



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 09:58 PM UTC

PDB ID : 1W5T / pdb_00001w5t
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	:	4-5-2 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

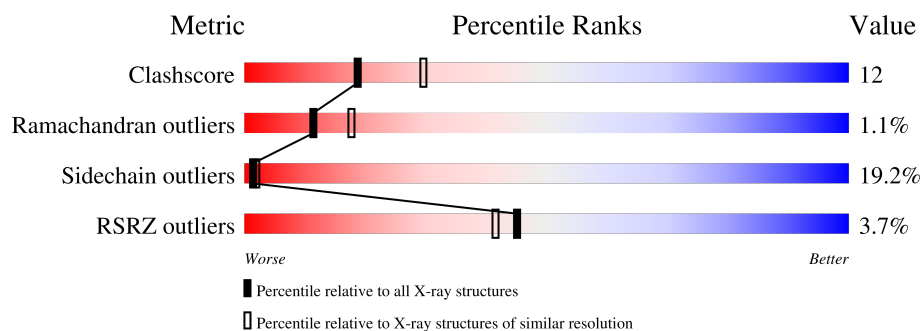
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	412	2% 68% 21% 6% .
1	B	412	2% 68% 21% 7% .
1	C	412	7% 55% 31% 8% . .

2 Entry composition [i](#)

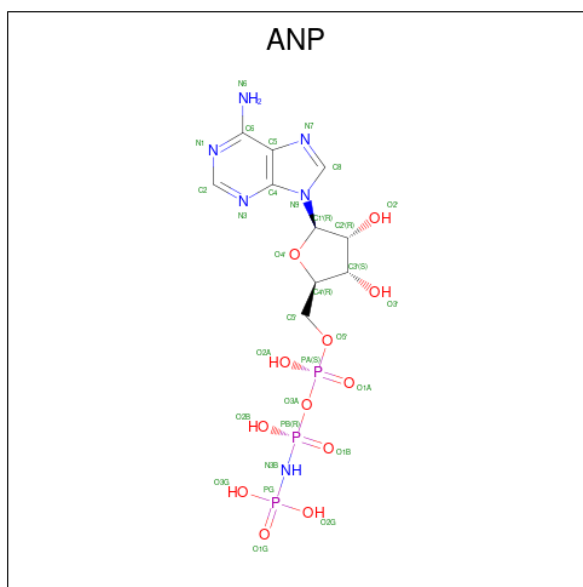
There are 5 unique types of molecules in this entry. The entry contains 9573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

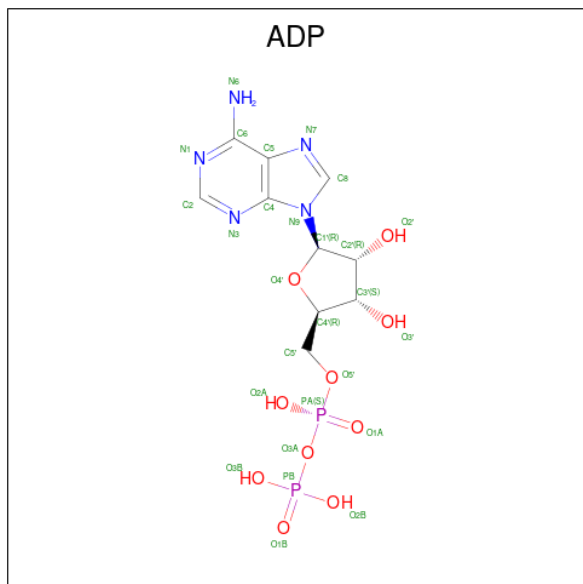


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: 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 (CCD ID: 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	

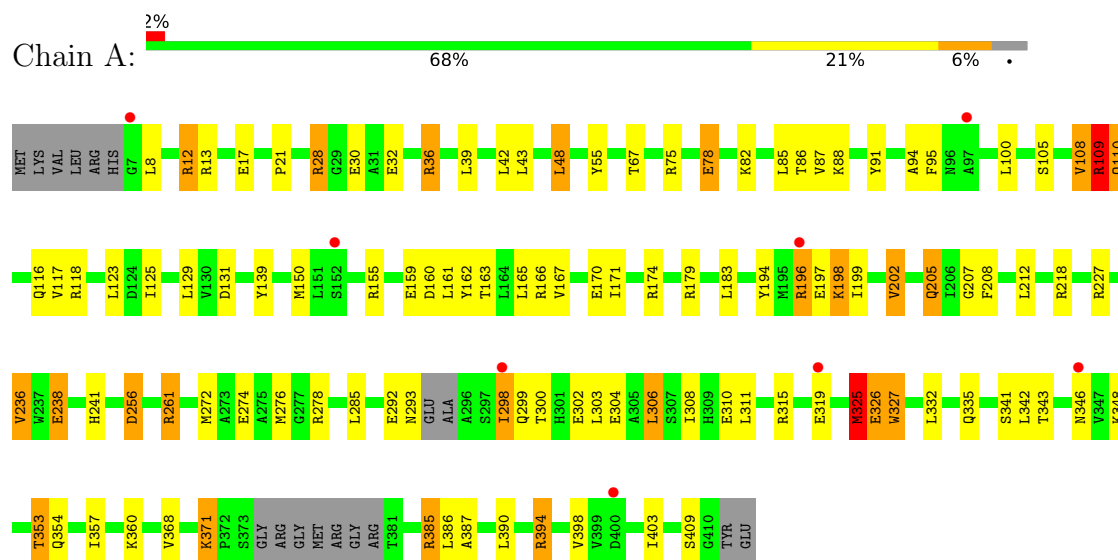
- Molecule 5 is water.

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

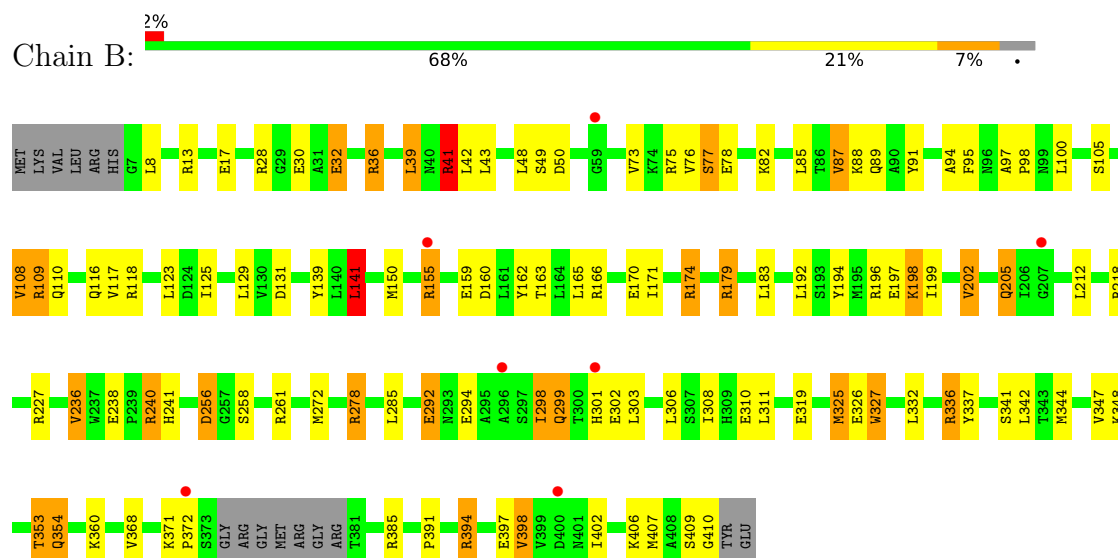
3 Residue-property plots [i](#)

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

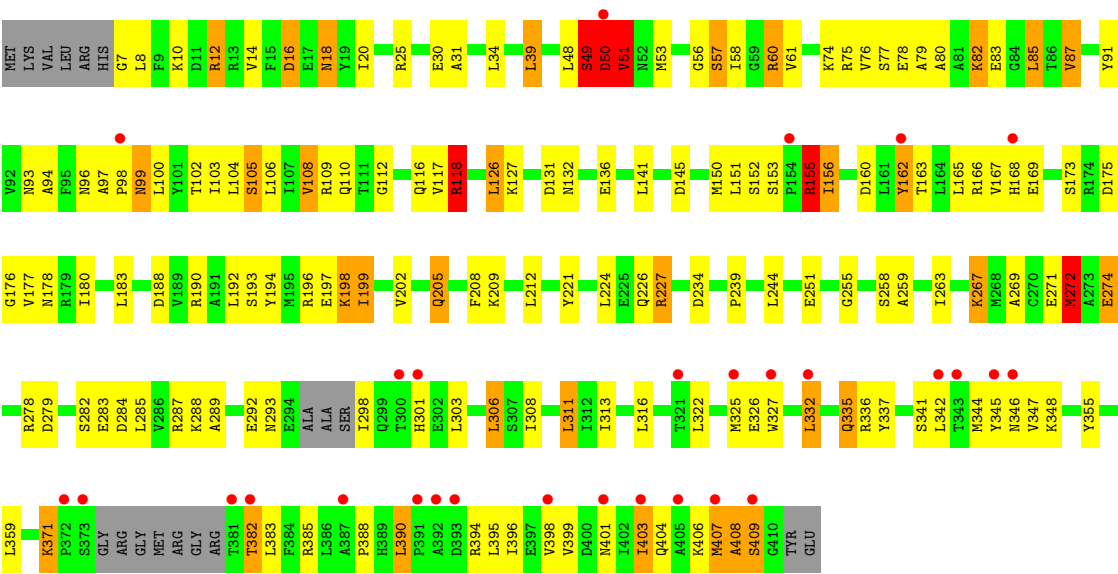


• Molecule 1: ORC2



• Molecule 1: ORC2





4 Data and refinement statistics

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 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.40) 90.5 (20.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.95	3/3159 (0.1%)	1.21	12/4272 (0.3%)
1	B	0.98	4/3174 (0.1%)	1.23	15/4294 (0.3%)
1	C	0.95	3/3149 (0.1%)	1.20	12/4259 (0.3%)
All	All	0.96	10/9482 (0.1%)	1.21	39/12825 (0.3%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	293	ASN	C-N	-6.94	1.23	1.33
1	C	409	SER	C-N	-6.67	1.24	1.33
1	A	325	MET	SD-CE	6.56	1.96	1.79
1	B	108	VAL	CA-CB	6.34	1.62	1.54
1	B	409	SER	C-N	-6.23	1.24	1.33
1	A	409	SER	C-N	-6.10	1.24	1.33
1	C	272	MET	SD-CE	-5.37	1.66	1.79
1	A	108	VAL	CA-CB	5.37	1.61	1.54
1	B	407	MET	SD-CE	5.17	1.92	1.79
1	B	141	LEU	C-O	5.10	1.29	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	SER	O-C-N	-9.21	108.26	123.00
1	B	85	LEU	N-CA-C	9.18	122.60	111.40
1	C	293	ASN	O-C-N	-9.06	108.51	123.00
1	A	85	LEU	N-CA-C	8.46	121.72	111.40
1	B	409	SER	O-C-N	-8.38	109.60	123.00
1	C	131	ASP	N-CA-C	7.57	119.17	111.07
1	B	179	ARG	NE-CZ-NH1	-6.99	114.51	121.50
1	B	179	ARG	NE-CZ-NH2	6.98	125.48	119.20
1	A	12	ARG	NE-CZ-NH2	6.37	124.93	119.20
1	C	53	MET	N-CA-C	6.33	119.82	109.06
1	C	103	ILE	N-CA-C	-6.29	104.62	110.53
1	C	156	ILE	N-CA-C	-6.21	99.79	108.12
1	A	12	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	A	28	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	B	240	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	A	110	GLN	N-CA-C	5.89	118.48	111.71
1	A	261	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	A	109	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	B	240	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	C	169	GLU	N-CA-C	-5.56	106.19	114.64
1	B	77	SER	N-CA-C	5.55	117.00	111.07
1	C	255	GLY	CA-C-N	5.54	127.96	120.38
1	C	255	GLY	C-N-CA	5.54	127.96	120.38
1	C	31	ALA	N-CA-C	-5.52	105.34	111.36
1	A	261	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	A	409	SER	CA-C-N	5.47	127.15	116.20
1	B	41	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	B	174	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	179	ARG	CD-NE-CZ	5.37	131.92	124.40
1	A	167	VAL	N-CA-C	5.37	116.74	110.62
1	B	109	ARG	NE-CZ-NH1	5.29	126.79	121.50
1	A	21	PRO	O-C-N	5.20	123.59	121.15
1	B	109	ARG	CD-NE-CZ	5.16	131.62	124.40
1	C	162	TYR	N-CA-C	-5.13	105.69	111.28
1	B	278	ARG	NE-CZ-NH2	5.11	123.79	119.20
1	B	87	VAL	N-CA-C	5.09	115.19	107.80
1	C	234	ASP	N-CA-C	5.05	117.52	111.71
1	C	293	ASN	CA-C-N	5.02	126.24	116.20
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	59	0
1	B	3123	0	3197	59	0
1	C	3099	0	3176	114	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	23	0
All	All	9573	0	9596	226	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 (226) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:166:ARG:CG	1:C:205:GLN:NE2	2.51	0.65
1:C:355:TYR:CE2	1:C:359:LEU:HD11	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:272:MET:HE1	1:C:289:ALA:HB2	1.80	0.63
1:B:117:VAL:HG23	1:B:125:ILE:HD13	1.81	0.62
1:C:94:ALA:HB2	1:C:150:MET:HE3	1.80	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:A:55:TYR:HH	1:C:209:LYS:HE3	1.68	0.59
1:B:89:GLN:HB3	5:B:2009:HOH:O	2.03	0.59
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:C:50:ASP:C	1:C:51:VAL:HG23	2.27	0.57
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:C:269:ALA:HA	1:C:272:MET:HE3	1.89	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:B:325:MET:HE1	1:B:336:ARG:HH22	1.73	0.54
1:A:8:LEU:HD23	1:A:236:VAL:HG13	1.90	0.53
1:C:91:TYR:OH	5:C:2020:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:108:VAL:O	1:C:109:ARG:C	2.54	0.51
1:C:151:LEU:C	1:C:153:SER:H	2.19	0.50
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:344:MET:HE1	5:C:2043:HOH:O	2.11	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:99:ASN:O	1:C:100:LEU:C	2.56	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:175:ASP:C	1:C:177:VAL:H	2.23	0.47
1:C:112:GLY:HA2	5:C:2023:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:163:THR:HG22	1:B:170:GLU:CD	2.41	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:A:150:MET:HE2	1:A:161:LEU:HD21	1.98	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:159:GLU:CD	5:A:2033:HOH:O	2.57	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:A:163:THR:HG22	1:A:170:GLU:CD	2.43	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:97:ALA:N	1:C:98:PRO:HD3	2.33	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:A:325:MET:HE3	1:A:325:MET:HB3	1.88	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:50:ASP:C	1:C:51:VAL:CG2	2.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:159:GLU:O	1:B:163:THR:HG23	2.21	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: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

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	389/412 (94%)	375 (96%)	11 (3%)	3 (1%)	16	25
1	B	393/412 (95%)	371 (94%)	19 (5%)	3 (1%)	16	25
1	C	388/412 (94%)	354 (91%)	27 (7%)	7 (2%)	6	9
All	All	1170/1236 (95%)	1100 (94%)	57 (5%)	13 (1%)	11	18

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

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Mol	Chain	Res	Type
1	B	327	TRP
1	A	327	TRP
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 ⓘ

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%)	274 (83%)	57 (17%)	2	2
1	B	332/344 (96%)	272 (82%)	60 (18%)	2	2
1	C	330/344 (96%)	256 (78%)	74 (22%)	1	1
All	All	993/1032 (96%)	802 (81%)	191 (19%)	1	2

All (191) 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	42	LEU
1	A	43	LEU
1	A	48	LEU
1	A	78	GLU
1	A	82	LYS
1	A	87	VAL
1	A	88	LYS
1	A	95	PHE

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Mol	Chain	Res	Type
1	A	108	VAL
1	A	109	ARG
1	A	129	LEU
1	A	131	ASP
1	A	155	ARG
1	A	165	LEU
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	236	VAL
1	A	238	GLU
1	A	274	GLU
1	A	278	ARG
1	A	292	GLU
1	A	298	ILE
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	343	THR
1	A	346	ASN
1	A	348	LYS
1	A	353	THR
1	A	357	ILE
1	A	360	LYS
1	A	368	VAL
1	A	371	LYS
1	A	385	ARG

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Mol	Chain	Res	Type
1	A	394	ARG
1	B	13	ARG
1	B	17	GLU
1	B	30	GLU
1	B	32	GLU
1	B	36	ARG
1	B	39	LEU
1	B	41	ARG
1	B	42	LEU
1	B	43	LEU
1	B	75	ARG
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	108	VAL
1	B	129	LEU
1	B	131	ASP
1	B	141	LEU
1	B	155	ARG
1	B	165	LEU
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	236	VAL
1	B	240	ARG
1	B	261	ARG
1	B	278	ARG
1	B	292	GLU
1	B	298	ILE
1	B	299	GLN
1	B	302	GLU
1	B	306	LEU

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Mol	Chain	Res	Type
1	B	308	ILE
1	B	310	GLU
1	B	311	LEU
1	B	319	GLU
1	B	325	MET
1	B	332	LEU
1	B	336	ARG
1	B	342	LEU
1	B	344	MET
1	B	347	VAL
1	B	348	LYS
1	B	353	THR
1	B	354	GLN
1	B	360	LYS
1	B	368	VAL
1	B	394	ARG
1	B	397	GLU
1	B	398	VAL
1	B	406	LYS
1	C	10	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	74	LYS
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

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Mol	Chain	Res	Type
1	C	141	LEU
1	C	155	ARG
1	C	163	THR
1	C	165	LEU
1	C	167	VAL
1	C	173	SER
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	212	LEU
1	C	227	ARG
1	C	251	GLU
1	C	267	LYS
1	C	272	MET
1	C	274	GLU
1	C	279	ASP
1	C	283	GLU
1	C	288	LYS
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	313	ILE
1	C	322	LEU
1	C	325	MET
1	C	332	LEU
1	C	335	GLN
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

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Mol	Chain	Res	Type
1	C	390	LEU
1	C	394	ARG
1	C	398	VAL
1	C	401	ASN
1	C	403	ILE
1	C	404	GLN
1	C	406	LYS
1	C	407	MET
1	C	409	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	89	GLN
1	A	110	GLN
1	A	116	GLN
1	A	205	GLN
1	A	241	HIS
1	A	293	ASN
1	A	299	GLN
1	A	335	GLN
1	A	356	HIS
1	A	401	ASN
1	A	404	GLN
1	B	40	ASN
1	B	89	GLN
1	B	96	ASN
1	B	110	GLN
1	B	116	GLN
1	B	205	GLN
1	B	241	HIS
1	B	293	ASN
1	B	299	GLN
1	B	354	GLN
1	B	361	HIS
1	C	96	ASN
1	C	110	GLN
1	C	116	GLN
1	C	178	ASN
1	C	205	GLN
1	C	226	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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	33,33,33	2.99	10 (30%)	45,52,52	1.61	10 (22%)
4	ADP	C	700	3	28,29,29	1.24	4 (14%)	43,45,45	1.86	9 (20%)
2	ANP	A	700	3	33,33,33	2.82	13 (39%)	45,52,52	1.98	12 (26%)

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	-	2/18/38/38	0/3/3/3
4	ADP	C	700	3	-	2/16/32/32	0/3/3/3
2	ANP	A	700	3	-	2/18/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	ANP	PB-O1B	9.97	1.61	1.46
2	B	700	ANP	PG-O1G	9.77	1.61	1.46
2	A	700	ANP	PG-O1G	8.56	1.59	1.46
2	A	700	ANP	PB-O1B	8.18	1.58	1.46
2	B	700	ANP	C4-N3	4.60	1.43	1.34
2	A	700	ANP	C4-N3	4.33	1.42	1.34
2	A	700	ANP	C5-C4	4.03	1.46	1.39
2	B	700	ANP	C5-C4	3.87	1.46	1.39
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	C4-N9	-3.36	1.30	1.37
2	A	700	ANP	C5-C6	3.35	1.50	1.41
2	A	700	ANP	PB-O3A	3.22	1.63	1.59
2	A	700	ANP	PB-N3B	3.08	1.71	1.63
2	B	700	ANP	C5-C6	3.05	1.49	1.41
2	B	700	ANP	C8-N7	2.80	1.37	1.31
4	C	700	ADP	C2-N1	2.78	1.38	1.33
2	A	700	ANP	PA-O1A	2.78	1.60	1.50
2	B	700	ANP	PB-N3B	2.77	1.70	1.63
4	C	700	ADP	C2-N3	2.73	1.38	1.33
4	C	700	ADP	PA-O3A	2.62	1.62	1.59
2	A	700	ANP	C5-N7	-2.48	1.34	1.39
4	C	700	ADP	C5-N7	-2.42	1.34	1.39
2	B	700	ANP	C4-N9	-2.32	1.32	1.37
2	A	700	ANP	PA-O3A	2.30	1.62	1.59
2	A	700	ANP	C8-N7	2.28	1.36	1.31
2	B	700	ANP	PG-O2G	2.01	1.62	1.56

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	700	ADP	N3-C2-N1	-6.08	119.38	128.58
2	A	700	ANP	C4-C5-N7	-4.97	104.90	110.58
2	A	700	ANP	C5-C4-N9	4.64	110.87	105.81
2	A	700	ANP	C6-C5-N7	4.51	140.78	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	700	ADP	N9-C8-N7	-4.30	107.84	113.94
2	A	700	ANP	O1G-PG-N3B	-4.22	105.56	111.77
2	B	700	ANP	C5-C4-N9	4.07	110.25	105.81
2	A	700	ANP	C5-C4-N3	-3.98	121.23	126.72
4	C	700	ADP	C5-C4-N3	-3.92	121.32	126.72
2	B	700	ANP	C4-C5-N7	-3.71	106.34	110.58
2	B	700	ANP	C6-C5-N7	3.56	138.95	132.09
4	C	700	ADP	C2-N3-C4	3.51	120.40	111.83
2	A	700	ANP	N3-C2-N1	-3.38	123.47	128.58
2	B	700	ANP	C5-C4-N3	-3.36	122.10	126.72
4	C	700	ADP	C5-N7-C8	3.31	108.66	103.45
4	C	700	ADP	N3-C4-N9	2.92	132.13	127.17
2	A	700	ANP	C2-N3-C4	2.75	118.54	111.83
2	A	700	ANP	C2-N1-C6	2.63	123.05	118.73
2	B	700	ANP	C2-N1-C6	2.62	123.03	118.73
2	B	700	ANP	N3-C2-N1	-2.59	124.67	128.58
2	A	700	ANP	C5-N7-C8	2.58	107.50	103.45
4	C	700	ADP	O3'-C3'-C4'	-2.41	104.17	111.08
4	C	700	ADP	C4-N9-C8	2.37	108.22	105.74
2	A	700	ANP	O2A-PA-O3A	2.35	113.62	107.27
2	B	700	ANP	C3'-C2'-C1'	2.25	105.72	101.46
2	A	700	ANP	O2G-PG-O1G	-2.20	107.94	113.45
2	A	700	ANP	C6-C5-C4	-2.11	114.29	117.18
2	B	700	ANP	O3G-PG-O1G	-2.09	108.20	113.45
2	B	700	ANP	C2-N3-C4	2.09	116.94	111.83
2	B	700	ANP	O2G-PG-O3G	2.03	113.05	107.59
4	C	700	ADP	C6-C5-C4	2.01	119.92	117.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

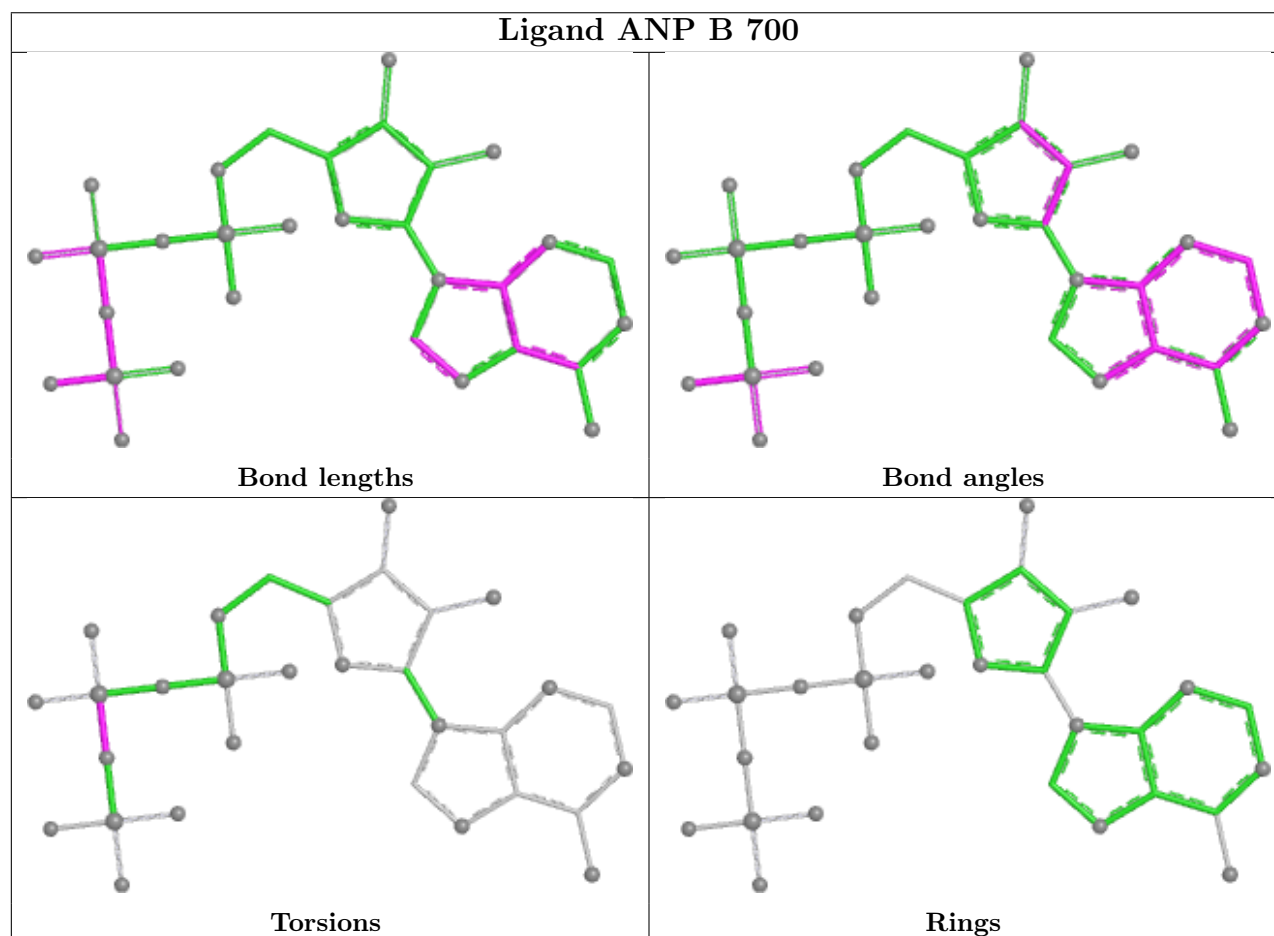
Mol	Chain	Res	Type	Atoms
2	A	700	ANP	PG-N3B-PB-O1B
2	A	700	ANP	PG-N3B-PB-O3A
2	B	700	ANP	PG-N3B-PB-O1B
2	B	700	ANP	PG-N3B-PB-O3A
4	C	700	ADP	PA-O3A-PB-O2B
4	C	700	ADP	PA-O3A-PB-O3B

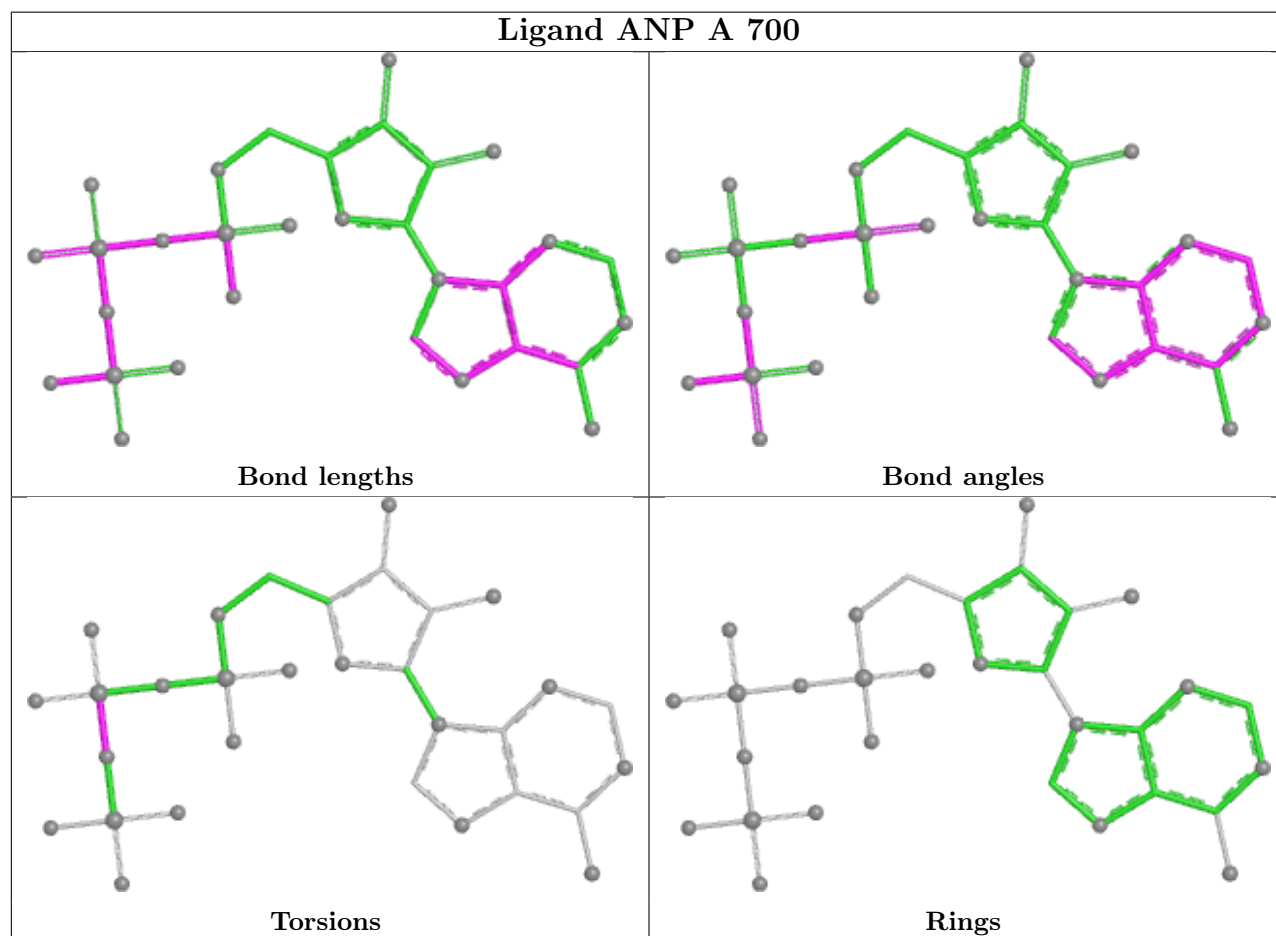
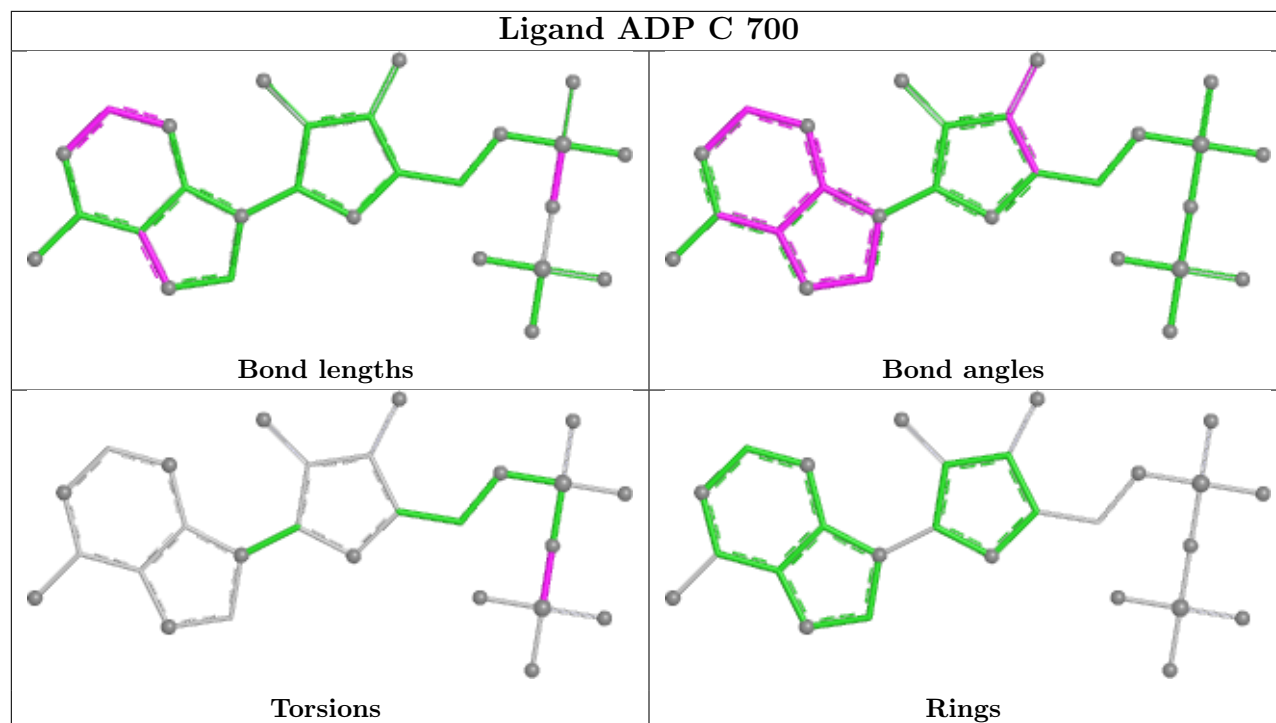
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	395/412 (95%)	0.12	8 (2%) 65 60	8, 25, 45, 57	0
1	B	397/412 (96%)	0.12	7 (1%) 67 63	9, 25, 46, 57	0
1	C	394/412 (95%)	0.42	29 (7%) 20 17	12, 32, 66, 80	0
All	All	1186/1236 (95%)	0.22	44 (3%) 45 41	8, 27, 56, 80	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	373	SER	4.5
1	C	381	THR	4.0
1	C	407	MET	3.8
1	A	7	GLY	3.8
1	C	154	PRO	3.8
1	C	50	ASP	3.7
1	C	391	PRO	3.2
1	C	342	LEU	3.1
1	C	372	PRO	3.1
1	C	98	PRO	3.0
1	C	332	LEU	2.9
1	C	162	TYR	2.9
1	B	207	GLY	2.8
1	C	398	VAL	2.7
1	C	392	ALA	2.7
1	A	400	ASP	2.6
1	C	327	TRP	2.6
1	A	298	ILE	2.6
1	A	97	ALA	2.5
1	C	168	HIS	2.5
1	C	393	ASP	2.4
1	C	403	ILE	2.4
1	C	301	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	382	THR	2.4
1	C	345	TYR	2.4
1	B	155	ARG	2.3
1	A	319	GLU	2.3
1	B	296	ALA	2.2
1	C	346	ASN	2.2
1	B	372	PRO	2.2
1	A	152	SER	2.2
1	C	387	ALA	2.2
1	C	401	ASN	2.2
1	C	300	THR	2.2
1	B	400	ASP	2.2
1	A	196	ARG	2.2
1	C	325	MET	2.1
1	C	409	SER	2.1
1	B	301	HIS	2.1
1	A	346	ASN	2.1
1	C	343	THR	2.1
1	C	405	ALA	2.0
1	B	59	GLY	2.0
1	C	321	THR	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.

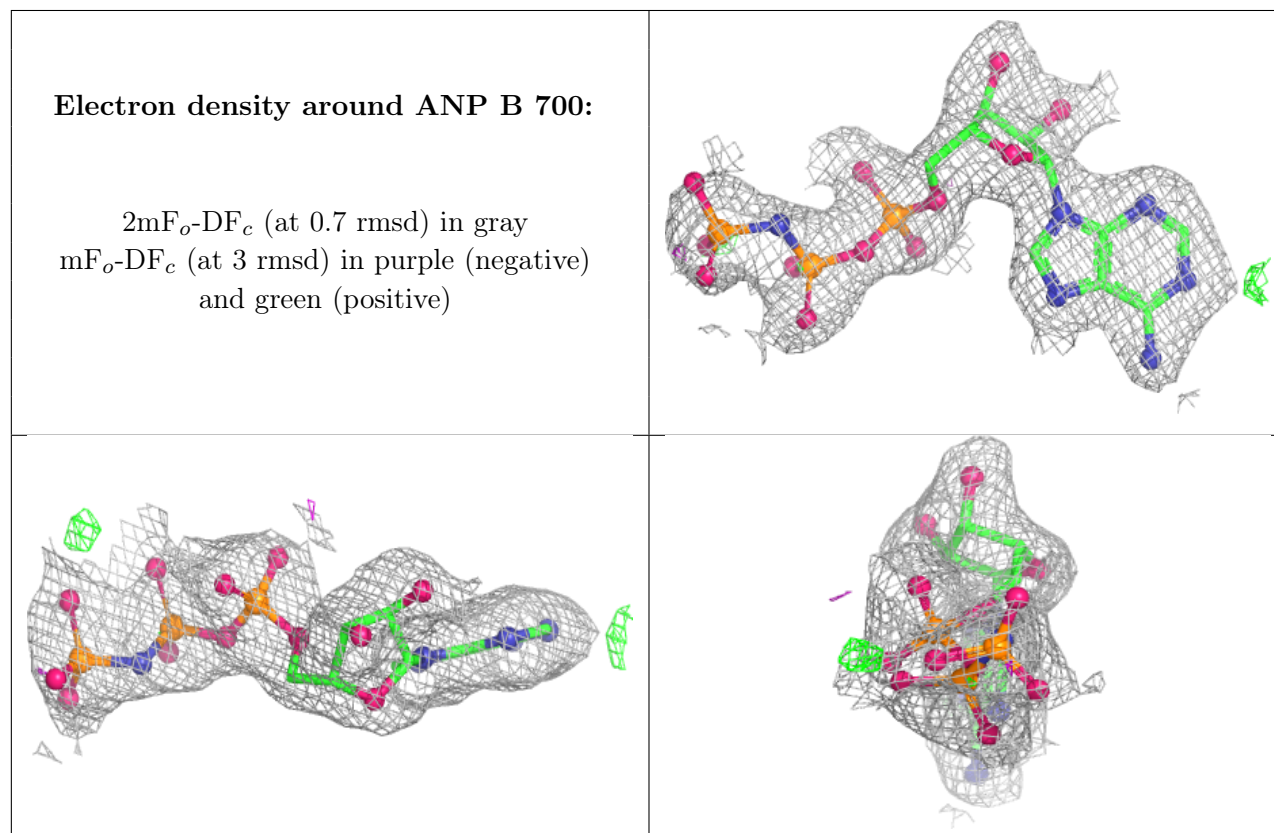
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	701	1/1	0.94	0.10	5,5,5,5	0
3	MG	A	701	1/1	0.96	0.15	3,3,3,3	0

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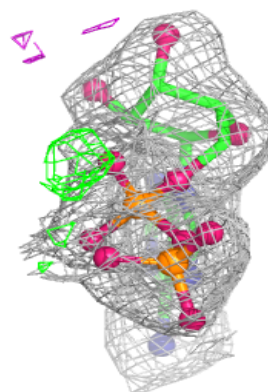
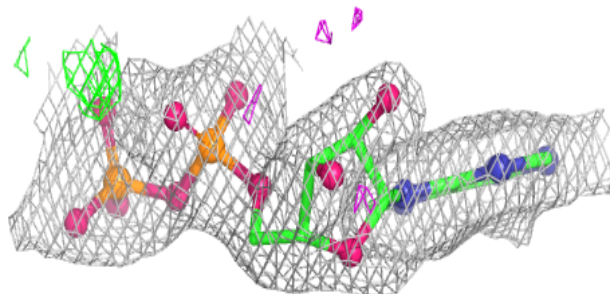
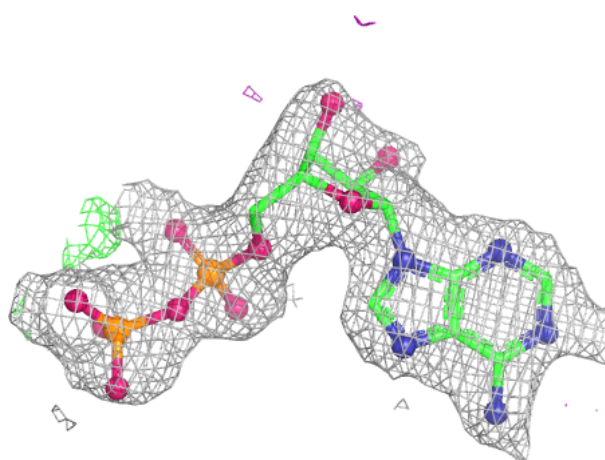
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	B	700	31/31	0.96	0.07	8,16,30,32	0
3	MG	C	701	1/1	0.96	0.16	19,19,19,19	0
4	ADP	C	700	27/27	0.97	0.06	15,20,26,28	0
2	ANP	A	700	31/31	0.98	0.06	5,9,14,19	0

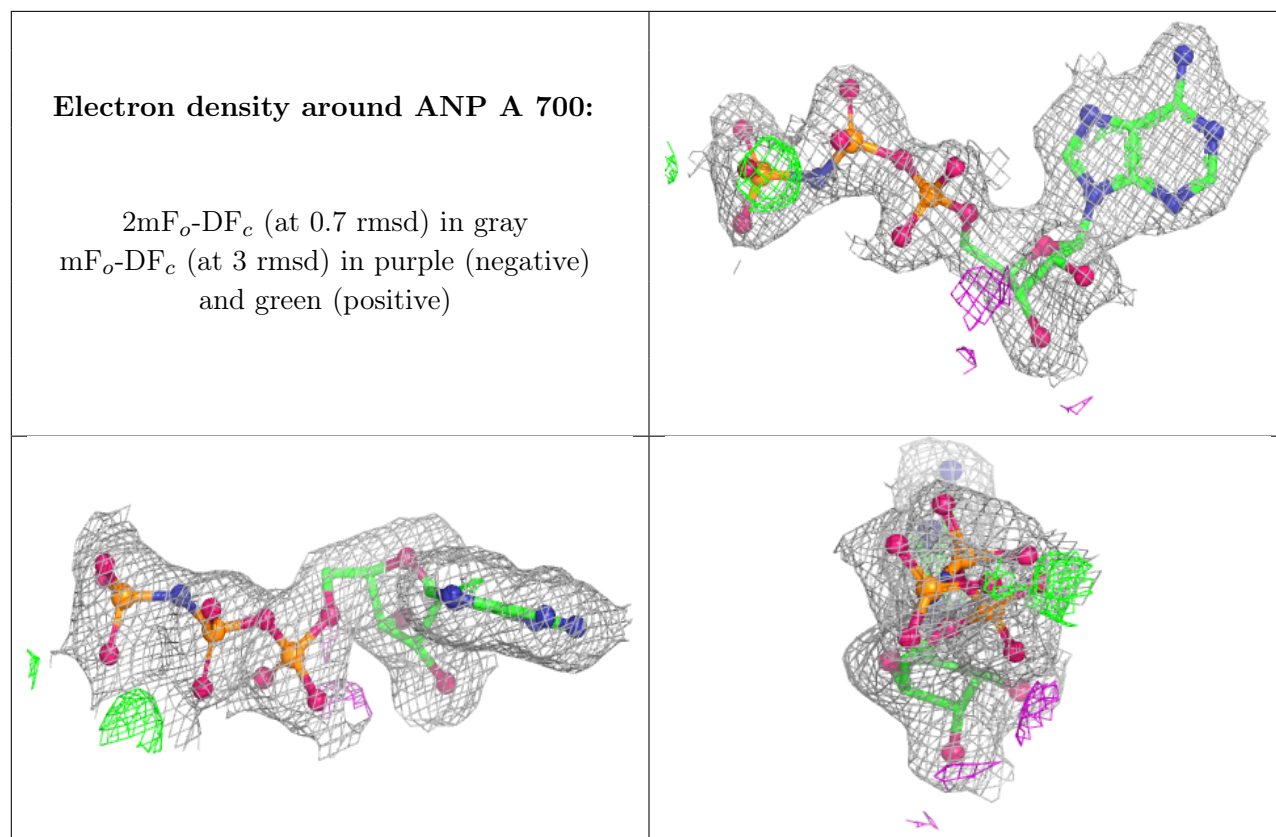
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around 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 ⓘ

There are no such residues in this entry.