ILE:HG22	2.22	0.40
1:A:67:THR:OG1	2:A:700:ANP:H2'	2.22	0.40
1:B:159:GLU:O	1:B:162:TYR:HB3	2.21	0.40
1:B:326:GLU:O	1:B:327:TRP:CB	2.67	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	389/412 (94%)	375 (96%)	11 (3%)	3 (1%)	19	29
1	B	393/412 (95%)	371 (94%)	19 (5%)	3 (1%)	19	29
1	C	388/412 (94%)	354 (91%)	27 (7%)	7 (2%)	8	10
All	All	1170/1236 (95%)	1100 (94%)	57 (5%)	13 (1%)	14	20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	49	SER
1	C	118	ARG
1	C	152	SER
1	A	256	ASP
1	B	256	ASP
1	B	327	TRP
1	A	327	TRP

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Mol	Chain	Res	Type
1	B	49	SER
1	C	408	ALA
1	A	86	THR
1	C	50	ASP
1	C	51	VAL
1	C	176	GLY

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	331/344 (96%)	280 (85%)	51 (15%)	2	3
1	B	332/344 (96%)	279 (84%)	53 (16%)	2	3
1	C	330/344 (96%)	264 (80%)	66 (20%)	1	1
All	All	993/1032 (96%)	823 (83%)	170 (17%)	2	2

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	ARG
1	A	17	GLU
1	A	30	GLU
1	A	36	ARG
1	A	39	LEU
1	A	41	ARG
1	A	42	LEU
1	A	43	LEU
1	A	48	LEU
1	A	78	GLU
1	A	82	LYS
1	A	88	LYS
1	A	95	PHE
1	A	129	LEU
1	A	131	ASP

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Mol	Chain	Res	Type
1	A	155	ARG
1	A	165	LEU
1	A	166	ARG
1	A	174	ARG
1	A	183	LEU
1	A	196	ARG
1	A	197	GLU
1	A	198	LYS
1	A	202	VAL
1	A	205	GLN
1	A	212	LEU
1	A	218	ARG
1	A	227	ARG
1	A	238	GLU
1	A	251	GLU
1	A	278	ARG
1	A	292	GLU
1	A	299	GLN
1	A	302	GLU
1	A	306	LEU
1	A	310	GLU
1	A	311	LEU
1	A	325	MET
1	A	326	GLU
1	A	332	LEU
1	A	335	GLN
1	A	341	SER
1	A	342	LEU
1	A	346	ASN
1	A	348	LYS
1	A	353	THR
1	A	360	LYS
1	A	368	VAL
1	A	371	LYS
1	A	394	ARG
1	B	10	LYS
1	B	13	ARG
1	B	17	GLU
1	B	30	GLU
1	B	36	ARG
1	B	39	LEU
1	B	41	ARG

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Mol	Chain	Res	Type
1	B	42	LEU
1	B	43	LEU
1	B	77	SER
1	B	78	GLU
1	B	82	LYS
1	B	87	VAL
1	B	88	LYS
1	B	95	PHE
1	B	129	LEU
1	B	131	ASP
1	B	155	ARG
1	B	165	LEU
1	B	166	ARG
1	B	174	ARG
1	B	183	LEU
1	B	196	ARG
1	B	197	GLU
1	B	198	LYS
1	B	202	VAL
1	B	205	GLN
1	B	212	LEU
1	B	218	ARG
1	B	227	ARG
1	B	240	ARG
1	B	251	GLU
1	B	261	ARG
1	B	278	ARG
1	B	292	GLU
1	B	298	ILE
1	B	302	GLU
1	B	306	LEU
1	B	310	GLU
1	B	311	LEU
1	B	315	ARG
1	B	319	GLU
1	B	325	MET
1	B	332	LEU
1	B	336	ARG
1	B	342	LEU
1	B	347	VAL
1	B	348	LYS
1	B	353	THR

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Mol	Chain	Res	Type
1	B	354	GLN
1	B	360	LYS
1	B	394	ARG
1	B	406	LYS
1	C	12	ARG
1	C	16	ASP
1	C	18	ASN
1	C	20	ILE
1	C	39	LEU
1	C	50	ASP
1	C	51	VAL
1	C	57	SER
1	C	58	ILE
1	C	60	ARG
1	C	75	ARG
1	C	82	LYS
1	C	85	LEU
1	C	87	VAL
1	C	96	ASN
1	C	99	ASN
1	C	105	SER
1	C	106	LEU
1	C	108	VAL
1	C	118	ARG
1	C	126	LEU
1	C	127	LYS
1	C	141	LEU
1	C	155	ARG
1	C	162	TYR
1	C	163	THR
1	C	165	LEU
1	C	167	VAL
1	C	173	SER
1	C	174	ARG
1	C	180	ILE
1	C	183	LEU
1	C	196	ARG
1	C	197	GLU
1	C	198	LYS
1	C	199	ILE
1	C	205	GLN
1	C	227	ARG

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Mol	Chain	Res	Type
1	C	251	GLU
1	C	267	LYS
1	C	279	ASP
1	C	292	GLU
1	C	298	ILE
1	C	301	HIS
1	C	306	LEU
1	C	308	ILE
1	C	311	LEU
1	C	322	LEU
1	C	325	MET
1	C	332	LEU
1	C	336	ARG
1	C	341	SER
1	C	342	LEU
1	C	346	ASN
1	C	347	VAL
1	C	348	LYS
1	C	371	LYS
1	C	382	THR
1	C	383	LEU
1	C	390	LEU
1	C	391	PRO
1	C	394	ARG
1	C	401	ASN
1	C	403	ILE
1	C	404	GLN
1	C	409	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	116	GLN
1	A	205	GLN
1	A	241	HIS
1	A	329	ASN
1	A	335	GLN
1	A	356	HIS
1	B	40	ASN
1	B	96	ASN
1	B	110	GLN

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Mol	Chain	Res	Type
1	B	116	GLN
1	B	201	GLN
1	B	205	GLN
1	B	241	HIS
1	B	293	ASN
1	B	329	ASN
1	B	354	GLN
1	C	96	ASN
1	C	110	GLN
1	C	116	GLN
1	C	205	GLN
1	C	241	HIS
1	C	293	ASN
1	C	299	GLN
1	C	335	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\|>2$
2	ANP	B	700	3	29,33,33	2.96	6 (20%)	31,52,52	1.45	7 (22%)
2	ANP	A	700	3	29,33,33	2.74	9 (31%)	31,52,52	1.67	6 (19%)
4	ADP	C	700	3	24,29,29	1.28	2 (8%)	29,45,45	1.58	4 (13%)

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	ANP	B	700	3	-	2/14/38/38	0/3/3/3
2	ANP	A	700	3	-	2/14/38/38	0/3/3/3
4	ADP	C	700	3	-	2/12/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	ANP	PB-O1B	9.52	1.61	1.46
2	B	700	ANP	PG-O1G	9.32	1.61	1.46
2	A	700	ANP	PG-O1G	8.17	1.59	1.46
2	A	700	ANP	PB-O1B	7.82	1.58	1.46
2	B	700	ANP	C4-N3	5.34	1.43	1.35
2	A	700	ANP	C4-N3	4.97	1.42	1.35
4	C	700	ADP	C2-N3	4.15	1.38	1.32
2	B	700	ANP	PG-N3B	3.44	1.72	1.63
2	A	700	ANP	PG-N3B	3.42	1.72	1.63
2	A	700	ANP	PB-O3A	3.18	1.63	1.59
2	A	700	ANP	PB-N3B	3.08	1.71	1.63
2	B	700	ANP	PB-N3B	2.77	1.70	1.63
2	A	700	ANP	PA-O1A	2.69	1.60	1.50
4	C	700	ADP	C2-N1	2.67	1.38	1.33
2	A	700	ANP	C2-N3	2.52	1.36	1.32
2	A	700	ANP	C5-C4	2.02	1.46	1.40
2	B	700	ANP	PG-O2G	2.00	1.62	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	700	ADP	N3-C2-N1	-5.95	119.38	128.68
2	A	700	ANP	C4-C5-N7	-4.32	104.90	109.40
2	A	700	ANP	O1G-PG-N3B	-4.22	105.56	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	ANP	N3-C2-N1	-3.33	123.47	128.68
2	B	700	ANP	C3'-C2'-C1'	3.15	105.72	100.98
2	B	700	ANP	C4-C5-N7	-2.94	106.34	109.40
2	B	700	ANP	N3-C2-N1	-2.57	124.67	128.68
2	A	700	ANP	C2-N1-C6	2.51	123.05	118.75
2	B	700	ANP	C2-N1-C6	2.50	123.03	118.75
4	C	700	ADP	PA-O3A-PB	-2.46	124.39	132.83
4	C	700	ADP	C3'-C2'-C1'	2.41	104.61	100.98
4	C	700	ADP	O3'-C3'-C4'	-2.38	104.17	111.05
2	A	700	ANP	O2G-PG-O1G	-2.19	107.94	113.45
2	B	700	ANP	PB-O3A-PA	-2.15	125.04	132.62
2	A	700	ANP	PB-O3A-PA	-2.13	125.10	132.62
2	B	700	ANP	O3G-PG-O1G	-2.09	108.20	113.45
2	B	700	ANP	O2G-PG-O3G	2.03	113.05	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	ANP	PG-N3B-PB-O1B
2	A	700	ANP	PG-N3B-PB-O3A
2	B	700	ANP	PG-N3B-PB-O1B
2	B	700	ANP	PG-N3B-PB-O3A
4	C	700	ADP	PA-O3A-PB-O2B
4	C	700	ADP	PA-O3A-PB-O3B

There are no ring outliers.

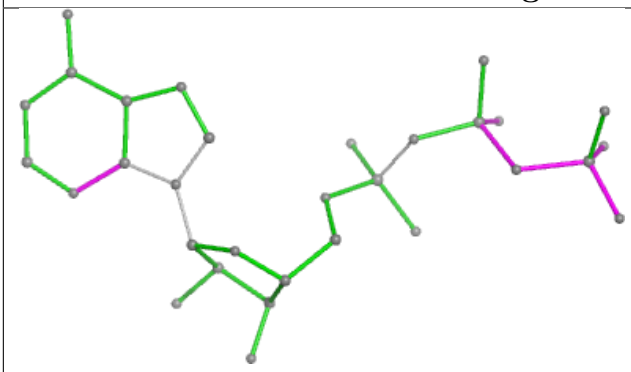
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	ANP	1	0
4	C	700	ADP	1	0

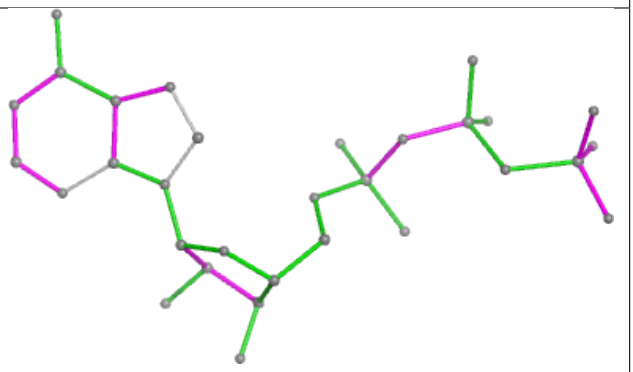
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

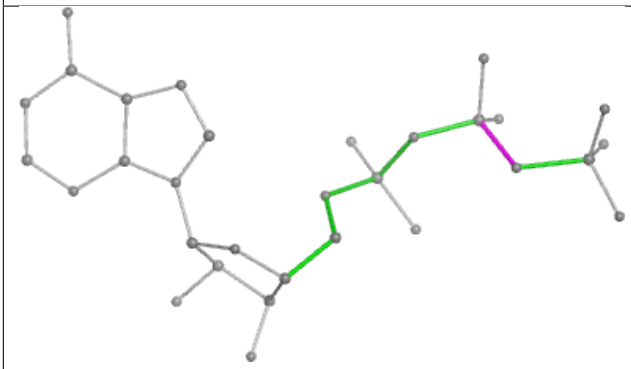
Ligand ANP B 700



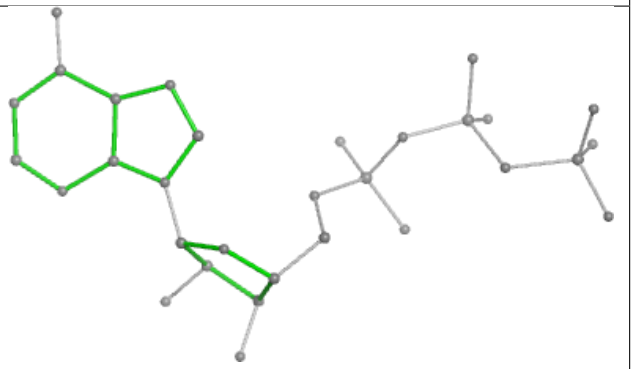
Bond lengths



Bond angles

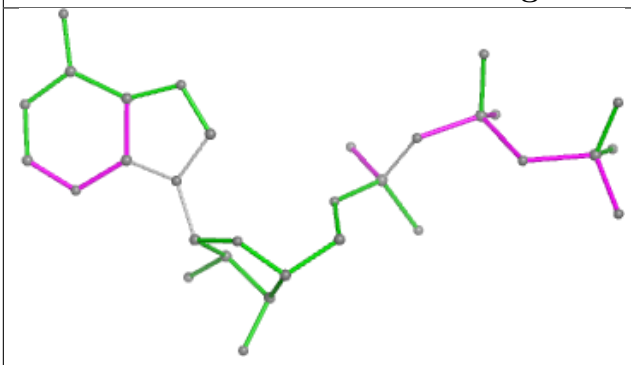


Torsions

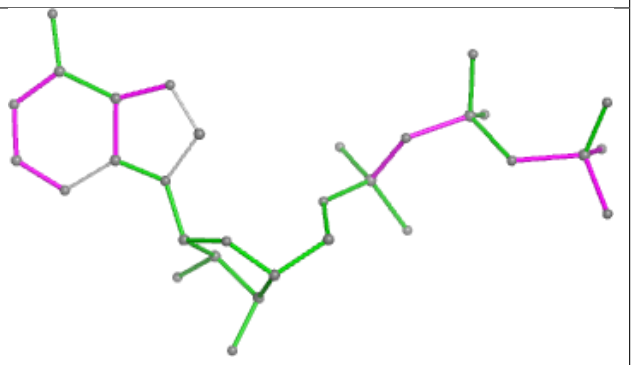


Rings

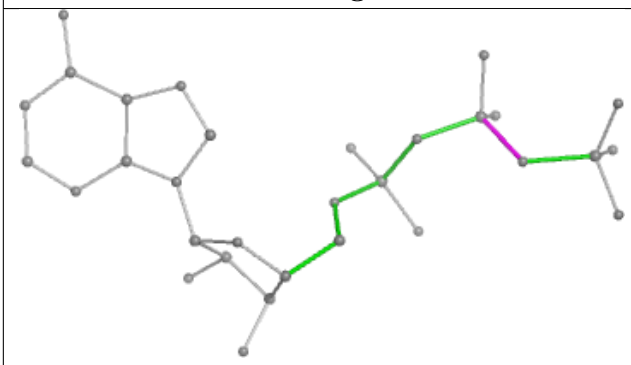
Ligand ANP A 700



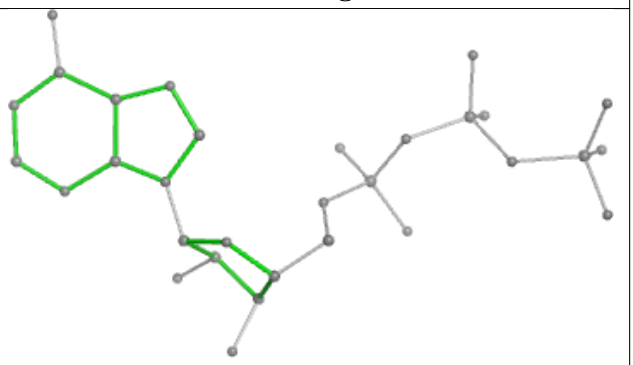
Bond lengths



Bond angles

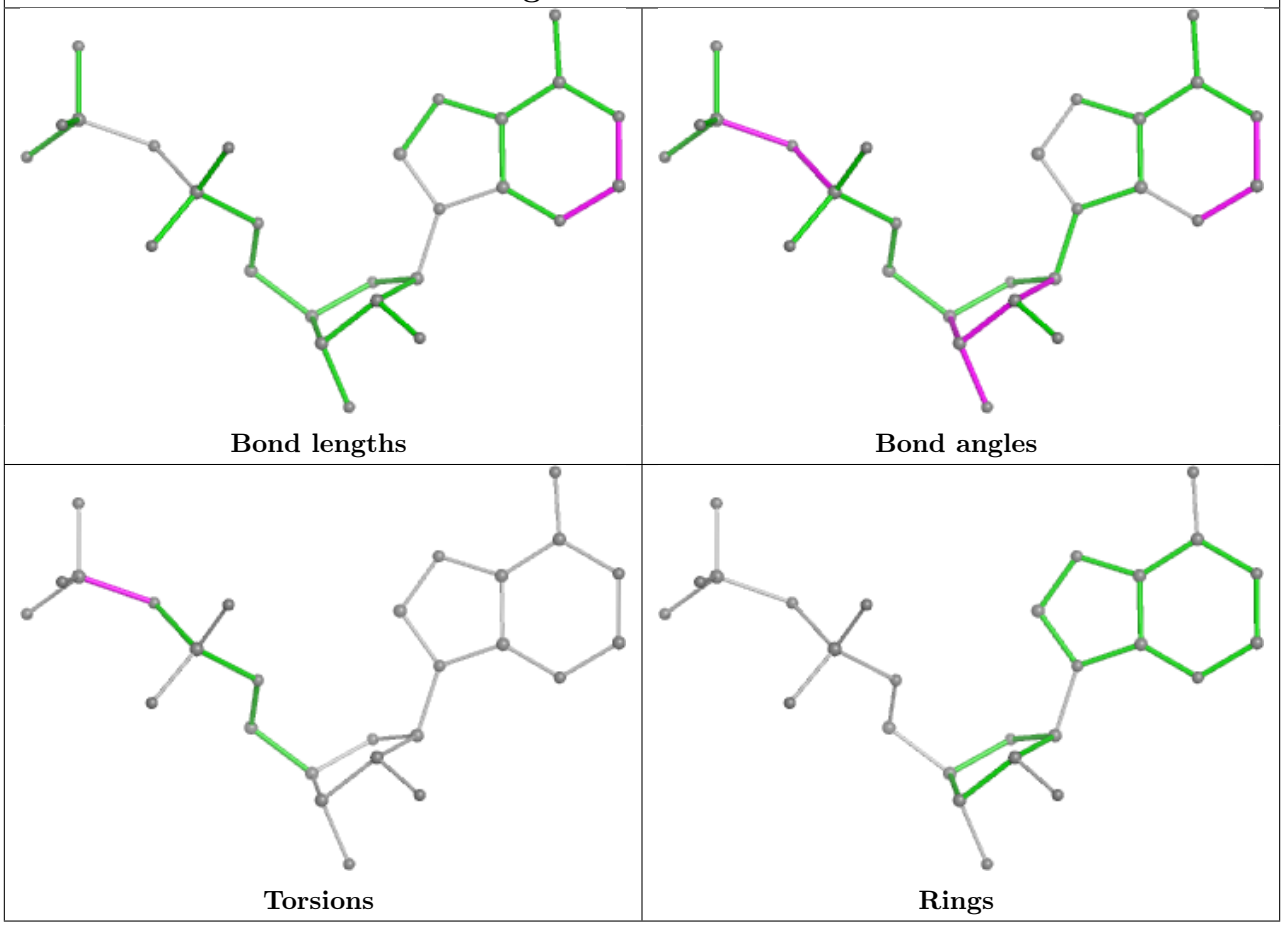


Torsions



Rings

Ligand ADP C 700



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	395/412 (95%)	-0.14	3 (0%)	86	84	8, 25, 45, 57	0
1	B	397/412 (96%)	-0.08	14 (3%)	44	43	9, 25, 46, 57	0
1	C	394/412 (95%)	0.16	27 (6%)	16	15	12, 32, 66, 80	0
All	All	1186/1236 (95%)	-0.02	44 (3%)	41	41	8, 27, 56, 80	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	373	SER	7.0
1	C	372	PRO	5.9
1	C	407	MET	5.4
1	C	154	PRO	4.9
1	A	7	GLY	4.9
1	C	342	LEU	4.7
1	C	381	THR	4.1
1	C	346	ASN	4.1
1	B	294	GLU	3.9
1	C	404	GLN	3.7
1	C	343	THR	3.4
1	C	352	TYR	3.3
1	B	373	SER	3.3
1	C	391	PRO	3.2
1	B	155	ARG	3.2
1	B	301	HIS	3.2
1	B	324	GLY	3.0
1	C	168	HIS	2.9
1	A	154	PRO	2.7
1	B	154	PRO	2.7
1	B	297	SER	2.7
1	C	382	THR	2.7
1	C	409	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	298	ILE	2.6
1	C	325	MET	2.6
1	C	408	ALA	2.6
1	C	401	ASN	2.6
1	C	332	LEU	2.5
1	B	325	MET	2.4
1	B	296	ALA	2.4
1	B	326	GLU	2.4
1	C	50	ASP	2.3
1	C	119	GLY	2.3
1	C	405	ALA	2.3
1	C	301	HIS	2.3
1	B	295	ALA	2.3
1	C	383	LEU	2.2
1	B	322	LEU	2.2
1	B	372	PRO	2.2
1	C	174	ARG	2.1
1	C	321	THR	2.1
1	A	325	MET	2.1
1	B	196	ARG	2.1
1	C	410	GLY	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 monosaccharides 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, 95^{th} 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	ANP	B	700	31/31	0.95	0.11	8,16,30,32	0
3	MG	C	701	1/1	0.95	0.16	19,19,19,19	0

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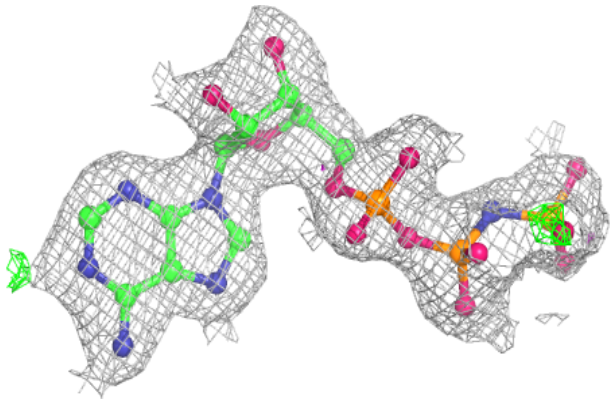
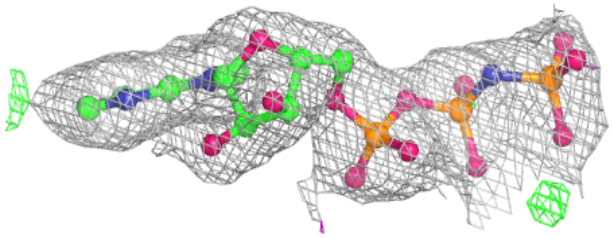
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	701	1/1	0.97	0.17	3,3,3,3	0
2	ANP	A	700	31/31	0.97	0.10	5,9,14,19	0
4	ADP	C	700	27/27	0.98	0.10	15,20,26,28	0
3	MG	B	701	1/1	0.99	0.14	5,5,5,5	0

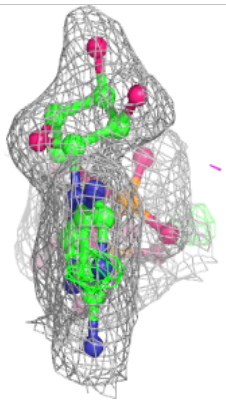
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 700:

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

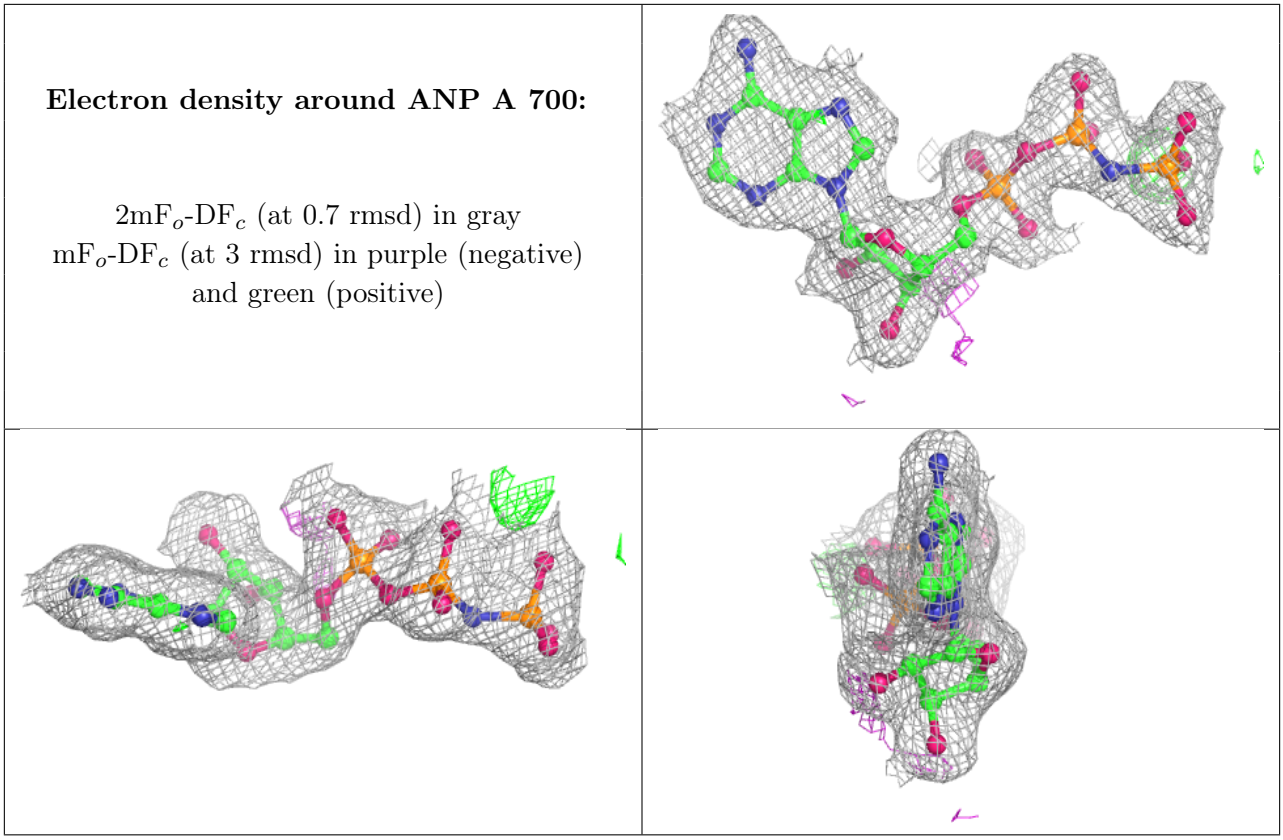






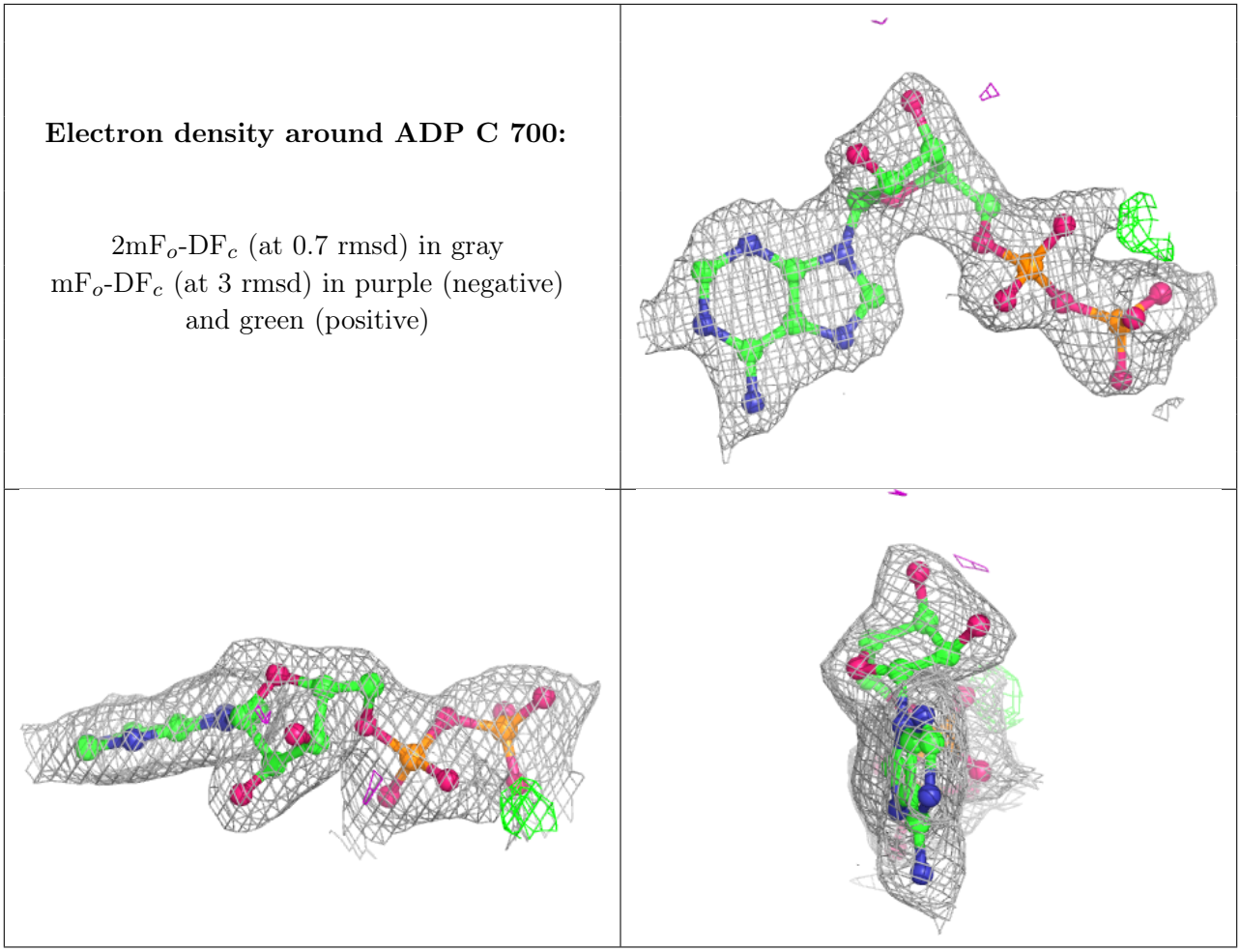
Electron density around ANP A 700:

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



Electron density around ADP C 700:

$2mF_o$-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.