



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 09:47 am GMT

PDB ID : 2JDI
Title : Ground state structure of F1-ATPase from bovine heart mitochondria (Bovine F1-ATPase crystallised in the absence of azide)
Authors : Bowler, M.W.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2007-01-09
Resolution : 1.90 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

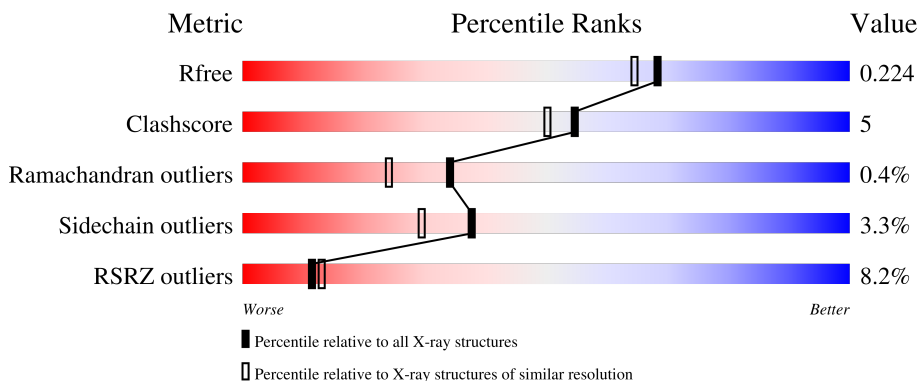
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

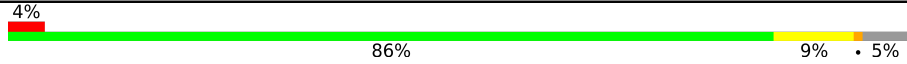
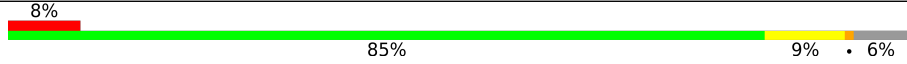



The reported resolution of this entry is 1.90 Å.

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.



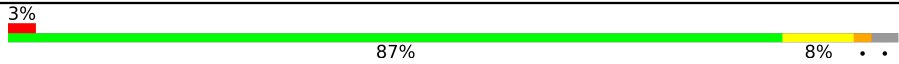

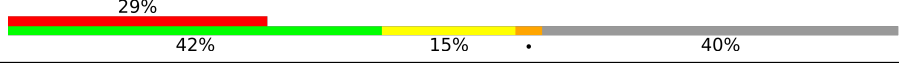

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	510	 4% 86% 9% • 5%
1	B	510	 8% 85% 9% • 6%
1	C	510	 3% 86% 8% • 5%
2	D	482	 2% 89% 7% • 5%
2	E	482	 11% 84% 9% • 5%

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Mol	Chain	Length	Quality of chain
2	F	482	
3	G	273	
4	H	146	
5	I	50	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26426 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 ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	Total 3726	C 2348	N 659	O 707	S 12	0	2	0
1	B	480	Total 3663	C 2308	N 648	O 695	S 12	0	0	0
1	C	487	Total 3715	C 2341	N 656	O 706	S 12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	SEE REMARK 999	UNP P19483
B	481	GLY	SER	SEE REMARK 999	UNP P19483
C	481	GLY	SER	SEE REMARK 999	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	467	Total 3544	C 2248	N 601	O 684	S 11	3	1	0
2	E	458	Total 3481	C 2207	N 593	O 671	S 10	5	2	0
2	F	466	Total 3538	C 2246	N 600	O 681	S 11	1	2	0

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	184	Total 1417	C 894	N 252	O 265	S 6	0	0	0

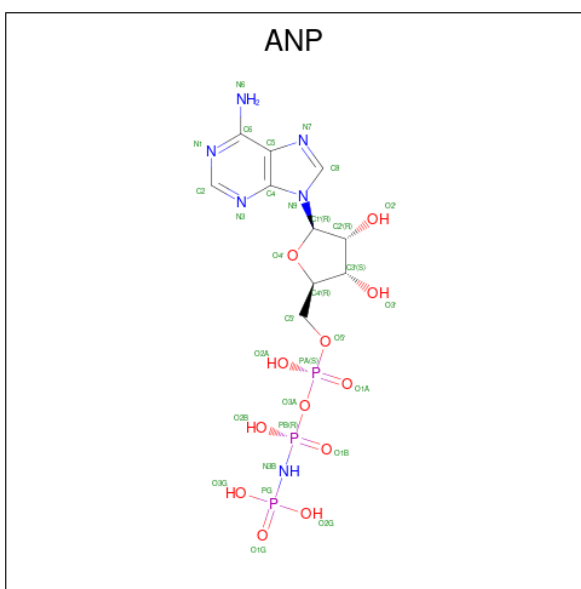
- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	88	657	417	108	131	1	0	0	0

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	I	25	203	130	38	34	1	0	0	0

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

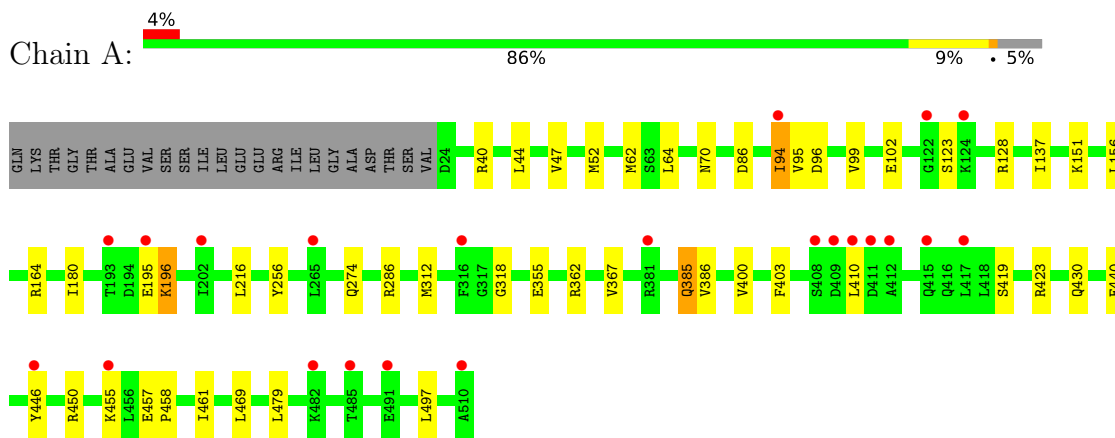
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	354	Total O 354 354	0	0
8	B	348	Total O 348 348	0	0
8	C	367	Total O 367 367	0	0
8	D	389	Total O 389 389	0	0
8	E	267	Total O 267 267	0	0
8	F	436	Total O 436 436	0	0
8	G	114	Total O 114 114	0	0
8	H	31	Total O 31 31	0	0
8	I	16	Total O 16 16	0	0

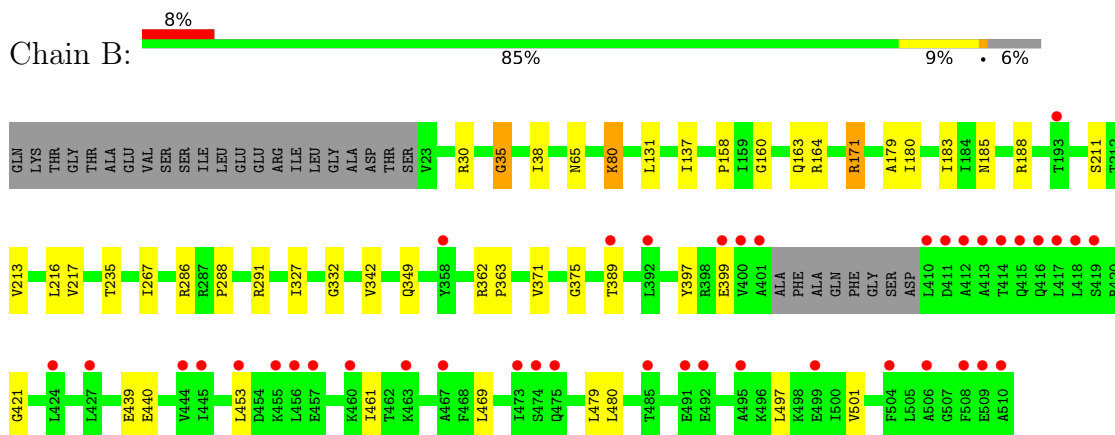
3 Residue-property plots [i](#)

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.

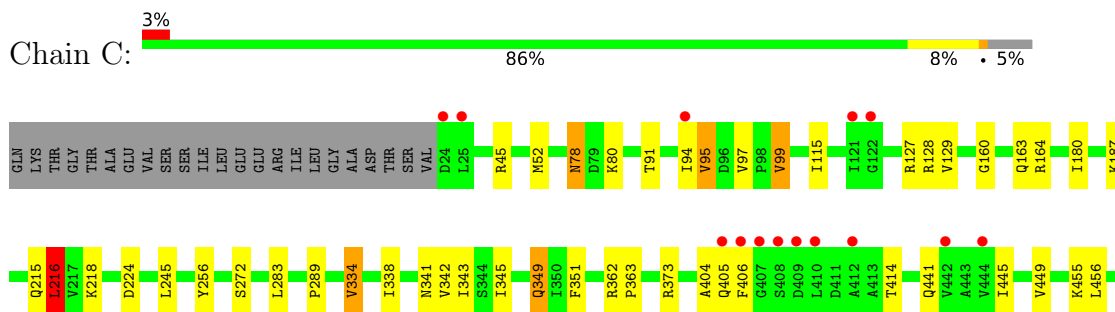
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM



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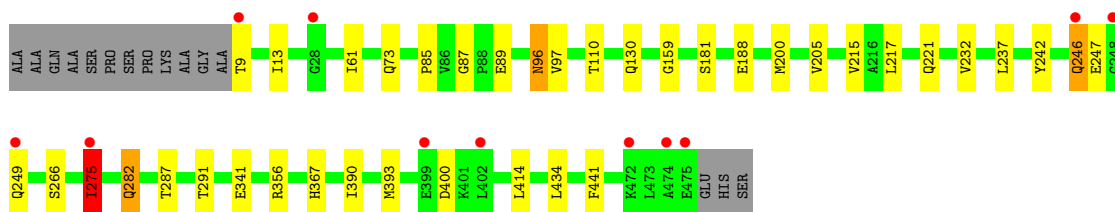
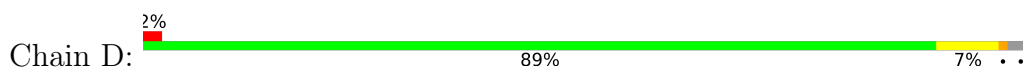


- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

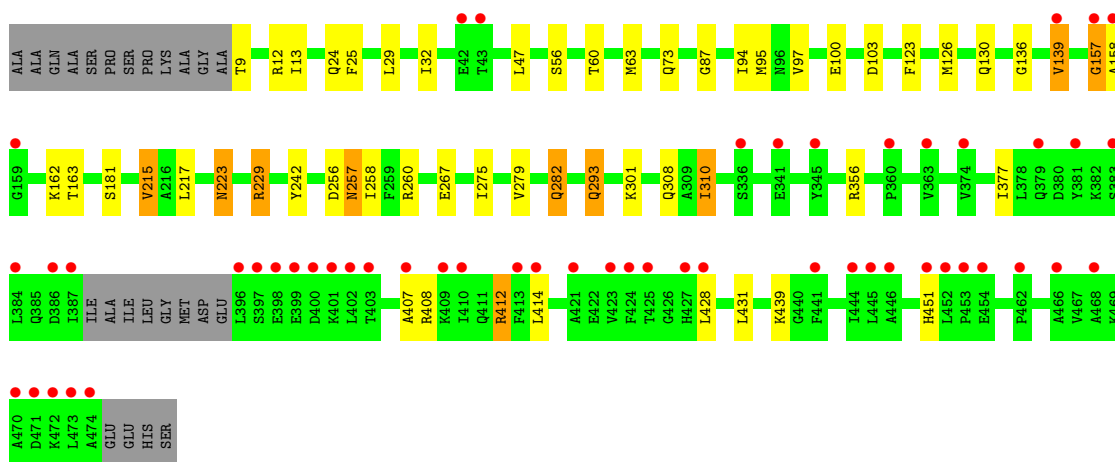
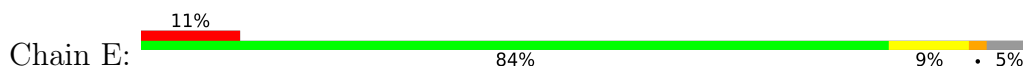




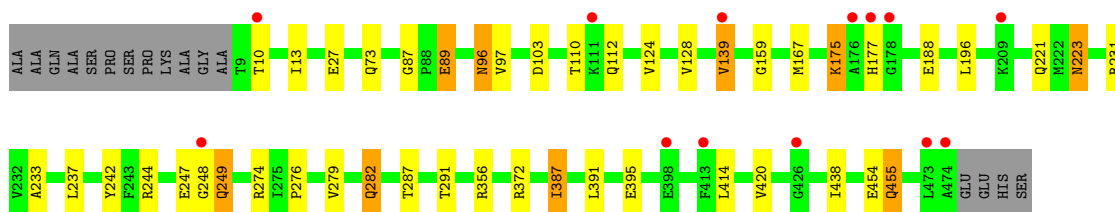
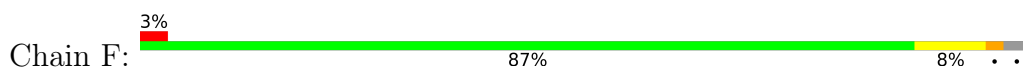
- Molecule 2: ATP SYNTHASE SUBUNIT BETA



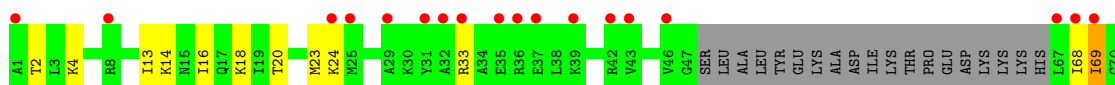
- Molecule 2: ATP SYNTHASE SUBUNIT BETA

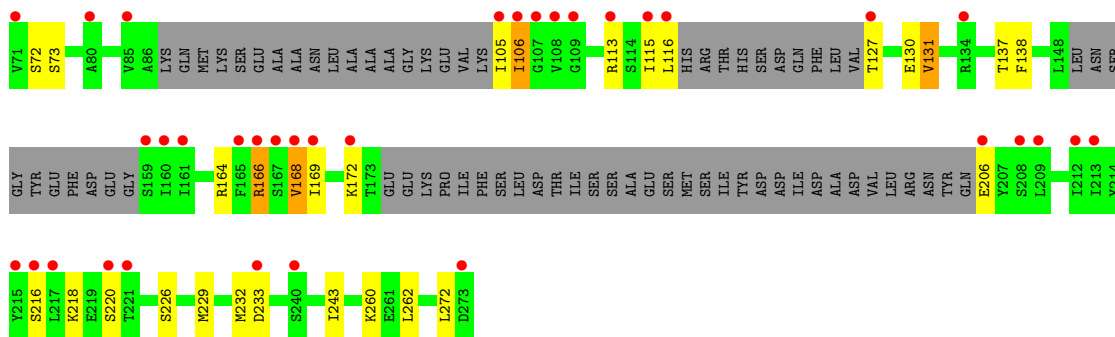


- Molecule 2: ATP SYNTHASE SUBUNIT BETA

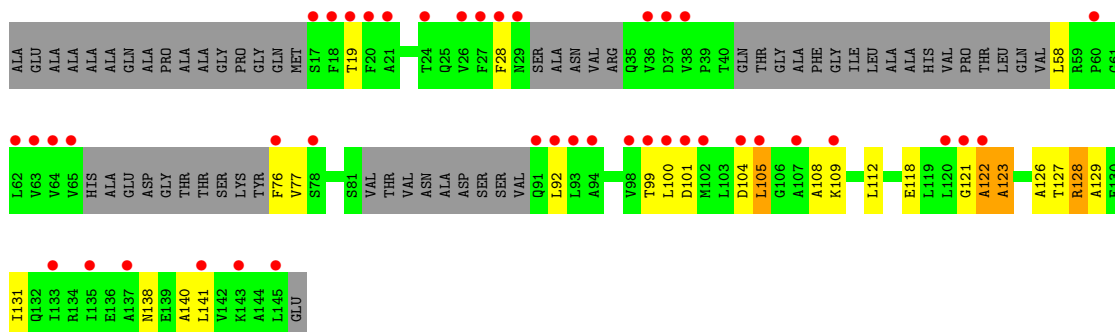
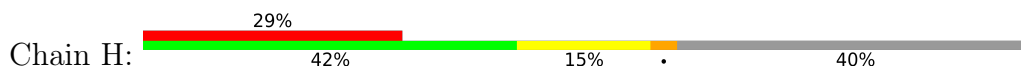


- Molecule 3: ATP SYNTHASE GAMMA CHAIN

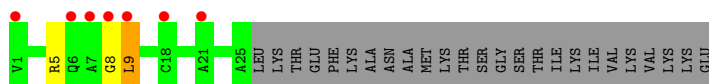
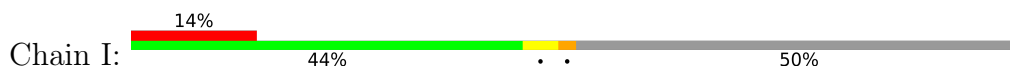




• Molecule 4: ATP SYNTHASE DELTA CHAIN



• Molecule 5: ATP SYNTHASE EPSILON CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.61Å 123.13Å 261.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 23.15 – 1.85	Depositor EDS
% Data completeness (in resolution range)	72.7 (20.00-1.90) 67.6 (23.15-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.220 0.178 , 0.224	Depositor DCC
R_{free} test set	9843 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26426	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.37	0/3783	0.53	0/5102
1	B	0.39	0/3711	0.53	0/5005
1	C	0.39	0/3766	0.56	1/5080 (0.0%)
2	D	1.57	2/3604 (0.1%)	0.64	6/4891 (0.1%)
2	E	0.37	0/3543	0.54	1/4807 (0.0%)
2	F	0.41	0/3601	1.44	2/4887 (0.0%)
3	G	0.35	0/1426	0.49	0/1907
4	H	0.37	0/660	0.63	0/890
5	I	0.31	0/207	0.61	0/279
All	All	0.70	2/24301 (0.0%)	0.76	10/32848 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	275[A]	ILE	CB-CG2	64.47	3.52	1.52
2	D	275[B]	ILE	CB-CG2	64.47	3.52	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	97[A]	VAL	CG1-CB-CG2	-65.79	5.64	110.90
2	F	97[B]	VAL	CG1-CB-CG2	-65.79	5.64	110.90
2	D	275[A]	ILE	CA-CB-CG2	-13.16	84.58	110.90
2	D	275[B]	ILE	CA-CB-CG2	-13.16	84.58	110.90
2	D	275[A]	ILE	CG1-CB-CG2	6.93	126.64	111.40
2	D	275[B]	ILE	CG1-CB-CG2	6.93	126.64	111.40
2	D	275[A]	ILE	CB-CA-C	6.71	125.01	111.60
2	D	275[B]	ILE	CB-CA-C	6.71	125.01	111.60
1	C	216	LEU	CA-CB-CG	6.02	129.14	115.30
2	E	229	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	3726	0	3832	32	0
1	B	3663	0	3774	30	0
1	C	3715	0	3814	32	0
2	D	3544	0	3603	35	0
2	E	3481	0	3539	39	0
2	F	3538	0	3604	41	0
3	G	1417	0	1501	32	0
4	H	657	0	663	28	0
5	I	203	0	205	2	0
6	A	31	0	13	0	0
6	B	31	0	13	0	0
6	C	31	0	13	0	0
6	D	31	0	13	3	0
6	F	31	0	13	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	354	0	0	6	0
8	B	348	0	0	5	0
8	C	367	0	0	11	0
8	D	389	0	0	4	0
8	E	267	0	0	5	0
8	F	436	0	0	8	0
8	G	114	0	0	3	0
8	H	31	0	0	1	0
8	I	16	0	0	0	0
All	All	26426	0	24600	254	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 5.

All (254) 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)
3:G:68:ILE:HB	3:G:69:ILE:HA	1.29	1.11
4:H:104:ASP:HA	4:H:105:LEU:CB	1.80	1.10
4:H:104:ASP:CA	4:H:105:LEU:HB2	1.82	1.08
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.31	1.07
4:H:122:ALA:HA	4:H:123:ALA:HB2	1.09	1.05
4:H:122:ALA:HA	4:H:123:ALA:CB	1.82	1.04
2:E:282:GLN:H	2:E:282:GLN:HE21	1.04	1.01
2:F:356:ARG:HD2	8:F:2347:HOH:O	1.64	0.98
4:H:99:THR:HB	4:H:101:ASP:H	1.31	0.93
2:D:282:GLN:H	2:D:282:GLN:HE21	1.01	0.93
4:H:99:THR:HA	4:H:100:LEU:HB2	1.48	0.93
1:A:99:VAL:HG11	1:A:256:TYR:HB2	1.52	0.91
2:D:159:GLY:H	6:D:1480:ANP:HNB1	1.14	0.89
2:F:282:GLN:H	2:F:282:GLN:HE21	0.91	0.87
2:F:282:GLN:HE21	2:F:282:GLN:N	1.73	0.87
1:C:52:MET:SD	8:C:2016:HOH:O	2.32	0.85
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.57	0.84
8:A:2187:HOH:O	2:D:291:THR:HG22	1.76	0.84
1:C:449:VAL:HB	8:C:2323:HOH:O	1.78	0.83
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.59	0.82
1:C:338:ILE:HG21	8:C:2195:HOH:O	1.81	0.80
4:H:126:ALA:HA	4:H:129:ALA:HB3	1.62	0.80
3:G:20:THR:HG22	3:G:232:MET:HE1	1.63	0.80
2:E:63:MET:HE3	2:E:97:VAL:HG21	1.63	0.79
2:F:282:GLN:H	2:F:282:GLN:NE2	1.76	0.78
1:C:95:VAL:HG22	8:C:2025:HOH:O	1.80	0.78
4:H:104:ASP:HA	4:H:105:LEU:HB2	0.88	0.78
4:H:121:GLY:HA3	4:H:122:ALA:HB3	1.66	0.77
1:A:151:LYS:H	1:A:430:GLN:HE22	1.32	0.76
2:D:97:VAL:HG23	8:D:2198:HOH:O	1.87	0.73
8:A:2213:HOH:O	2:D:275[A]:ILE:HG23	1.88	0.73
1:A:44:LEU:O	1:A:47:VAL:HG22	1.89	0.73
2:F:438:ILE:HG13	8:F:2361:HOH:O	1.87	0.73
1:A:99:VAL:CG1	1:A:256:TYR:HB2	2.19	0.72
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.71	0.71
4:H:99:THR:HB	4:H:101:ASP:N	2.04	0.71
3:G:68:ILE:CB	3:G:69:ILE:HA	2.12	0.71
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.26	0.70
2:F:223:ASN:HD22	2:F:223:ASN:H	1.37	0.70
2:E:158:ALA:HB3	8:E:2134:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:99:THR:CA	4:H:100:LEU:HB2	2.20	0.69
4:H:122:ALA:CA	4:H:123:ALA:CB	2.66	0.69
2:E:293:GLN:HE22	2:E:308:GLN:HE22	1.40	0.69
1:C:362:ARG:HH12	2:F:372:ARG:CZ	2.06	0.69
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.23	0.69
2:D:282:GLN:H	2:D:282:GLN:NE2	1.85	0.68
1:C:94:ILE:HG22	8:C:2068:HOH:O	1.93	0.68
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.29	0.68
2:F:395:GLU:HB3	8:F:2384:HOH:O	1.94	0.67
1:A:419:SER:O	1:A:423:ARG:HD3	1.93	0.67
2:D:97:VAL:HG22	2:D:232:VAL:HB	1.77	0.67
4:H:127:THR:N	4:H:128:ARG:HB2	2.10	0.66
1:B:217:VAL:HG11	2:E:123:PHE:HZ	1.60	0.66
1:C:160:GLY:H	1:C:163:GLN:NE2	1.92	0.66
4:H:105:LEU:H	4:H:108:ALA:H	1.43	0.65
2:F:249:GLN:OE1	2:F:249:GLN:HA	1.95	0.65
1:B:137:ILE:HG13	2:F:103:ASP:HA	1.79	0.65
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.77	0.65
1:C:272:SER:HA	8:C:2195:HOH:O	1.96	0.65
1:B:35:GLY:O	8:B:2011:HOH:O	2.14	0.64
2:D:85:PRO:HB3	2:D:110:THR:HG21	1.78	0.64
2:F:287:THR:O	2:F:291:THR:HG23	1.97	0.64
1:A:86:ASP:HB3	8:A:2068:HOH:O	1.99	0.63
4:H:126:ALA:HA	4:H:129:ALA:CB	2.28	0.62
1:C:95:VAL:CG2	8:C:2025:HOH:O	2.43	0.62
2:E:157:GLY:HA2	2:E:162:LYS:HE3	1.81	0.62
2:D:275[A]:ILE:HG22	3:G:272:LEU:HD13	1.81	0.62
4:H:127:THR:H	4:H:128:ARG:HB2	1.65	0.61
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.35	0.61
2:F:223:ASN:HD22	2:F:223:ASN:N	1.99	0.60
1:C:95:VAL:O	8:C:2068:HOH:O	2.16	0.60
2:E:223:ASN:HD22	2:E:223:ASN:H	1.48	0.60
3:G:20:THR:HG22	3:G:232:MET:CE	2.32	0.60
1:A:446:TYR:CE1	1:A:450:ARG:HD2	2.35	0.60
2:E:63:MET:HE3	2:E:97:VAL:CG2	2.30	0.60
3:G:168:VAL:HG23	3:G:169:ILE:HD12	1.84	0.59
1:A:99:VAL:CG1	1:A:256:TYR:CB	2.81	0.59
4:H:99:THR:HA	4:H:100:LEU:CB	2.28	0.59
4:H:99:THR:CB	4:H:101:ASP:H	2.12	0.59
2:E:356:ARG:NH2	8:E:2249:HOH:O	2.34	0.58
2:F:96:ASN:C	2:F:96:ASN:HD22	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:SER:HB2	2:E:215:VAL:HG13	1.84	0.58
2:E:282:GLN:H	2:E:282:GLN:NE2	1.87	0.58
1:C:215:GLN:HB3	2:F:356:ARG:HH22	1.69	0.57
2:E:229:ARG:HH22	2:E:267:GLU:CD	2.08	0.57
2:E:377:ILE:HG12	2:E:407:ALA:HB2	1.85	0.57
2:D:159:GLY:N	6:D:1480:ANP:HNB1	1.93	0.57
8:C:2175:HOH:O	2:F:291:THR:HG22	2.04	0.57
3:G:166:ARG:HE	3:G:172:LYS:HB2	1.70	0.57
4:H:127:THR:H	4:H:128:ARG:CB	2.17	0.57
3:G:113:ARG:HD3	3:G:127:THR:HG21	1.87	0.56
1:B:160:GLY:H	1:B:163:GLN:NE2	2.03	0.56
1:B:160:GLY:H	1:B:163:GLN:HE21	1.53	0.56
2:F:139:VAL:HG13	2:F:414:LEU:HD22	1.86	0.56
3:G:73:SER:HA	3:G:131:VAL:CG2	2.36	0.56
2:E:47:LEU:HB3	2:E:60[B]:THR:CG2	2.37	0.55
2:E:282:GLN:HE21	2:E:282:GLN:N	1.89	0.55
2:E:47:LEU:HB3	2:E:60[B]:THR:HG21	1.88	0.55
1:A:446:TYR:CE2	1:A:497:LEU:HB3	2.42	0.55
2:D:287:THR:O	2:D:291:THR:HG23	2.07	0.55
1:B:179:ALA:HB1	1:B:267:ILE:HG12	1.88	0.54
3:G:2:THR:HG22	3:G:4:LYS:H	1.72	0.54
2:F:233:ALA:O	2:F:237:LEU:HD13	2.07	0.54
1:A:40:ARG:HD2	1:A:70:ASN:OD1	2.08	0.54
4:H:122:ALA:HB3	8:H:2007:HOH:O	2.07	0.54
2:E:223:ASN:HD22	2:E:223:ASN:N	2.05	0.54
2:D:205:VAL:CG1	2:D:215:VAL:HG23	2.38	0.54
2:D:390:ILE:HD12	3:G:16:ILE:CD1	2.37	0.54
2:E:258:ILE:HG21	2:E:310:ILE:HD13	1.90	0.54
1:A:423:ARG:HG3	1:A:461:ILE:HD11	1.89	0.54
1:A:355:GLU:HG3	8:A:2131:HOH:O	2.08	0.53
2:D:96:ASN:C	2:D:96:ASN:HD22	2.11	0.53
2:D:188:GLU:O	2:D:221:GLN:HB3	2.08	0.53
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.44	0.53
2:D:390:ILE:HD12	3:G:16:ILE:HD13	1.91	0.53
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.91	0.52
1:A:102:GLU:HG3	1:A:123:SER:HA	1.91	0.52
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.91	0.52
3:G:229:MET:HB2	8:G:2014:HOH:O	2.09	0.52
1:B:158:PRO:O	1:B:375:GLY:HA3	2.10	0.52
2:F:391:LEU:HB3	2:F:395:GLU:HG3	1.93	0.51
1:B:213:VAL:O	1:B:217:VAL:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:115:ILE:HG22	3:G:116:LEU:HD12	1.92	0.51
4:H:58:LEU:HD21	4:H:92:LEU:HD11	1.93	0.51
1:C:441:GLN:O	1:C:445:ILE:HG12	2.10	0.51
1:B:183:ILE:HD11	1:B:267:ILE:HD13	1.93	0.50
1:C:218:LYS:HD3	2:F:128:VAL:HG21	1.93	0.50
4:H:127:THR:H	4:H:129:ALA:H	1.59	0.50
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.45	0.50
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.93	0.50
1:C:362:ARG:HA	1:C:363:PRO:C	2.31	0.50
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.76	0.50
2:F:244:ARG:O	2:F:248:GLY:HA2	2.10	0.50
1:B:171:ARG:HD3	8:E:2234:HOH:O	2.10	0.50
2:D:275[A]:ILE:CG2	3:G:272:LEU:HD13	2.41	0.50
2:E:13:ILE:HD12	2:E:73:GLN:HB3	1.94	0.50
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.77	0.50
2:D:85:PRO:HB3	2:D:110:THR:CG2	2.41	0.49
5:I:5:ARG:HA	5:I:9:LEU:H	1.76	0.49
2:E:408:ARG:O	2:E:412:ARG:NE	2.45	0.49
1:A:286:ARG:HG2	2:D:275[A]:ILE:HG21	1.94	0.49
2:D:130:GLN:HE22	2:D:356:ARG:HD2	1.77	0.49
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.39	0.49
2:D:414:LEU:HD23	2:D:441:PHE:CZ	2.48	0.49
2:F:159:GLY:HA2	6:F:1479:ANP:HNB1	1.77	0.48
1:B:30:ARG:HB3	8:B:2062:HOH:O	2.13	0.48
2:D:61:ILE:HD13	8:D:2057:HOH:O	2.12	0.48
1:B:349:GLN:NE2	8:B:2298:HOH:O	2.31	0.48
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.39	0.48
1:B:497:LEU:O	1:B:501:VAL:HG23	2.14	0.48
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.96	0.47
3:G:137:THR:HG22	3:G:138:PHE:N	2.29	0.47
3:G:68:ILE:HB	3:G:69:ILE:CA	2.21	0.47
1:A:62:MET:CE	1:A:64:LEU:HD21	2.45	0.47
3:G:164:ARG:HH12	3:G:172:LYS:HE2	1.79	0.47
1:B:332:GLY:HA2	8:B:2283:HOH:O	2.13	0.47
2:F:188:GLU:O	2:F:221:GLN:HB3	2.14	0.47
2:F:454:GLU:HG2	8:F:2388:HOH:O	2.13	0.47
4:H:128:ARG:H	4:H:131:ILE:HD12	1.80	0.47
3:G:24:LYS:HG3	3:G:233:ASP:HB2	1.97	0.47
2:E:47:LEU:CB	2:E:60[B]:THR:HG21	2.45	0.46
2:F:223:ASN:H	2:F:223:ASN:ND2	2.11	0.46
3:G:260:LYS:HD2	8:G:2043:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:69:ILE:HG21	3:G:106:ILE:HD12	1.98	0.46
1:C:78:ASN:HD22	1:C:80:LYS:H	1.61	0.46
2:F:139:VAL:CG1	2:F:414:LEU:HD22	2.46	0.46
1:A:362:ARG:NH1	8:A:2283:HOH:O	2.48	0.46
3:G:14:LYS:O	3:G:18:LYS:HE3	2.14	0.46
3:G:23:MET:SD	3:G:232:MET:HE2	2.55	0.46
2:D:89:GLU:CD	2:D:89:GLU:H	2.19	0.46
1:A:457:GLU:HA	1:A:458:PRO:HD2	1.79	0.46
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.98	0.45
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.99	0.45
1:B:362:ARG:HA	1:B:363:PRO:C	2.36	0.45
1:C:115:ILE:O	2:F:124:VAL:HG13	2.16	0.45
2:D:205:VAL:CG1	2:D:215:VAL:CG2	2.95	0.45
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.80	0.45
2:D:275[A]:ILE:CG2	2:D:275[A]:ILE:H	2.28	0.45
2:F:13:ILE:HD12	2:F:73:GLN:HB3	1.97	0.45
2:F:175:LYS:C	2:F:177:HIS:H	2.18	0.45
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.97	0.45
1:A:400:VAL:HG13	1:A:403:PHE:CE1	2.52	0.45
4:H:121:GLY:CA	4:H:122:ALA:HB3	2.40	0.45
2:E:9:THR:N	8:E:2001:HOH:O	2.49	0.45
1:A:286:ARG:CZ	2:D:275[A]:ILE:HG21	2.47	0.45
1:C:94:ILE:HD11	8:C:2023:HOH:O	2.16	0.45
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.98	0.45
3:G:69:ILE:HG13	3:G:106:ILE:HG13	1.99	0.45
2:F:231:ARG:NH1	8:F:2250:HOH:O	2.50	0.44
1:B:211:SER:HA	2:E:126:MET:HE2	1.98	0.44
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.99	0.44
3:G:73:SER:HA	3:G:131:VAL:HG23	1.98	0.44
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.98	0.44
3:G:106:ILE:HG22	3:G:127:THR:N	2.31	0.44
2:F:455:GLN:H	2:F:455:GLN:CD	2.20	0.44
1:A:128:ARG:NE	8:A:2105:HOH:O	2.48	0.44
1:B:371:VAL:HG21	8:F:2436:HOH:O	2.17	0.44
1:A:385:GLN:HG3	1:A:386:VAL:HG13	1.99	0.44
2:E:139:VAL:HG13	2:E:414:LEU:HB3	1.98	0.44
2:D:242:TYR:CD1	2:D:246:GLN:HG3	2.53	0.44
1:A:62:MET:HE2	1:A:64:LEU:HD21	2.00	0.44
1:C:99:VAL:HG21	1:C:127:ARG:HB2	1.99	0.44
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.00	0.44
1:C:404:ALA:O	1:C:406:PHE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:GLU:HG2	8:F:2013:HOH:O	2.18	0.44
1:C:128:ARG:NH1	8:C:2101:HOH:O	2.51	0.43
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.49	0.43
1:C:52:MET:O	1:C:91:THR:HB	2.17	0.43
1:B:440:GLU:HB3	1:B:469:LEU:HD11	2.00	0.43
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.01	0.43
3:G:216:SER:O	3:G:220:SER:HB2	2.18	0.43
1:A:195:GLU:O	1:A:196:LYS:HB2	2.19	0.43
2:E:25:PHE:O	2:E:56:SER:HB3	2.19	0.43
2:E:95:MET:HA	2:E:100:GLU:O	2.18	0.43
2:F:291:THR:HG21	8:F:2161:HOH:O	2.17	0.43
1:C:160:GLY:H	1:C:163:GLN:HE21	1.61	0.43
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.49	0.43
2:E:256:ASP:HA	2:E:257[A]:ASN:HA	1.67	0.43
1:C:187:LYS:HE2	1:C:224:ASP:HB3	2.00	0.43
1:B:327:ILE:HD11	1:B:342:VAL:HG21	2.02	0.42
1:A:312:MET:O	1:A:318:GLY:HA2	2.19	0.42
2:F:249:GLN:OE1	2:F:249:GLN:CA	2.66	0.42
2:D:367:HIS:CE1	2:D:434:LEU:HD11	2.54	0.42
2:F:188:GLU:H	2:F:221:GLN:NE2	2.18	0.42
3:G:69:ILE:HD11	3:G:105:ILE:N	2.34	0.42
4:H:19:THR:HA	4:H:28:PHE:O	2.18	0.42
5:I:8:GLY:HA3	5:I:9:LEU:CD1	2.50	0.42
1:A:94:ILE:CD1	1:A:96:ASP:HB3	2.49	0.42
1:B:180:ILE:HG13	1:B:216:LEU:HD21	2.02	0.42
3:G:166:ARG:HH21	3:G:172:LYS:HB2	1.85	0.42
1:C:343:ILE:HG23	1:C:349:GLN:NE2	2.34	0.42
1:C:373:ARG:HA	6:D:1480:ANP:O3'	2.20	0.42
3:G:69:ILE:HG23	3:G:69:ILE:O	2.20	0.42
3:G:13:ILE:HG22	3:G:243:ILE:HG13	2.02	0.42
1:B:286:ARG:HA	2:E:275:ILE:HD12	2.01	0.41
1:C:414:THR:HG21	8:D:2367:HOH:O	2.19	0.41
4:H:138:ASN:HA	4:H:141:LEU:HD12	2.00	0.41
1:B:235:THR:HG22	8:B:2182:HOH:O	2.20	0.41
4:H:58:LEU:HD13	4:H:77:VAL:HG11	2.02	0.41
2:F:89:GLU:HG3	2:F:110:THR:HA	2.02	0.41
2:F:167:MET:CE	2:F:196:LEU:HD13	2.50	0.41
1:C:99:VAL:HG13	1:C:256:TYR:HB2	2.02	0.41
2:E:260:ARG:HD2	8:E:2086:HOH:O	2.20	0.41
2:F:387:ILE:H	2:F:387:ILE:HG13	1.70	0.41
1:B:288:PRO:HB3	2:F:276:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:76:PHE:CZ	4:H:140:ALA:O	2.73	0.41
1:A:137:ILE:HD11	2:E:103:ASP:HA	2.04	0.40
1:B:439:GLU:HG3	1:B:480:LEU:HB3	2.02	0.40
3:G:226:SER:HB2	8:G:2075:HOH:O	2.21	0.40
1:A:151:LYS:H	1:A:430:GLN:NE2	2.10	0.40
1:B:80:LYS:HA	2:E:32:ILE:HB	2.02	0.40
2:D:9:THR:N	8:D:2001:HOH:O	2.54	0.40
1:B:453:LEU:HB3	1:B:461:ILE:HD12	2.04	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	487/510 (96%)	475 (98%)	11 (2%)	1 (0%)	47	38
1	B	476/510 (93%)	463 (97%)	12 (2%)	1 (0%)	47	38
1	C	485/510 (95%)	474 (98%)	10 (2%)	1 (0%)	47	38
2	D	466/482 (97%)	450 (97%)	16 (3%)	0	100	100
2	E	456/482 (95%)	442 (97%)	12 (3%)	2 (0%)	34	24
2	F	466/482 (97%)	453 (97%)	12 (3%)	1 (0%)	47	38
3	G	172/273 (63%)	163 (95%)	8 (5%)	1 (1%)	25	15
4	H	78/146 (53%)	65 (83%)	9 (12%)	4 (5%)	2	0
5	I	23/50 (46%)	22 (96%)	1 (4%)	0	100	100
All	All	3109/3445 (90%)	3007 (97%)	91 (3%)	11 (0%)	34	24

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	C	405	GLN
4	H	105	LEU
4	H	123	ALA
1	B	35	GLY
4	H	128	ARG
3	G	72	SER
4	H	122	ALA
2	E	279	VAL
2	F	279	VAL
2	E	157	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	395/412 (96%)	388 (98%)	7 (2%)	59 55
1	B	389/412 (94%)	379 (97%)	10 (3%)	46 39
1	C	393/412 (95%)	379 (96%)	14 (4%)	35 26
2	D	378/386 (98%)	367 (97%)	11 (3%)	42 35
2	E	372/386 (96%)	357 (96%)	15 (4%)	31 22
2	F	378/386 (98%)	364 (96%)	14 (4%)	34 25
3	G	154/231 (67%)	144 (94%)	10 (6%)	17 8
4	H	70/109 (64%)	67 (96%)	3 (4%)	29 19
5	I	19/41 (46%)	18 (95%)	1 (5%)	22 13
All	All	2548/2775 (92%)	2463 (97%)	85 (3%)	38 29

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	164	ARG
1	A	274	GLN
1	A	385	GLN

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Mol	Chain	Res	Type
1	A	410	LEU
1	A	455	LYS
1	A	479	LEU
1	B	38	ILE
1	B	65	ASN
1	B	80	LYS
1	B	131	LEU
1	B	164	ARG
1	B	171	ARG
1	B	291	ARG
1	B	389	THR
1	B	399	GLU
1	B	479	LEU
1	C	45	ARG
1	C	78	ASN
1	C	95	VAL
1	C	97	VAL
1	C	99	VAL
1	C	164	ARG
1	C	216	LEU
1	C	334	VAL
1	C	341	ASN
1	C	349	GLN
1	C	455	LYS
1	C	456	LEU
1	C	479	LEU
1	C	505	LEU
2	D	96	ASN
2	D	237	LEU
2	D	246	GLN
2	D	247	GLU
2	D	249	GLN
2	D	275[A]	ILE
2	D	275[B]	ILE
2	D	282	GLN
2	D	341	GLU
2	D	393	MET
2	D	400	ASP
2	E	130	GLN
2	E	139	VAL
2	E	163	THR
2	E	215	VAL

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Mol	Chain	Res	Type
2	E	223	ASN
2	E	257[A]	ASN
2	E	257[B]	ASN
2	E	282	GLN
2	E	293	GLN
2	E	301	LYS
2	E	310	ILE
2	E	412	ARG
2	E	428	LEU
2	E	439	LYS
2	E	451	HIS
2	F	10	THR
2	F	89	GLU
2	F	96	ASN
2	F	112	GLN
2	F	139	VAL
2	F	175	LYS
2	F	223	ASN
2	F	247	GLU
2	F	249	GLN
2	F	274	ARG
2	F	282	GLN
2	F	387	ILE
2	F	420	VAL
2	F	455	GLN
3	G	33	ARG
3	G	69	ILE
3	G	106	ILE
3	G	130	GLU
3	G	131	VAL
3	G	166	ARG
3	G	168	VAL
3	G	206	GLU
3	G	218	LYS
3	G	262	LEU
4	H	109	LYS
4	H	112	LEU
4	H	118	GLU
5	I	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	A	396	GLN
1	A	430	GLN
1	A	477	GLN
1	B	65	ASN
1	B	163	GLN
1	B	208	GLN
1	B	471	HIS
1	B	503	ASN
1	C	48	GLN
1	C	78	ASN
1	C	163	GLN
1	C	263	HIS
1	C	341	ASN
1	C	349	GLN
1	C	476	HIS
2	D	73	GLN
2	D	96	ASN
2	D	112	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	282	GLN
2	E	130	GLN
2	E	194	ASN
2	E	223	ASN
2	E	249	GLN
2	E	282	GLN
2	E	293	GLN
2	E	379	GLN
2	F	51	GLN
2	F	73	GLN
2	F	96	ASN
2	F	112	GLN
2	F	194	ASN
2	F	198	HIS
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	379	GLN
2	F	443	GLN
3	G	15	ASN
3	G	211	ASN

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Mol	Chain	Res	Type
4	H	91	GLN
5	I	16	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
6	ANP	C	1511	7	29,33,33	1.85	8 (27%)	31,52,52	1.92	4 (12%)
6	ANP	B	1511	7	29,33,33	1.80	8 (27%)	31,52,52	1.82	6 (19%)
6	ANP	A	1511	7	29,33,33	1.80	7 (24%)	31,52,52	2.07	7 (22%)
6	ANP	F	1479	7	29,33,33	1.76	8 (27%)	31,52,52	1.97	6 (19%)
6	ANP	D	1480	7	29,33,33	1.80	7 (24%)	31,52,52	2.12	7 (22%)

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
6	ANP	C	1511	7	-	3/14/38/38	0/3/3/3
6	ANP	B	1511	7	-	2/14/38/38	0/3/3/3
6	ANP	A	1511	7	-	3/14/38/38	0/3/3/3
6	ANP	F	1479	7	-	3/14/38/38	0/3/3/3
6	ANP	D	1480	7	-	4/14/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1511	ANP	PB-N3B	4.40	1.74	1.63
6	B	1511	ANP	PB-N3B	4.40	1.74	1.63
6	C	1511	ANP	PG-N3B	4.38	1.74	1.63
6	F	1479	ANP	PB-O1B	4.28	1.52	1.46
6	B	1511	ANP	PG-N3B	4.11	1.74	1.63
6	A	1511	ANP	PB-N3B	4.10	1.74	1.63
6	A	1511	ANP	PG-N3B	3.95	1.73	1.63
6	D	1480	ANP	PG-N3B	3.93	1.73	1.63
6	C	1511	ANP	PB-O1B	3.70	1.52	1.46
6	D	1480	ANP	PB-N3B	3.68	1.73	1.63
6	F	1479	ANP	PG-N3B	3.68	1.73	1.63
6	D	1480	ANP	PB-O1B	3.66	1.52	1.46
6	F	1479	ANP	PB-N3B	3.61	1.72	1.63
6	A	1511	ANP	PG-O1G	3.57	1.51	1.46
6	A	1511	ANP	PB-O1B	3.44	1.51	1.46
6	D	1480	ANP	PG-O1G	3.38	1.51	1.46
6	B	1511	ANP	PG-O1G	3.37	1.51	1.46
6	C	1511	ANP	PG-O1G	3.36	1.51	1.46
6	B	1511	ANP	PB-O1B	3.09	1.51	1.46
6	F	1479	ANP	PG-O1G	2.81	1.50	1.46
6	D	1480	ANP	C5-C4	2.66	1.48	1.40
6	D	1480	ANP	PB-O2B	-2.59	1.49	1.56
6	C	1511	ANP	C5-C4	2.56	1.47	1.40
6	F	1479	ANP	C5-C4	2.56	1.47	1.40
6	A	1511	ANP	C5-C4	2.55	1.47	1.40
6	F	1479	ANP	PG-O2G	-2.54	1.49	1.56
6	B	1511	ANP	C5-C4	2.51	1.47	1.40
6	A	1511	ANP	PG-O2G	-2.39	1.50	1.56
6	F	1479	ANP	PB-O2B	-2.28	1.50	1.56
6	A	1511	ANP	PB-O2B	-2.26	1.50	1.56
6	B	1511	ANP	PB-O2B	-2.22	1.50	1.56
6	C	1511	ANP	PG-O3G	-2.19	1.50	1.56
6	C	1511	ANP	PB-O2B	-2.17	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1480	ANP	PG-O2G	-2.16	1.50	1.56
6	B	1511	ANP	PG-O2G	-2.10	1.51	1.56
6	F	1479	ANP	PG-O3G	-2.08	1.51	1.56
6	B	1511	ANP	PG-O3G	-2.07	1.51	1.56
6	C	1511	ANP	PG-O2G	-2.02	1.51	1.56

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1480	ANP	O1G-PG-N3B	-9.07	98.41	111.77
6	C	1511	ANP	O1G-PG-N3B	-7.84	100.22	111.77
6	F	1479	ANP	O1G-PG-N3B	-7.63	100.54	111.77
6	A	1511	ANP	O1G-PG-N3B	-7.54	100.67	111.77
6	B	1511	ANP	O1G-PG-N3B	-6.53	102.15	111.77
6	A	1511	ANP	O2B-PB-O1B	4.11	118.54	109.92
6	A	1511	ANP	N3-C2-N1	-3.65	122.97	128.68
6	B	1511	ANP	N3-C2-N1	-3.54	123.14	128.68
6	C	1511	ANP	N3-C2-N1	-3.43	123.32	128.68
6	D	1480	ANP	N3-C2-N1	-3.42	123.33	128.68
6	F	1479	ANP	N3-C2-N1	-3.41	123.34	128.68
6	F	1479	ANP	O2B-PB-O1B	3.35	116.94	109.92
6	B	1511	ANP	O2B-PB-O1B	3.32	116.88	109.92
6	A	1511	ANP	O1B-PB-N3B	-3.17	107.10	111.77
6	F	1479	ANP	O3A-PB-N3B	-2.96	98.37	106.59
6	C	1511	ANP	O2B-PB-O1B	2.90	116.00	109.92
6	B	1511	ANP	C4-C5-N7	-2.75	106.53	109.40
6	A	1511	ANP	C4-C5-N7	-2.54	106.75	109.40
6	D	1480	ANP	O2B-PB-O1B	2.48	115.11	109.92
6	F	1479	ANP	C4-C5-N7	-2.40	106.90	109.40
6	C	1511	ANP	C4-C5-N7	-2.37	106.93	109.40
6	D	1480	ANP	C2-N1-C6	2.34	122.75	118.75
6	D	1480	ANP	C4-C5-N7	-2.22	107.08	109.40
6	D	1480	ANP	O2B-PB-O3A	2.18	111.91	104.64
6	B	1511	ANP	C3'-C2'-C1'	2.14	104.19	100.98
6	A	1511	ANP	PB-O3A-PA	-2.13	125.11	132.62
6	A	1511	ANP	C2-N1-C6	2.13	122.39	118.75
6	D	1480	ANP	O2G-PG-O3G	2.09	113.20	107.64
6	B	1511	ANP	PB-O3A-PA	-2.09	125.27	132.62
6	F	1479	ANP	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (15) torsion outliers are listed below:

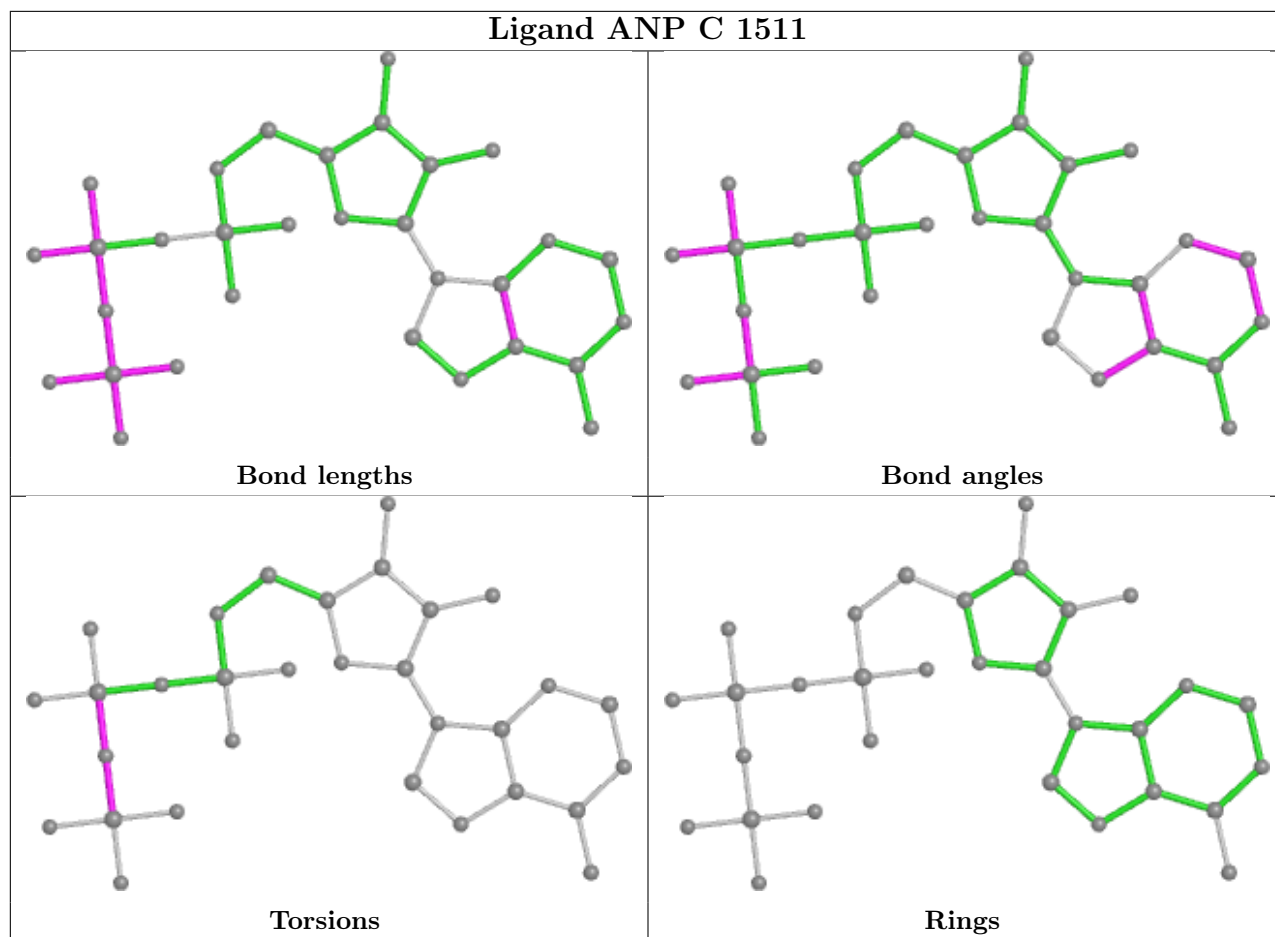
Mol	Chain	Res	Type	Atoms
6	A	1511	ANP	PG-N3B-PB-O1B
6	A	1511	ANP	PG-N3B-PB-O3A
6	B	1511	ANP	PG-N3B-PB-O1B
6	B	1511	ANP	PG-N3B-PB-O3A
6	C	1511	ANP	PB-N3B-PG-O1G
6	C	1511	ANP	PG-N3B-PB-O1B
6	D	1480	ANP	PG-N3B-PB-O1B
6	D	1480	ANP	PA-O3A-PB-O1B
6	D	1480	ANP	PA-O3A-PB-O2B
6	F	1479	ANP	PG-N3B-PB-O1B
6	F	1479	ANP	PA-O3A-PB-O1B
6	F	1479	ANP	PA-O3A-PB-O2B
6	A	1511	ANP	PB-N3B-PG-O1G
6	C	1511	ANP	PG-N3B-PB-O3A
6	D	1480	ANP	PB-N3B-PG-O1G

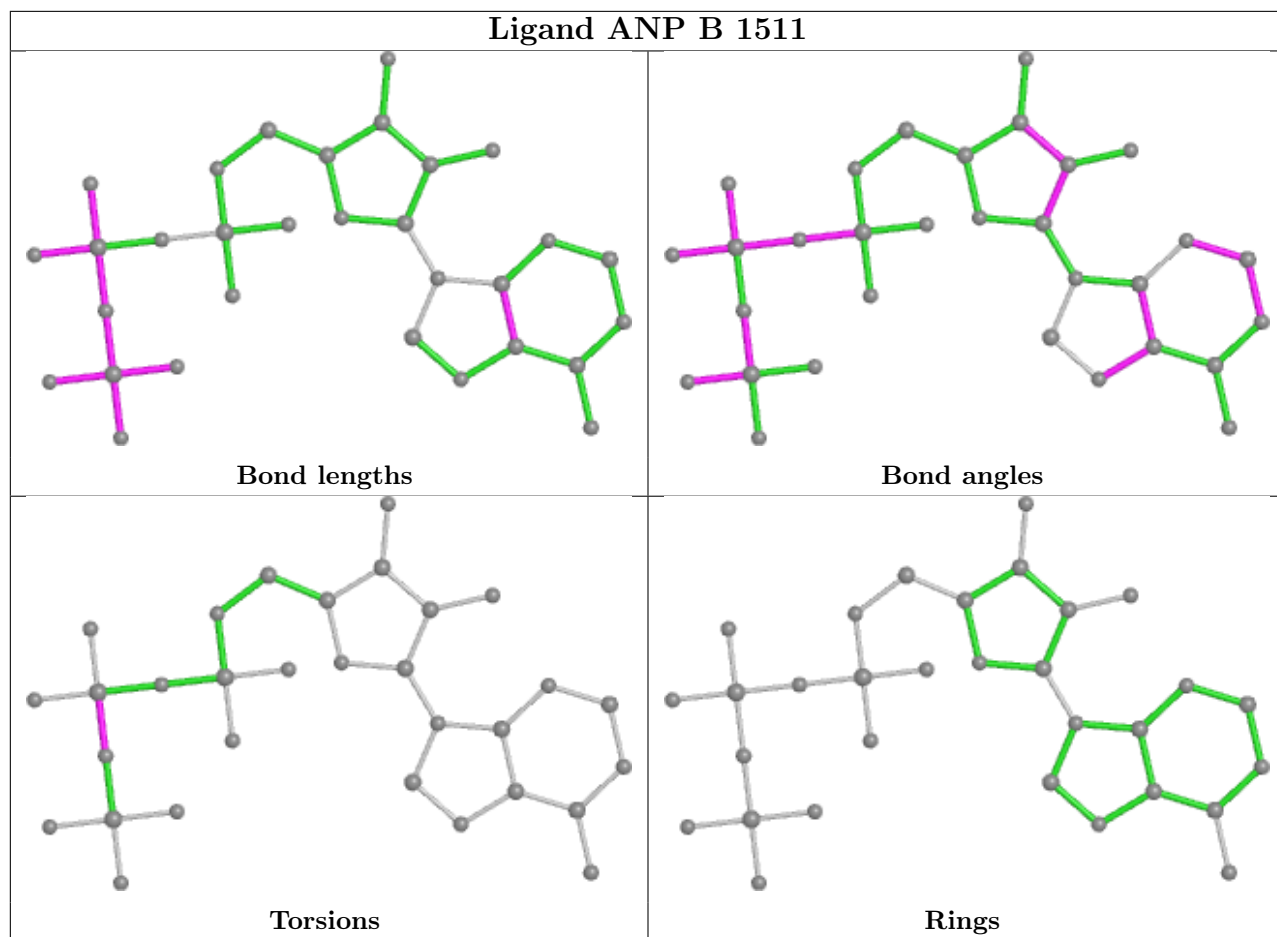
There are no ring outliers.

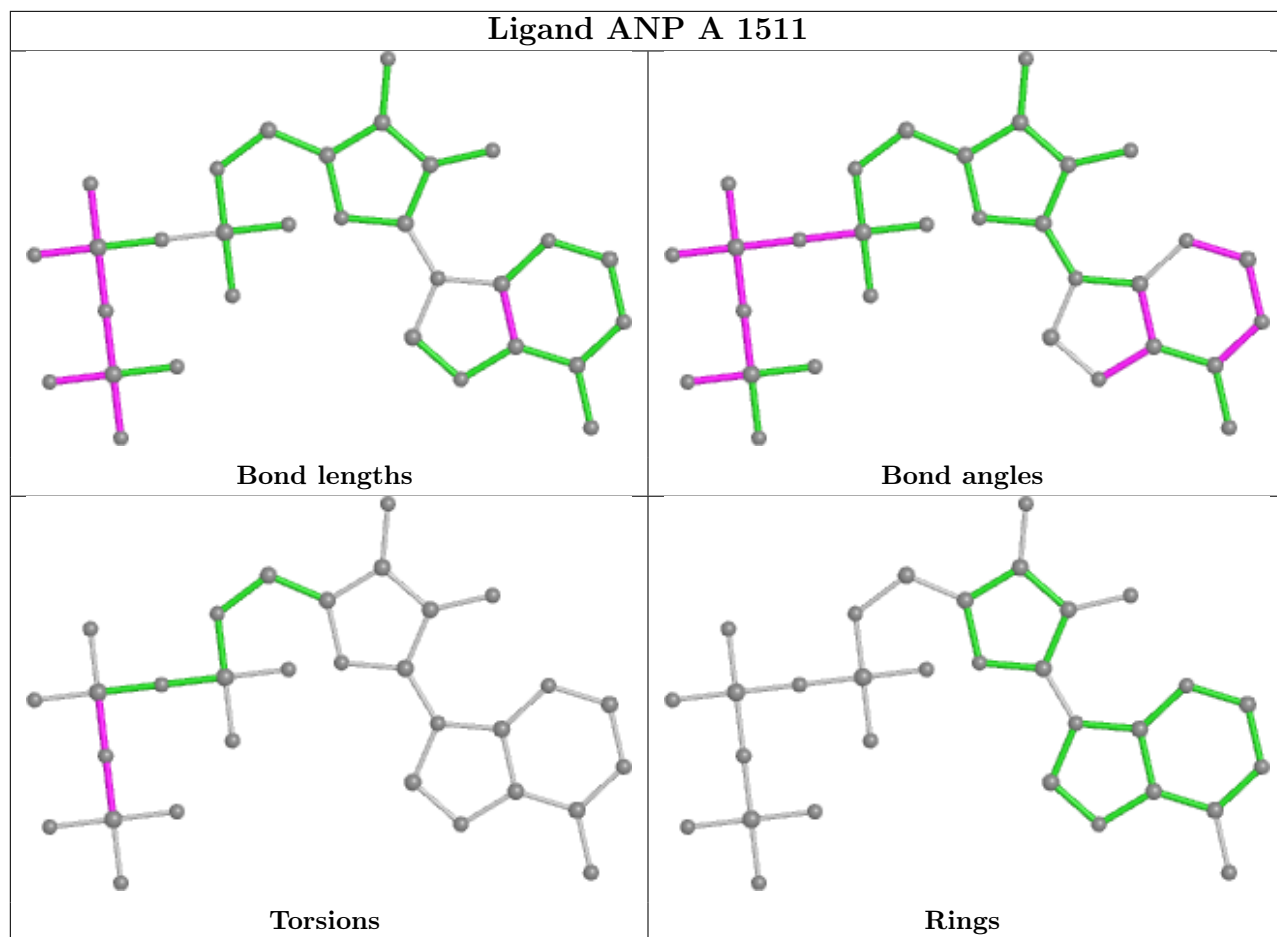
2 monomers are involved in 4 short contacts:

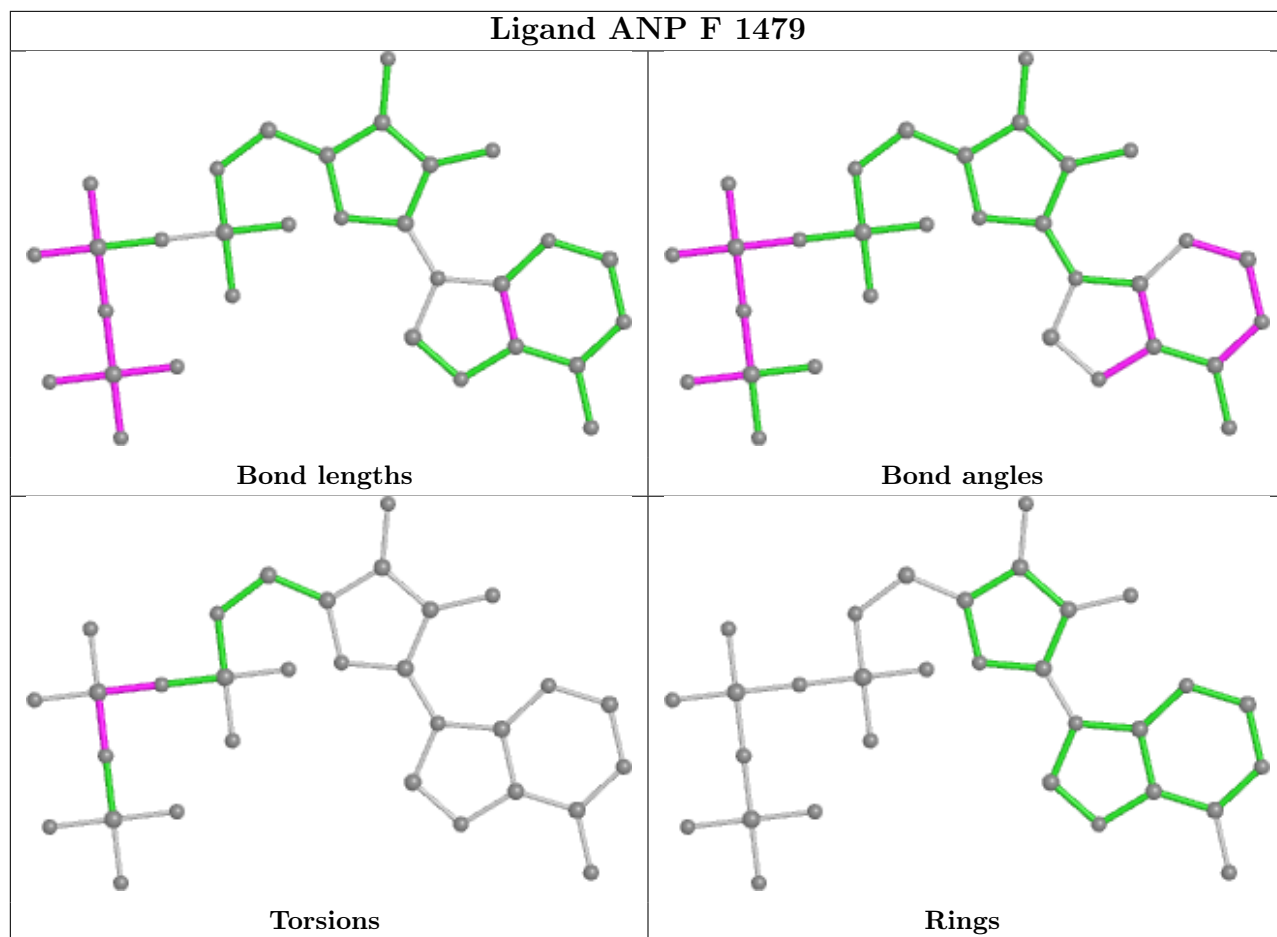
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1479	ANP	1	0
6	D	1480	ANP	3	0

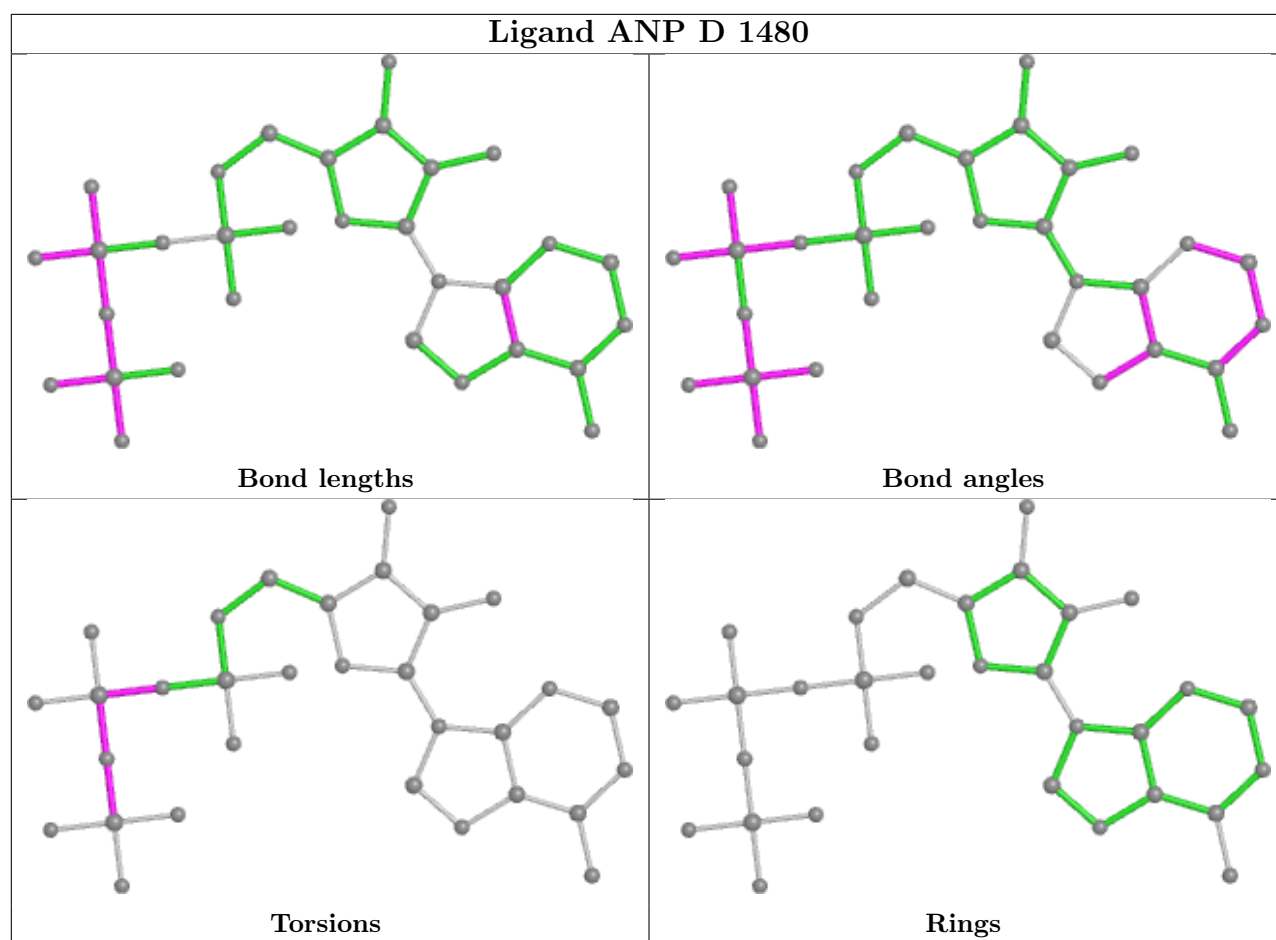
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/510 (95%)	-0.02	22 (4%) 33 36	5, 15, 36, 66	3 (0%)
1	B	480/510 (94%)	0.12	41 (8%) 10 12	5, 14, 48, 78	1 (0%)
1	C	487/510 (95%)	-0.16	16 (3%) 46 49	8, 15, 32, 70	0
2	D	467/482 (96%)	-0.22	11 (2%) 59 62	6, 14, 34, 71	1 (0%)
2	E	458/482 (95%)	0.44	53 (11%) 4 5	7, 18, 60, 81	2 (0%)
2	F	466/482 (96%)	-0.17	13 (2%) 53 56	8, 14, 38, 59	1 (0%)
3	G	184/273 (67%)	1.47	53 (28%) 0 0	5, 32, 48, 54	1 (0%)
4	H	88/146 (60%)	2.50	42 (47%) 0 0	2, 20, 42, 50	0
5	I	25/50 (50%)	1.64	7 (28%) 0 0	2, 7, 32, 34	0
All	All	3142/3445 (91%)	0.17	258 (8%) 11 13	2, 15, 45, 81	9 (0%)

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	273	ASP	11.9
1	B	412	ALA	9.8
2	E	402	LEU	9.0
1	C	407	GLY	8.4
4	H	63	VAL	8.0
1	C	406	PHE	7.7
4	H	18	PHE	7.7
4	H	27	PHE	7.6
2	E	451	HIS	7.6
4	H	105	LEU	7.5
2	E	424	PHE	7.4
2	E	384	LEU	7.3
2	F	474	ALA	6.9
4	H	64	VAL	6.7
5	I	8	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
2	E	423	VAL	6.7
2	E	383	SER	6.6
4	H	65	VAL	6.6
2	E	398	GLU	6.5
3	G	85	VAL	6.3
1	B	400	VAL	6.3
2	D	475	GLU	6.2
1	C	409	ASP	6.2
4	H	145	LEU	6.0
3	G	1	ALA	5.9
1	B	414	THR	5.7
1	B	455	LYS	5.7
5	I	7	ALA	5.6
1	B	413	ALA	5.6
2	E	470	ALA	5.6
2	F	176	ALA	5.6
2	E	400	ASP	5.5
3	G	169	ILE	5.5
1	B	416	GLN	5.3
3	G	159	SER	5.3
2	E	472	LYS	5.2
4	H	26	VAL	5.2
4	H	62	LEU	5.2
3	G	106	ILE	5.2
3	G	25	MET	5.2
1	B	417	LEU	5.1
5	I	1	VAL	5.1
2	E	410	ILE	5.1
1	B	358	TYR	5.1
4	H	36	VAL	5.0
3	G	217	LEU	5.0
4	H	28	PHE	5.0
1	B	411	ASP	4.9
3	G	172	LYS	4.9
2	E	414	LEU	4.9
1	B	506	ALA	4.9
2	D	248	GLY	4.9
3	G	160	ILE	4.8
2	E	468	ALA	4.8
3	G	116	LEU	4.8
3	G	29	ALA	4.8
2	E	399	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
3	G	32	ALA	4.7
2	E	474	ALA	4.6
2	E	413	PHE	4.6
4	H	17	SER	4.6
1	B	510	ALA	4.6
2	E	159	GLY	4.5
1	B	419	SER	4.5
1	A	410	LEU	4.5
2	E	473	LEU	4.5
4	H	100	LEU	4.5
3	G	36	ARG	4.4
4	H	102	MET	4.4
4	H	107	ALA	4.4
4	H	99	THR	4.3
2	E	441	PHE	4.2
2	E	379	GLN	4.2
3	G	209	LEU	4.2
1	C	24	ASP	4.1
1	B	474	SER	4.1
3	G	67	LEU	4.1
3	G	46	VAL	4.1
2	E	42	GLU	4.1
3	G	168	VAL	4.1
2	E	425	THR	4.1
1	C	122	GLY	4.1
1	A	408	SER	4.0
2	D	249	GLN	4.0
4	H	76	PHE	4.0
4	H	122	ALA	4.0
1	A	193	THR	4.0
3	G	208	SER	4.0
2	F	248	GLY	4.0
3	G	68	ILE	3.9
4	H	29	ASN	3.9
3	G	167	SER	3.9
1	C	405	GLN	3.9
1	B	410	LEU	3.9
1	C	412	ALA	3.9
3	G	43	VAL	3.9
1	B	460	LYS	3.8
2	F	473	LEU	3.8
4	H	120	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
4	H	37	ASP	3.7
2	E	139	VAL	3.7
2	D	275[A]	ILE	3.7
1	B	457	GLU	3.7
1	B	427	LEU	3.7
1	A	94	ILE	3.7
3	G	105	ILE	3.7
1	B	392	LEU	3.6
1	A	122	GLY	3.6
1	B	492	GLU	3.6
2	E	401	LYS	3.6
2	F	178	GLY	3.5
3	G	39	LYS	3.5
3	G	221	THR	3.5
1	A	417	LEU	3.5
1	B	418	LEU	3.5
3	G	108	VAL	3.5
2	E	427	HIS	3.5
1	B	509	GLU	3.5
4	H	92	LEU	3.5
1	B	473	ILE	3.5
4	H	91	GLN	3.5
2	E	386	ASP	3.5
2	D	9	THR	3.5
3	G	69	ILE	3.4
2	E	452	LEU	3.4
1	B	444	VAL	3.4
2	E	446	ALA	3.4
2	E	396	LEU	3.4
2	D	474	ALA	3.4
1	B	475	GLN	3.3
2	E	444	ILE	3.3
2	E	43	THR	3.3
2	E	471	ASP	3.3
2	E	407	ALA	3.2
1	B	504	PHE	3.2
1	A	381	ARG	3.2
3	G	127	THR	3.2
4	H	135	ILE	3.2
4	H	141	LEU	3.2
4	H	19	THR	3.2
1	B	467	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
5	I	6	GLN	3.1
1	B	508	PHE	3.1
3	G	213	ILE	3.1
2	E	428	LEU	3.1
3	G	115	ILE	3.1
2	D	472	LYS	3.1
5	I	9	LEU	3.1
1	B	399	GLU	3.0
1	B	495	ALA	3.0
1	A	455	LYS	3.0
3	G	33	ARG	3.0
4	H	20	PHE	3.0
4	H	137	ALA	3.0
3	G	134	ARG	2.9
4	H	98	VAL	2.9
3	G	206	GLU	2.9
2	F	426	GLY	2.9
3	G	220	SER	2.9
1	A	491	GLU	2.9
3	G	161	ILE	2.9
2	E	454	GLU	2.8
3	G	215	TYR	2.8
3	G	31	TYR	2.8
1	B	445	ILE	2.8
3	G	24	LYS	2.7
1	A	510	ALA	2.7
2	E	360	PRO	2.7
4	H	38	VAL	2.7
2	E	409	LYS	2.7
1	B	424	LEU	2.7
3	G	71	VAL	2.7
1	A	412	ALA	2.7
3	G	216	SER	2.7
4	H	21	ALA	2.7
1	B	415	GLN	2.7
2	E	363	VAL	2.7
3	G	240	SER	2.7
2	E	387	ILE	2.6
4	H	104	ASP	2.6
4	H	133	ILE	2.6
2	D	399	GLU	2.6
2	E	341	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	316	PHE	2.6
4	H	109	LYS	2.6
1	A	409	ASP	2.6
2	E	397	SER	2.6
1	A	202	ILE	2.6
3	G	212	ILE	2.6
1	C	510	ALA	2.6
3	G	107	GLY	2.6
3	G	8	ARG	2.5
1	C	408	SER	2.5
1	A	482	LYS	2.5
2	F	209	LYS	2.5
2	F	398	GLU	2.5
2	E	158	ALA	2.5
1	B	401	ALA	2.5
4	H	121	GLY	2.5
1	B	453	LEU	2.5
2	F	111	LYS	2.5
3	G	35	GLU	2.5
2	F	139	VAL	2.5
3	G	233	ASP	2.5
1	C	410	LEU	2.4
2	E	345	TYR	2.4
3	G	165	PHE	2.4
2	E	453	PRO	2.4
1	B	463	LYS	2.4
2	F	413	PHE	2.4
2	E	157	GLY	2.4
2	E	466	ALA	2.4
1	B	193	THR	2.4
2	E	374	VAL	2.4
2	D	402	LEU	2.4
2	F	177	HIS	2.4
3	G	109	GLY	2.3
5	I	18	CYS	2.3
1	B	491	GLU	2.3
2	E	381	TYR	2.3
4	H	78	SER	2.3
1	A	446	TYR	2.3
1	A	411	ASP	2.3
1	C	94	ILE	2.3
2	E	445	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	468	PHE	2.3
4	H	93	LEU	2.3
1	A	415	GLN	2.2
1	B	499	GLU	2.2
2	F	10	THR	2.2
1	A	195	GLU	2.2
1	B	456	LEU	2.2
4	H	143	LYS	2.2
3	G	166	ARG	2.2
4	H	101	ASP	2.2
3	G	42	ARG	2.2
2	E	462	PRO	2.2
2	E	403	THR	2.2
1	C	444	VAL	2.2
4	H	60	PRO	2.2
1	B	485	THR	2.2
2	E	421	ALA	2.1
1	A	265	LEU	2.1
1	A	485	THR	2.1
1	B	389	THR	2.1
2	D	246	GLN	2.1
1	C	25	LEU	2.1
3	G	113	ARG	2.1
3	G	37	GLU	2.1
1	C	121	ILE	2.1
4	H	94	ALA	2.1
5	I	21	ALA	2.1
1	C	442	VAL	2.0
1	A	124	LYS	2.0
2	D	28	GLY	2.0
3	G	80	ALA	2.0
2	E	336	SER	2.0
4	H	24	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](#)

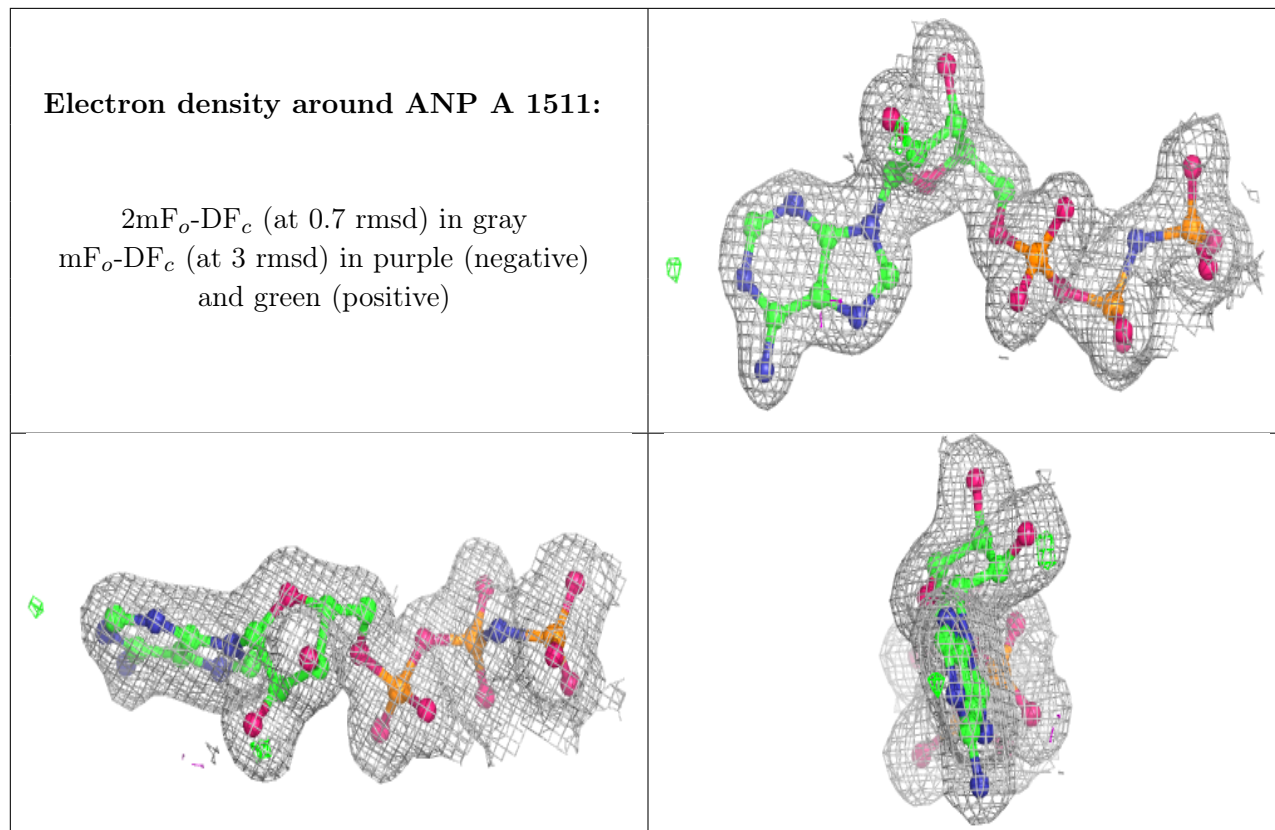
There are no monosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

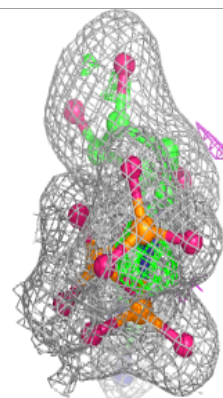
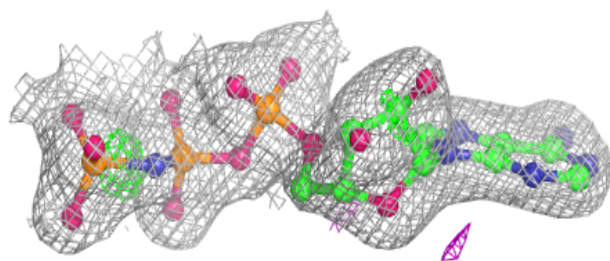
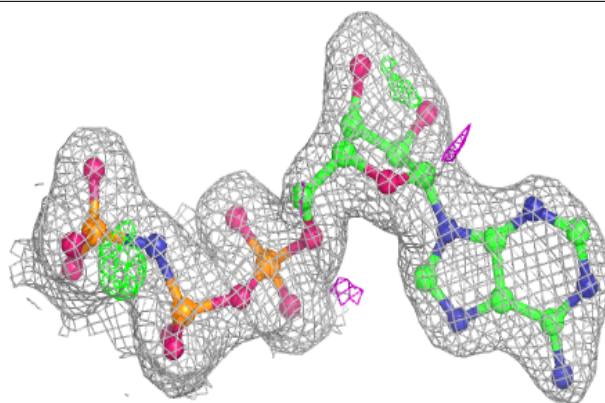
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ANP	A	1511	31/31	0.98	0.08	8,12,19,21	0
6	ANP	B	1511	31/31	0.98	0.07	8,15,24,33	0
6	ANP	F	1479	31/31	0.98	0.08	8,12,18,21	0
7	MG	B	1512	1/1	0.98	0.05	15,15,15,15	0
7	MG	F	1480	1/1	0.98	0.10	13,13,13,13	0
7	MG	A	1512	1/1	0.99	0.09	16,16,16,16	0
6	ANP	D	1480	31/31	0.99	0.07	6,10,14,16	0
7	MG	C	1512	1/1	0.99	0.07	13,13,13,13	0
7	MG	D	1481	1/1	0.99	0.10	14,14,14,14	0
6	ANP	C	1511	31/31	0.99	0.07	8,12,17,25	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.

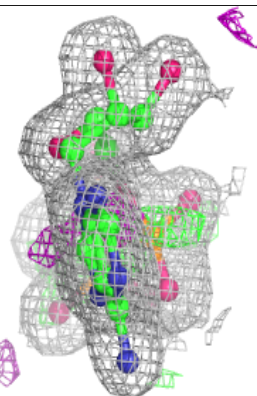
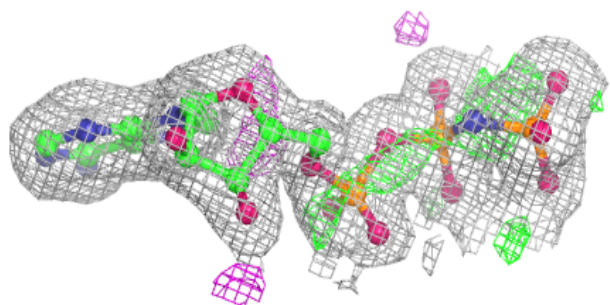
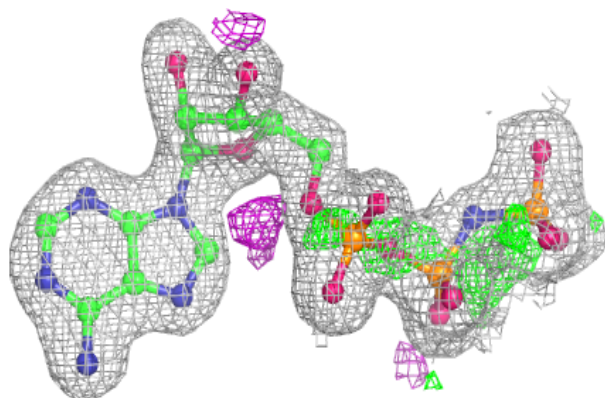


Electron density around ANP B 1511:

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

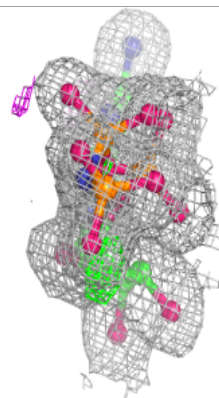
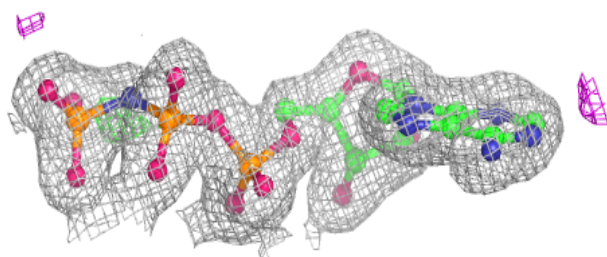
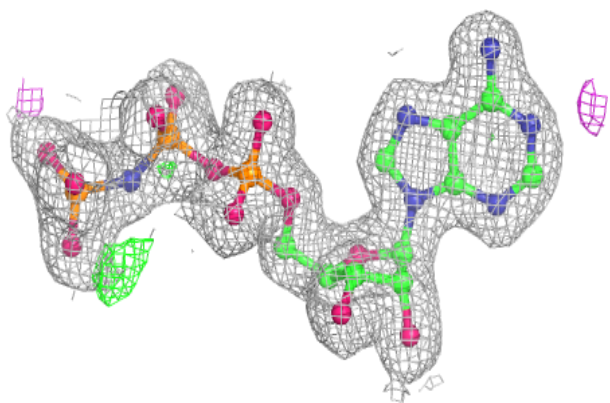
**Electron density around ANP F 1479:**

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

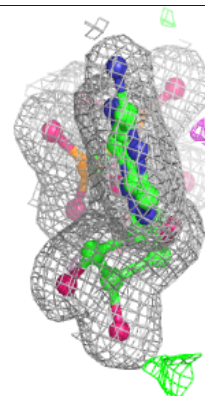
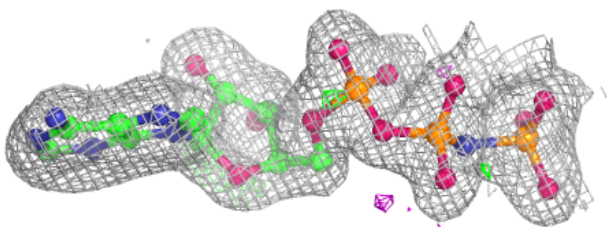
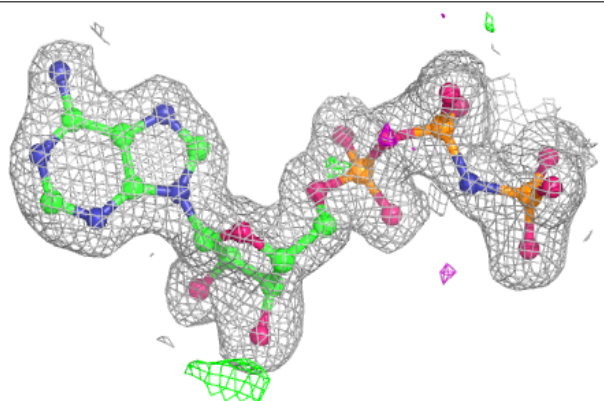


Electron density around ANP D 1480:

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

**Electron density around ANP C 1511:**

$2mF_o-DF_c$ (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.