



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 1OHH / pdb_00001ohh
Title : BOVINE MITOCHONDRIAL F1-ATPASE complexed with the inhibitor protein IF1
Authors : Cabezon, E.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2003-05-27
Resolution : 2.80 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

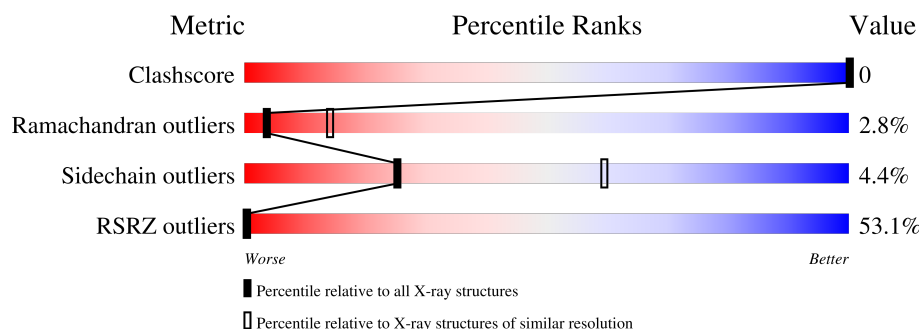
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1-A	510	51% 87% 9% 5%
1	1-B	510	45% 88% 5% 6%
1	1-C	510	42% 86% 9% .
1	2-A	510	88% 6% 6%
1	2-B	510	89% 6% 5%
1	2-C	510	84% 11% 6%
2	1-D	482	61% 93% 5% .

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Mol	Chain	Length	Quality of chain
2	1-E	482	67% 92% 5% .
2	1-F	482	39% 91% 6% .
2	2-D	482	91% 5% .
2	2-E	482	92% 5% ..
2	2-F	482	91% 6% .
3	1-G	272	19% 33% . 65%
3	2-G	272	33% . 65%
4	1-H	84	29% 35% 10% 56%
4	2-H	84	46% 6% 48%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45703 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	2-A	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	1-B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	2-B	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	1-C	488	Total	C	N	O	S	0	0	0
			3718	2341	656	709	12			
1	2-C	480	Total	C	N	O	S	0	0	0
			3661	2304	648	697	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

- Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-D	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			
2	2-D	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	1-E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	2-E	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	1-F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2-F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

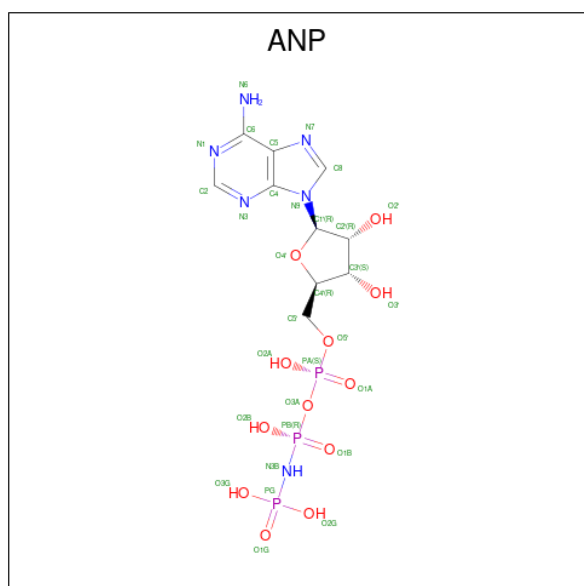
- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1-G	94	Total	C	N	O	S	0	0	0
			709	437	130	136	6			
3	2-G	94	Total	C	N	O	S	0	0	0
			717	444	129	138	6			

- Molecule 4 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	1-H	37	Total	C	N	O	0	0	0
			283	167	59	57			
4	2-H	44	Total	C	N	O	0	0	0
			336	202	69	65			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	1-A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	2-A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

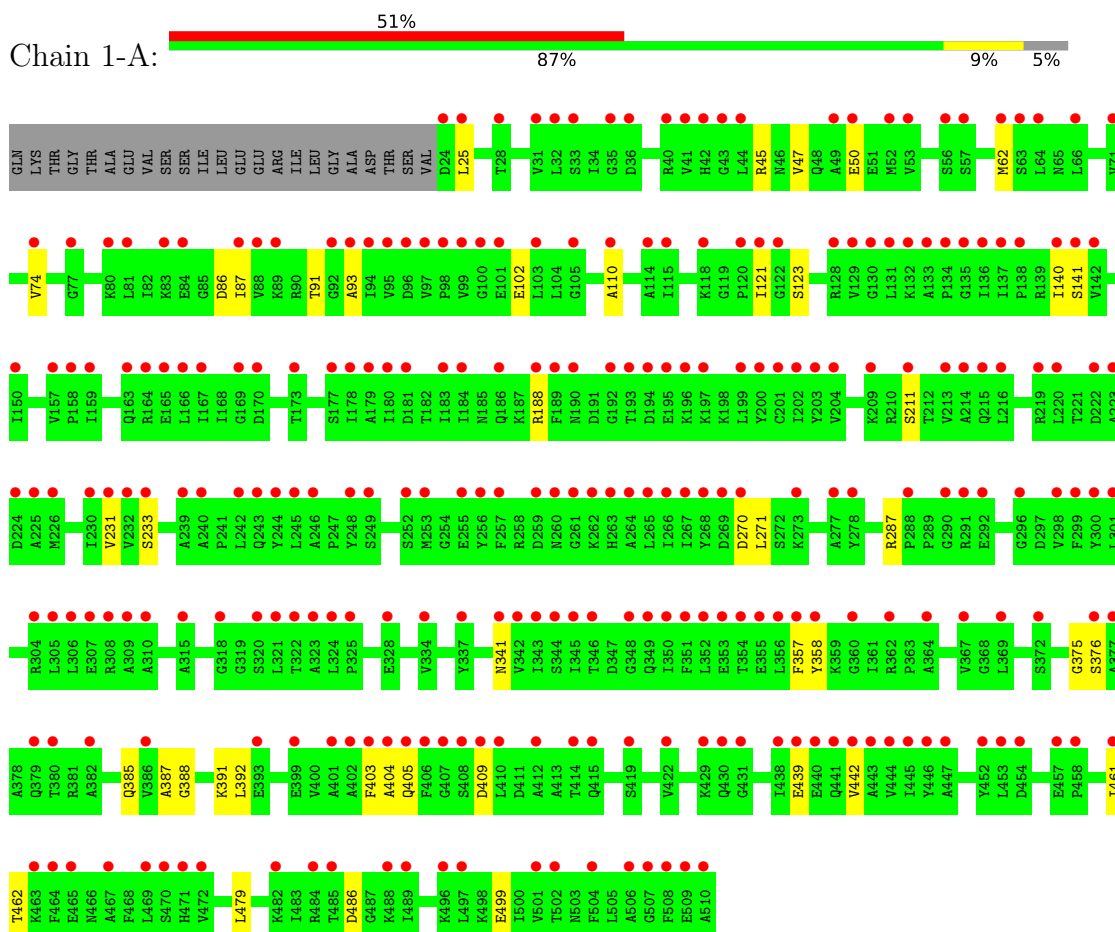
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-A	1	Total	Mg	0	0
			1	1		
6	2-A	1	Total	Mg	0	0
			1	1		
6	1-B	1	Total	Mg	0	0
			1	1		
6	2-B	1	Total	Mg	0	0
			1	1		
6	1-C	1	Total	Mg	0	0
			1	1		
6	2-C	1	Total	Mg	0	0
			1	1		
6	1-D	1	Total	Mg	0	0
			1	1		
6	2-D	1	Total	Mg	0	0
			1	1		
6	1-F	1	Total	Mg	0	0
			1	1		
6	2-F	1	Total	Mg	0	0
			1	1		

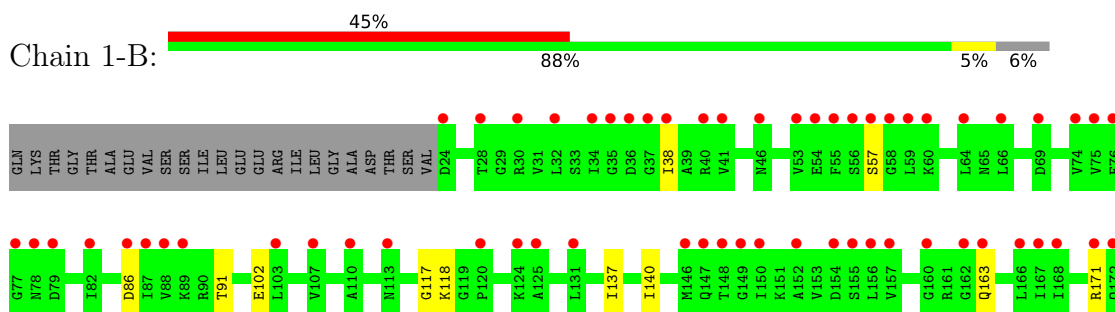
3 Residue-property plots [i](#)

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, mitochondrial

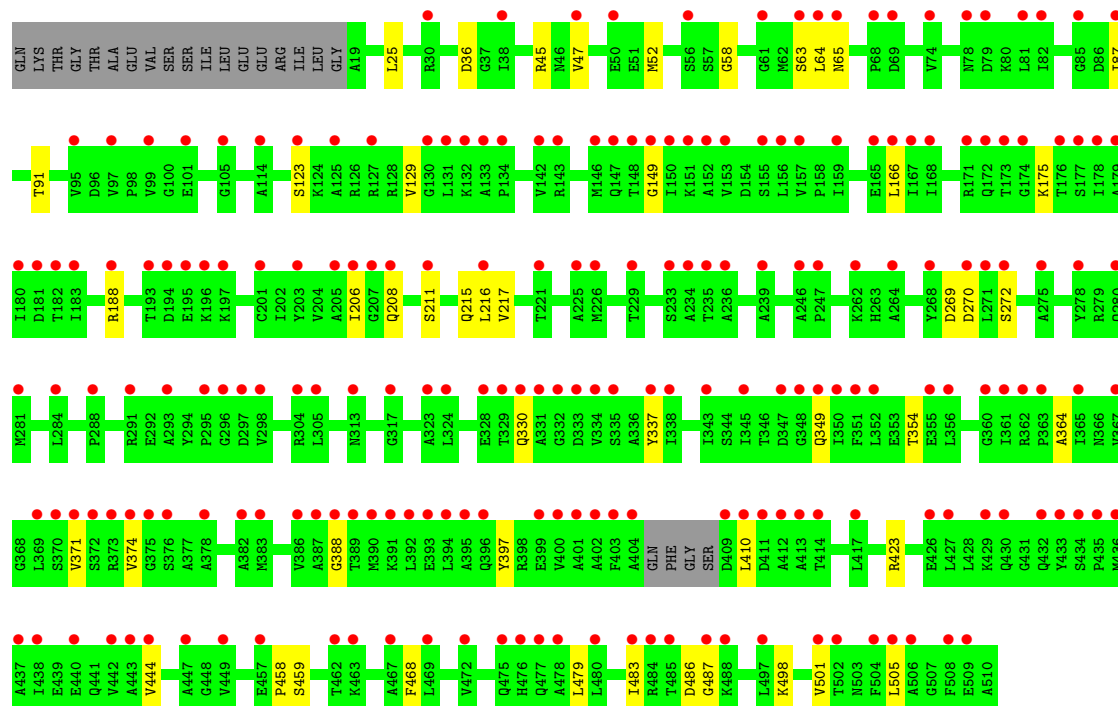
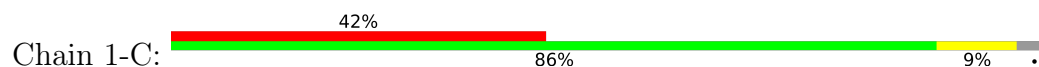


- Molecule 1: ATP synthase subunit alpha, mitochondrial



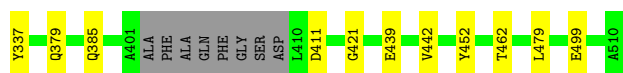


- Molecule 1: ATP synthase subunit alpha, mitochondrial



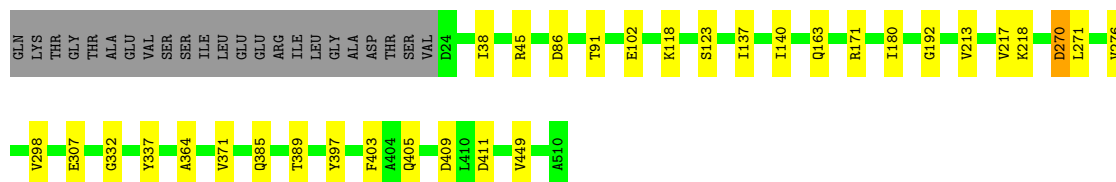
- Molecule 1: ATP synthase subunit alpha, mitochondrial





- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain 2-B: 89% 6% 5%



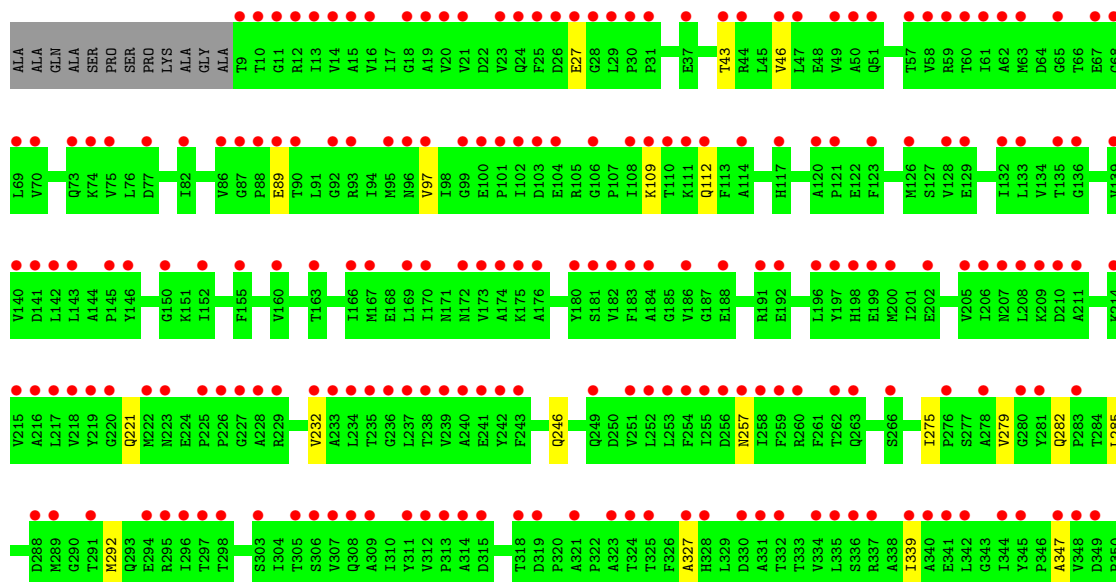
- Molecule 1: ATP synthase subunit alpha, mitochondrial

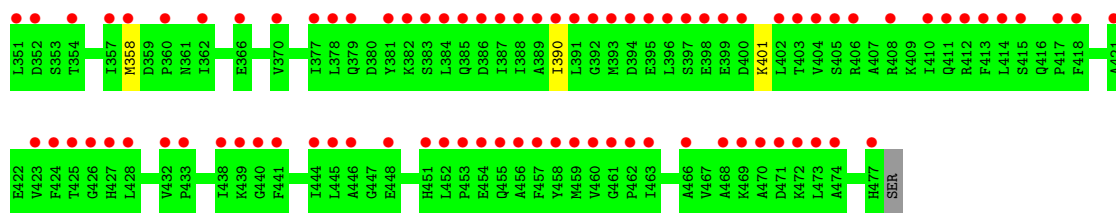
Chain 2-C: 84% 11% 6%



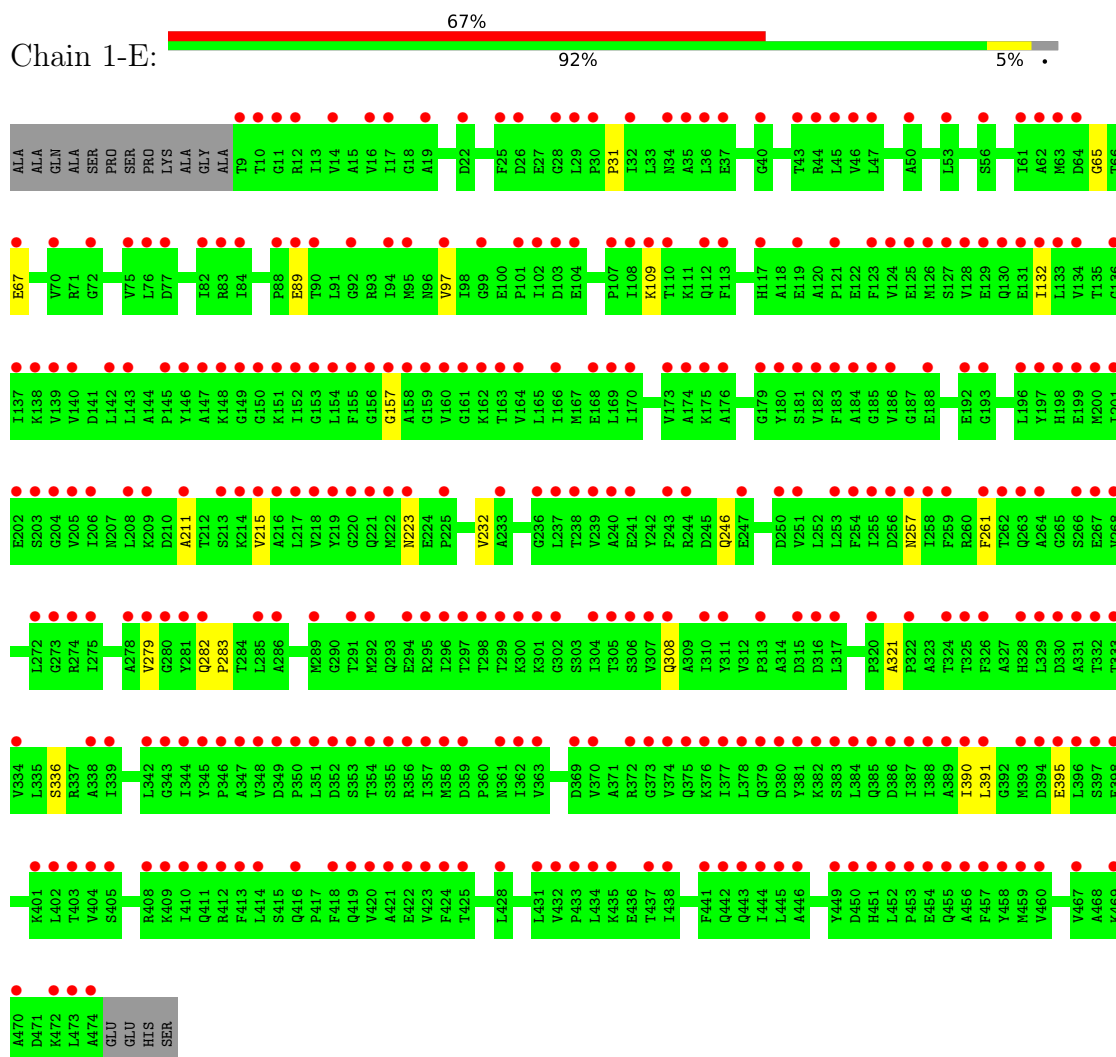
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain 1-D: 61% 93% 5%

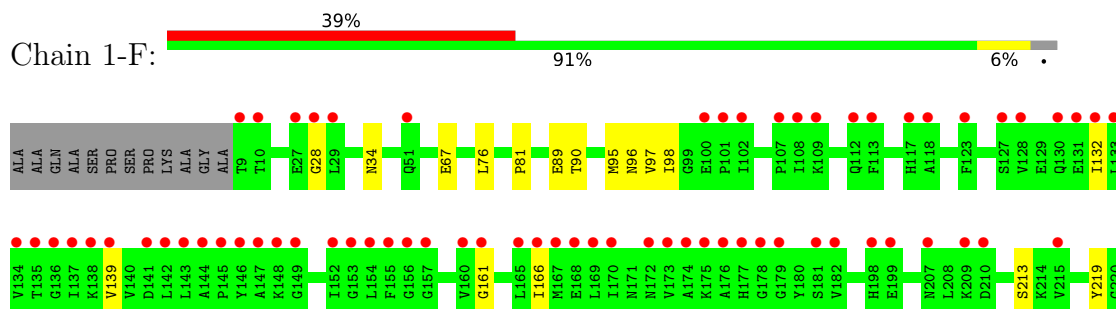


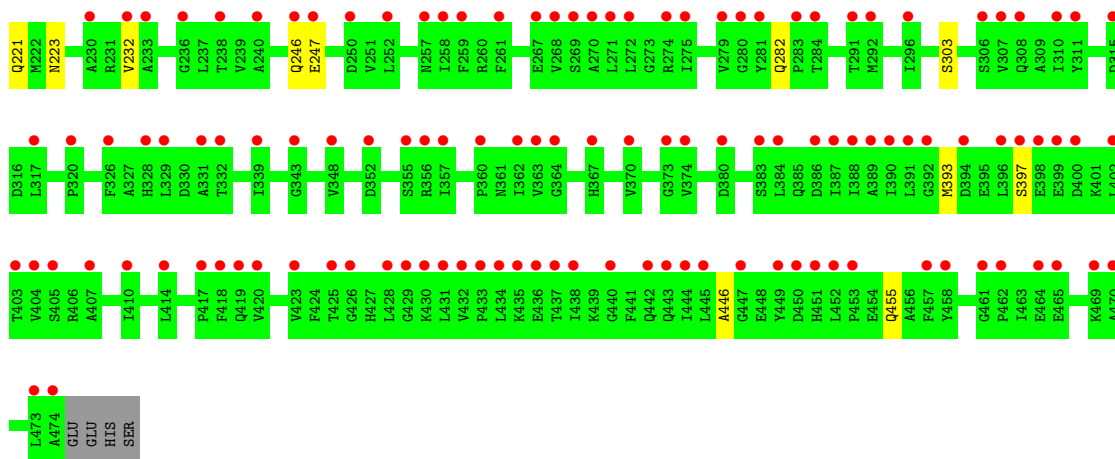


• Molecule 2: ATP synthase subunit beta, mitochondrial



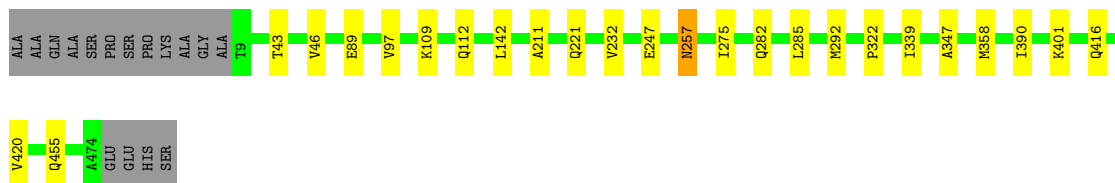
• Molecule 2: ATP synthase subunit beta, mitochondrial





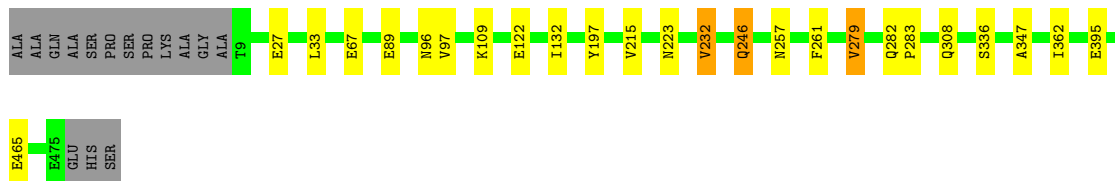
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain 2-D: 91% 5% .



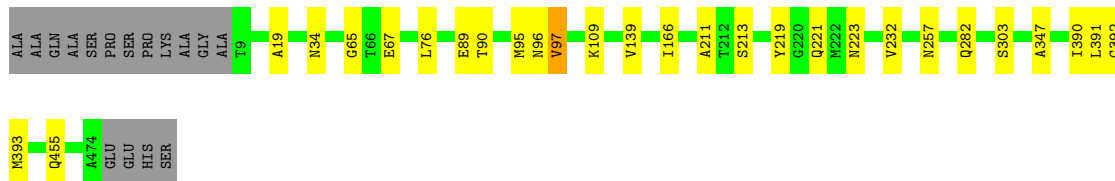
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain 2-E: 92% 5% . .



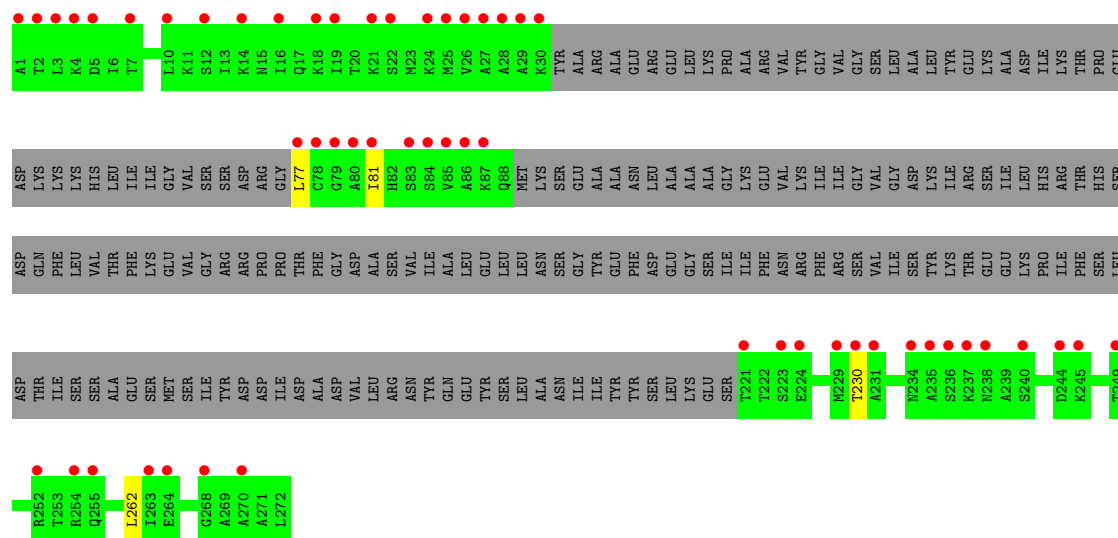
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain 2-F: 91% 6% .



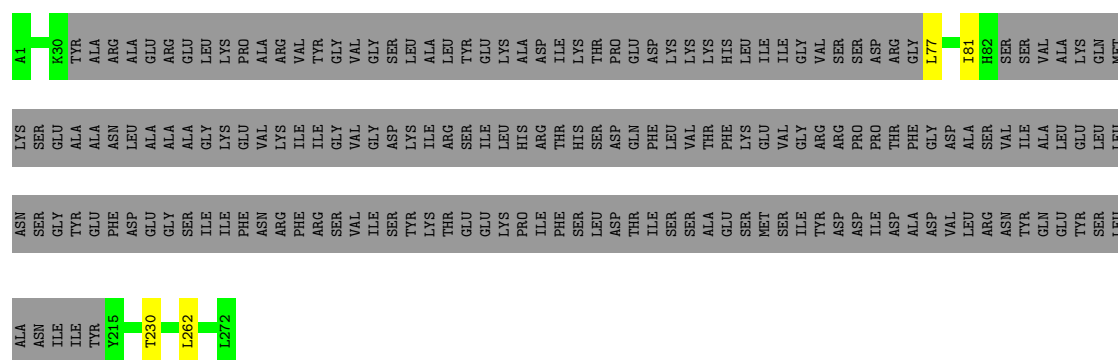
- Molecule 3: ATP synthase subunit gamma, mitochondrial

Chain 1-G: 19% 33% 65%



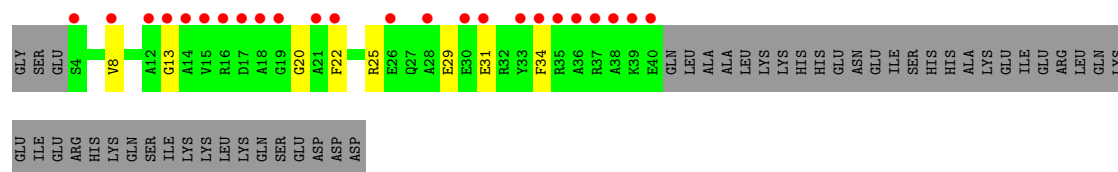
• Molecule 3: ATP synthase subunit gamma, mitochondrial

Chain 2-G: 33% 65%



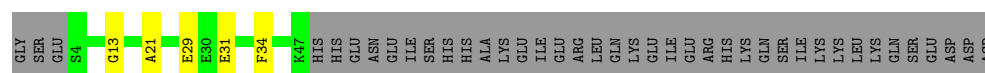
• Molecule 4: ATPase inhibitor, mitochondrial

Chain 1-H: 29% 35% 10% 56%



• Molecule 4: ATPase inhibitor, mitochondrial

Chain 2-H: 46% 6% 48%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	272.30Å 107.20Å 152.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.50 – 2.80 39.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.50-2.80) 99.0 (39.50-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.280 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	45703	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

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	1-A	0.30	0/3766	0.71	4/5080 (0.1%)
1	1-B	0.32	0/3704	0.71	3/4995 (0.1%)
1	1-C	0.34	0/3767	0.73	5/5082 (0.1%)
1	2-A	0.30	0/3704	0.70	3/4995 (0.1%)
1	2-B	0.32	0/3766	0.71	4/5080 (0.1%)
1	2-C	0.32	0/3709	0.73	5/5002 (0.1%)
2	1-D	0.32	0/3616	0.71	3/4906 (0.1%)
2	1-E	0.28	0/3587	0.69	2/4867 (0.0%)
2	1-F	0.33	0/3587	0.72	2/4867 (0.0%)
2	2-D	0.32	0/3587	0.71	3/4867 (0.1%)
2	2-E	0.28	0/3596	0.69	2/4879 (0.0%)
2	2-F	0.33	0/3587	0.72	2/4867 (0.0%)
3	1-G	0.36	0/708	0.70	0/941
3	2-G	0.36	0/717	0.68	0/953
4	1-H	0.40	0/285	0.83	1/376 (0.3%)
4	2-H	0.39	0/338	0.82	1/446 (0.2%)
All	All	0.32	0/46024	0.71	40/62203 (0.1%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-E	261	PHE	N-CA-C	-7.68	101.34	111.24
2	2-E	261	PHE	N-CA-C	-7.68	101.34	111.24
1	1-C	374	VAL	N-CA-C	-7.64	106.04	113.53
1	2-C	374	VAL	N-CA-C	-7.64	106.04	113.53
1	1-A	271	LEU	N-CA-C	-7.46	104.18	113.28
1	2-A	271	LEU	N-CA-C	-7.46	104.18	113.28
1	1-C	149	GLY	N-CA-C	-6.49	106.12	115.27
1	2-C	149	GLY	N-CA-C	-6.49	106.12	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-B	271	LEU	N-CA-C	-6.48	105.37	113.28
1	2-B	271	LEU	N-CA-C	-6.48	105.37	113.28
1	1-B	91	THR	N-CA-C	-6.43	106.02	114.31
1	2-B	91	THR	N-CA-C	-6.43	106.02	114.31
4	1-H	31	GLU	N-CA-C	-5.92	104.95	111.82
4	2-H	31	GLU	N-CA-C	-5.92	104.95	111.82
1	1-B	213	VAL	N-CA-C	-5.84	104.83	110.72
1	2-B	213	VAL	N-CA-C	-5.84	104.83	110.72
2	1-D	275	ILE	N-CA-C	-5.78	102.60	108.96
2	2-D	275	ILE	N-CA-C	-5.78	102.60	108.96
1	1-A	91	THR	N-CA-C	-5.73	106.63	113.97
1	2-A	91	THR	N-CA-C	-5.73	106.63	113.97
1	1-A	405	GLN	N-CA-C	5.44	117.97	111.71
1	1-C	215	GLN	N-CA-C	-5.38	105.52	111.71
1	2-C	215	GLN	N-CA-C	-5.38	105.52	111.71
2	1-D	221	GLN	N-CA-C	5.36	118.15	109.79
2	2-D	221	GLN	N-CA-C	5.36	118.15	109.79
2	1-F	219	TYR	N-CA-C	5.35	118.17	109.24
2	2-F	219	TYR	N-CA-C	5.35	118.17	109.24
1	1-C	58	GLY	N-CA-C	-5.32	107.77	115.27
1	2-C	58	GLY	N-CA-C	-5.32	107.77	115.27
1	1-A	233	SER	N-CA-C	5.17	118.50	107.70
1	2-A	233	SER	N-CA-C	5.17	118.50	107.70
2	1-E	283	PRO	N-CA-C	-5.09	106.46	113.53
2	2-E	283	PRO	N-CA-C	-5.09	106.46	113.53
2	1-D	46	VAL	N-CA-C	5.07	115.88	108.58
2	2-D	46	VAL	N-CA-C	5.07	115.88	108.58
2	1-F	90	THR	N-CA-C	-5.04	105.49	111.69
2	2-F	90	THR	N-CA-C	-5.04	105.49	111.69
1	2-B	405	GLN	N-CA-C	5.01	117.48	111.71
1	1-C	498	LYS	N-CA-C	-5.00	106.02	111.82
1	2-C	498	LYS	N-CA-C	-5.00	106.02	111.82

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	1-A	3715	0	3814	0	0
1	1-B	3656	0	3766	0	0
1	1-C	3718	0	3818	0	0
1	2-A	3656	0	3765	0	0
1	2-B	3715	0	3814	0	0
1	2-C	3661	0	3766	0	0
2	1-D	3558	0	3605	0	0
2	1-E	3530	0	3587	0	0
2	1-F	3530	0	3586	0	0
2	2-D	3530	0	3586	0	0
2	2-E	3539	0	3592	0	0
2	2-F	3530	0	3587	0	0
3	1-G	709	0	771	0	0
3	2-G	717	0	775	0	0
4	1-H	283	0	265	0	0
4	2-H	336	0	331	0	0
5	1-A	31	0	13	0	0
5	1-B	31	0	13	0	0
5	1-C	31	0	13	0	0
5	1-D	31	0	13	0	0
5	1-F	31	0	13	0	0
5	2-A	31	0	13	0	0
5	2-B	31	0	13	0	0
5	2-C	31	0	13	0	0
5	2-D	31	0	13	0	0
5	2-F	31	0	13	0	0
6	1-A	1	0	0	0	0
6	1-B	1	0	0	0	0
6	1-C	1	0	0	0	0
6	1-D	1	0	0	0	0
6	1-F	1	0	0	0	0
6	2-A	1	0	0	0	0
6	2-B	1	0	0	0	0
6	2-C	1	0	0	0	0
6	2-D	1	0	0	0	0
6	2-F	1	0	0	0	0
All	All	45703	0	46558	0	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 0.

There are no clashes within the asymmetric unit.

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	1-A	485/510 (95%)	398 (82%)	63 (13%)	24 (5%)	1	6
1	1-B	475/510 (93%)	408 (86%)	56 (12%)	11 (2%)	5	18
1	1-C	484/510 (95%)	411 (85%)	58 (12%)	15 (3%)	3	12
1	2-A	475/510 (93%)	416 (88%)	48 (10%)	11 (2%)	5	18
1	2-B	485/510 (95%)	413 (85%)	59 (12%)	13 (3%)	4	15
1	2-C	476/510 (93%)	390 (82%)	64 (13%)	22 (5%)	2	6
2	1-D	467/482 (97%)	411 (88%)	50 (11%)	6 (1%)	9	31
2	1-E	464/482 (96%)	396 (85%)	59 (13%)	9 (2%)	6	22
2	1-F	464/482 (96%)	400 (86%)	54 (12%)	10 (2%)	5	19
2	2-D	464/482 (96%)	408 (88%)	46 (10%)	10 (2%)	5	19
2	2-E	465/482 (96%)	400 (86%)	52 (11%)	13 (3%)	4	14
2	2-F	464/482 (96%)	400 (86%)	53 (11%)	11 (2%)	4	17
3	1-G	88/272 (32%)	78 (89%)	9 (10%)	1 (1%)	11	36
3	2-G	88/272 (32%)	76 (86%)	11 (12%)	1 (1%)	11	36
4	1-H	35/84 (42%)	20 (57%)	10 (29%)	5 (14%)	0	0
4	2-H	42/84 (50%)	30 (71%)	10 (24%)	2 (5%)	2	6
All	All	5921/6664 (89%)	5055 (85%)	702 (12%)	164 (3%)	4	14

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	123	SER
1	1-A	141	SER
1	1-A	270	ASP
1	1-A	387	ALA
1	1-A	404	ALA
1	1-A	409	ASP

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Mol	Chain	Res	Type
1	1-C	25	LEU
1	1-C	123	SER
1	1-C	337	TYR
1	1-C	483	ILE
2	1-D	27	GLU
2	1-D	109	LYS
2	1-E	65	GLY
2	1-E	109	LYS
1	2-A	270	ASP
1	2-B	332	GLY
1	2-B	337	TYR
1	2-C	337	TYR
1	2-C	364	ALA
2	2-D	347	ALA
2	2-E	109	LYS
2	2-E	246	GLN
2	2-F	391	LEU
4	2-H	13	GLY
1	1-A	341	ASN
1	1-A	357	PHE
1	1-B	57	SER
1	1-B	118	LYS
1	1-B	270	ASP
1	1-B	337	TYR
1	1-B	459	SER
1	1-C	45	ARG
1	1-C	270	ASP
1	1-C	364	ALA
1	1-C	388	GLY
2	1-D	246	GLN
2	1-E	157	GLY
2	1-E	211	ALA
2	1-F	28	GLY
2	1-F	455	GLN
4	1-H	13	GLY
1	2-A	57	SER
1	2-A	337	TYR
1	2-A	379	GLN
1	2-A	452	TYR
1	2-B	45	ARG
1	2-B	192	GLY
1	2-B	270	ASP

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Mol	Chain	Res	Type
1	2-B	409	ASP
1	2-C	20	ASP
1	2-C	236	ALA
1	2-C	361	ILE
1	2-C	373	ARG
1	2-C	388	GLY
1	2-C	431	GLY
2	2-D	211	ALA
2	2-D	247	GLU
2	2-D	420	VAL
2	2-E	27	GLU
2	2-F	19	ALA
2	2-F	109	LYS
2	2-F	211	ALA
2	2-F	347	ALA
2	2-F	390	ILE
3	2-G	81	ILE
1	1-A	50	GLU
1	1-A	110	ALA
1	1-A	188	ARG
1	1-A	358	TYR
1	1-A	388	GLY
1	1-A	391	LYS
1	1-A	392	LEU
1	1-B	384	LYS
1	1-C	175	LYS
1	1-C	269	ASP
1	1-C	459	SER
1	1-C	487	GLY
2	1-F	246	GLN
2	1-F	247	GLU
4	1-H	22	PHE
1	2-A	154	ASP
1	2-A	175	LYS
1	2-A	195	GLU
1	2-A	385	GLN
1	2-B	123	SER
1	2-B	397	TYR
1	2-B	411	ASP
1	2-C	45	ARG
1	2-C	141	SER
1	2-C	246	ALA

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Mol	Chain	Res	Type
1	2-C	288	PRO
1	2-C	377	ALA
2	2-D	257	ASN
2	2-D	455	GLN
2	2-E	33	LEU
2	2-E	96	ASN
2	2-E	122	GLU
2	2-E	347	ALA
2	2-F	257	ASN
2	2-F	392	GLY
2	2-F	455	GLN
4	2-H	21	ALA
1	1-A	25	LEU
1	1-A	376	SER
1	1-A	385	GLN
2	1-D	327	ALA
2	1-E	391	LEU
2	1-F	397	SER
2	1-F	446	ALA
4	1-H	25	ARG
1	2-B	118	LYS
1	2-B	364	ALA
1	2-C	79	ASP
1	2-C	270	ASP
1	2-C	295	PRO
1	2-C	458	PRO
1	2-C	491	GLU
2	2-D	142	LEU
1	1-A	287	ARG
1	1-A	375	GLY
1	1-A	486	ASP
1	1-B	236	ALA
1	1-C	188	ARG
1	1-C	468	PHE
2	1-D	347	ALA
2	1-E	257	ASN
2	1-E	390	ILE
2	1-F	81	PRO
1	2-A	411	ASP
1	2-C	95	VAL
2	2-D	109	LYS
2	2-E	197	TYR

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Mol	Chain	Res	Type
2	2-E	257	ASN
2	2-E	465	GLU
1	1-A	86	ASP
1	1-A	93	ALA
2	1-F	132	ILE
2	1-F	161	GLY
4	1-H	20	GLY
1	2-B	385	GLN
2	2-D	416	GLN
1	1-B	178	ILE
2	2-F	97	VAL
1	1-B	246	ALA
1	1-C	458	PRO
4	1-H	8	VAL
1	2-A	421	GLY
1	2-C	438	ILE
1	2-C	461	ILE
2	2-D	322	PRO
1	1-B	117	GLY
2	1-D	279	VAL
2	1-F	98	ILE
1	2-C	180	ILE
2	2-E	279	VAL
2	2-F	65	GLY
1	1-A	461	ILE
1	1-B	458	PRO
2	1-E	31	PRO
2	1-E	321	ALA
3	1-G	81	ILE
1	2-B	449	VAL
2	2-E	232	VAL
2	2-E	362	ILE

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	1-A	393/412 (95%)	377 (96%)	16 (4%)	27	62
1	1-B	388/412 (94%)	372 (96%)	16 (4%)	27	62
1	1-C	394/412 (96%)	366 (93%)	28 (7%)	13	39
1	2-A	388/412 (94%)	373 (96%)	15 (4%)	28	64
1	2-B	393/412 (95%)	376 (96%)	17 (4%)	26	60
1	2-C	389/412 (94%)	362 (93%)	27 (7%)	14	41
2	1-D	379/386 (98%)	366 (97%)	13 (3%)	32	68
2	1-E	376/386 (97%)	363 (96%)	13 (4%)	32	67
2	1-F	376/386 (97%)	360 (96%)	16 (4%)	26	60
2	2-D	376/386 (97%)	363 (96%)	13 (4%)	32	67
2	2-E	377/386 (98%)	364 (97%)	13 (3%)	32	68
2	2-F	376/386 (97%)	360 (96%)	16 (4%)	26	60
3	1-G	78/230 (34%)	75 (96%)	3 (4%)	29	64
3	2-G	79/230 (34%)	76 (96%)	3 (4%)	29	64
4	1-H	25/68 (37%)	23 (92%)	2 (8%)	11	34
4	2-H	30/68 (44%)	28 (93%)	2 (7%)	15	42
All	All	4817/5384 (90%)	4604 (96%)	213 (4%)	25	59

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	45	ARG
1	1-A	47	VAL
1	1-A	62	MET
1	1-A	74	VAL
1	1-A	87	ILE
1	1-A	102	GLU
1	1-A	121	ILE
1	1-A	140	ILE
1	1-A	211	SER
1	1-A	231	VAL
1	1-A	403	PHE
1	1-A	439	GLU
1	1-A	442	VAL
1	1-A	462	THR
1	1-A	479	LEU
1	1-A	499	GLU

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Mol	Chain	Res	Type
1	1-B	38	ILE
1	1-B	86	ASP
1	1-B	102	GLU
1	1-B	137	ILE
1	1-B	140	ILE
1	1-B	163	GLN
1	1-B	171	ARG
1	1-B	180	ILE
1	1-B	217	VAL
1	1-B	218	LYS
1	1-B	270	ASP
1	1-B	276	VAL
1	1-B	298	VAL
1	1-B	307	GLU
1	1-B	371	VAL
1	1-B	389	THR
1	1-C	36	ASP
1	1-C	47	VAL
1	1-C	52	MET
1	1-C	63	SER
1	1-C	64	LEU
1	1-C	65	ASN
1	1-C	87	ILE
1	1-C	91	THR
1	1-C	129	VAL
1	1-C	166	LEU
1	1-C	206	ILE
1	1-C	208	GLN
1	1-C	211	SER
1	1-C	216	LEU
1	1-C	217	VAL
1	1-C	272	SER
1	1-C	330	GLN
1	1-C	349	GLN
1	1-C	354	THR
1	1-C	371	VAL
1	1-C	397	TYR
1	1-C	410	LEU
1	1-C	423	ARG
1	1-C	444	VAL
1	1-C	479	LEU
1	1-C	486	ASP

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Mol	Chain	Res	Type
1	1-C	501	VAL
1	1-C	505	LEU
2	1-D	43	THR
2	1-D	89	GLU
2	1-D	97	VAL
2	1-D	112	GLN
2	1-D	232	VAL
2	1-D	257	ASN
2	1-D	282	GLN
2	1-D	285	LEU
2	1-D	292	MET
2	1-D	339	ILE
2	1-D	358	MET
2	1-D	390	ILE
2	1-D	401	LYS
2	1-E	67	GLU
2	1-E	89	GLU
2	1-E	97	VAL
2	1-E	132	ILE
2	1-E	215	VAL
2	1-E	223	ASN
2	1-E	232	VAL
2	1-E	246	GLN
2	1-E	279	VAL
2	1-E	282	GLN
2	1-E	308	GLN
2	1-E	336	SER
2	1-E	395	GLU
2	1-F	34	ASN
2	1-F	67	GLU
2	1-F	76	LEU
2	1-F	89	GLU
2	1-F	95	MET
2	1-F	96	ASN
2	1-F	97	VAL
2	1-F	139	VAL
2	1-F	166	ILE
2	1-F	213	SER
2	1-F	221	GLN
2	1-F	223	ASN
2	1-F	232	VAL
2	1-F	282	GLN

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Mol	Chain	Res	Type
2	1-F	303	SER
2	1-F	393	MET
3	1-G	77	LEU
3	1-G	230	THR
3	1-G	262	LEU
4	1-H	29	GLU
4	1-H	34	PHE
1	2-A	45	ARG
1	2-A	47	VAL
1	2-A	62	MET
1	2-A	74	VAL
1	2-A	87	ILE
1	2-A	102	GLU
1	2-A	121	ILE
1	2-A	140	ILE
1	2-A	211	SER
1	2-A	231	VAL
1	2-A	439	GLU
1	2-A	442	VAL
1	2-A	462	THR
1	2-A	479	LEU
1	2-A	499	GLU
1	2-B	38	ILE
1	2-B	86	ASP
1	2-B	102	GLU
1	2-B	137	ILE
1	2-B	140	ILE
1	2-B	163	GLN
1	2-B	171	ARG
1	2-B	180	ILE
1	2-B	217	VAL
1	2-B	218	LYS
1	2-B	270	ASP
1	2-B	276	VAL
1	2-B	298	VAL
1	2-B	307	GLU
1	2-B	371	VAL
1	2-B	389	THR
1	2-B	403	PHE
1	2-C	36	ASP
1	2-C	47	VAL
1	2-C	52	MET

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Mol	Chain	Res	Type
1	2-C	63	SER
1	2-C	64	LEU
1	2-C	65	ASN
1	2-C	87	ILE
1	2-C	91	THR
1	2-C	129	VAL
1	2-C	166	LEU
1	2-C	206	ILE
1	2-C	208	GLN
1	2-C	211	SER
1	2-C	216	LEU
1	2-C	217	VAL
1	2-C	272	SER
1	2-C	330	GLN
1	2-C	349	GLN
1	2-C	354	THR
1	2-C	371	VAL
1	2-C	397	TYR
1	2-C	423	ARG
1	2-C	444	VAL
1	2-C	479	LEU
1	2-C	486	ASP
1	2-C	501	VAL
1	2-C	505	LEU
2	2-D	43	THR
2	2-D	89	GLU
2	2-D	97	VAL
2	2-D	112	GLN
2	2-D	232	VAL
2	2-D	257	ASN
2	2-D	282	GLN
2	2-D	285	LEU
2	2-D	292	MET
2	2-D	339	ILE
2	2-D	358	MET
2	2-D	390	ILE
2	2-D	401	LYS
2	2-E	67	GLU
2	2-E	89	GLU
2	2-E	97	VAL
2	2-E	132	ILE
2	2-E	215	VAL

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Mol	Chain	Res	Type
2	2-E	223	ASN
2	2-E	232	VAL
2	2-E	246	GLN
2	2-E	279	VAL
2	2-E	282	GLN
2	2-E	308	GLN
2	2-E	336	SER
2	2-E	395	GLU
2	2-F	34	ASN
2	2-F	67	GLU
2	2-F	76	LEU
2	2-F	89	GLU
2	2-F	95	MET
2	2-F	96	ASN
2	2-F	97	VAL
2	2-F	139	VAL
2	2-F	166	ILE
2	2-F	213	SER
2	2-F	221	GLN
2	2-F	223	ASN
2	2-F	232	VAL
2	2-F	282	GLN
2	2-F	303	SER
2	2-F	393	MET
3	2-G	77	LEU
3	2-G	230	THR
3	2-G	262	LEU
4	2-H	29	GLU
4	2-H	34	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	190	ASN
1	1-A	208	GLN
1	1-A	263	HIS
1	1-A	274	GLN
1	1-A	349	GLN
1	1-A	385	GLN
1	1-A	396	GLN
1	1-A	405	GLN
1	1-A	415	GLN

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Mol	Chain	Res	Type
1	1-B	42	HIS
1	1-B	46	ASN
1	1-B	65	ASN
1	1-B	215	GLN
1	1-B	341	ASN
1	1-B	396	GLN
1	1-B	475	GLN
1	1-B	503	ASN
1	1-C	48	GLN
1	1-C	65	ASN
1	1-C	208	GLN
1	1-C	215	GLN
1	1-C	263	HIS
1	1-C	330	GLN
1	1-C	349	GLN
1	1-C	432	GLN
1	1-C	441	GLN
1	1-C	471	HIS
1	1-C	476	HIS
2	1-D	39	GLN
2	1-D	177	HIS
2	1-D	194	ASN
2	1-D	249	GLN
2	1-D	282	GLN
2	1-E	194	ASN
2	1-E	223	ASN
2	1-E	246	GLN
2	1-E	257	ASN
2	1-E	263	GLN
2	1-E	282	GLN
2	1-E	293	GLN
2	1-E	328	HIS
2	1-E	367	HIS
2	1-E	411	GLN
2	1-E	442	GLN
2	1-E	455	GLN
2	1-F	96	ASN
2	1-F	221	GLN
2	1-F	223	ASN
2	1-F	249	GLN
2	1-F	282	GLN
2	1-F	308	GLN

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Mol	Chain	Res	Type
2	1-F	328	HIS
2	1-F	385	GLN
2	1-F	443	GLN
3	1-G	82	HIS
3	1-G	225	GLN
3	1-G	251	ASN
4	1-H	7	ASN
4	1-H	27	GLN
1	2-A	42	HIS
1	2-A	48	GLN
1	2-A	65	ASN
1	2-A	208	GLN
1	2-A	379	GLN
1	2-A	466	ASN
1	2-A	475	GLN
1	2-A	503	ASN
1	2-B	113	ASN
1	2-B	172	GLN
1	2-B	263	HIS
1	2-B	405	GLN
1	2-B	415	GLN
1	2-B	416	GLN
1	2-B	471	HIS
1	2-B	475	GLN
1	2-B	476	HIS
1	2-B	503	ASN
1	2-C	78	ASN
1	2-C	186	GLN
1	2-C	208	GLN
1	2-C	263	HIS
1	2-C	349	GLN
1	2-C	396	GLN
1	2-C	415	GLN
1	2-C	430	GLN
1	2-C	476	HIS
2	2-D	51	GLN
2	2-D	96	ASN
2	2-D	112	GLN
2	2-D	117	HIS
2	2-D	171	ASN
2	2-D	194	ASN
2	2-D	221	GLN

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Mol	Chain	Res	Type
2	2-D	223	ASN
2	2-D	249	GLN
2	2-D	282	GLN
2	2-D	308	GLN
2	2-D	385	GLN
2	2-D	411	GLN
2	2-D	419	GLN
2	2-D	427	HIS
2	2-E	24	GLN
2	2-E	39	GLN
2	2-E	177	HIS
2	2-E	194	ASN
2	2-E	198	HIS
2	2-E	221	GLN
2	2-E	223	ASN
2	2-E	249	GLN
2	2-E	282	GLN
2	2-E	367	HIS
2	2-E	379	GLN
2	2-E	442	GLN
2	2-F	24	GLN
2	2-F	96	ASN
2	2-F	194	ASN
2	2-F	221	GLN
2	2-F	223	ASN
2	2-F	246	GLN
2	2-F	257	ASN
2	2-F	282	GLN
2	2-F	308	GLN
2	2-F	367	HIS
2	2-F	375	GLN
2	2-F	411	GLN
2	2-F	455	GLN
3	2-G	234	ASN
3	2-G	255	GLN
4	2-H	41	GLN

5.3.3 RNA ⓘ

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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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
5	ANP	1-A	1511	6	33,33,33	1.43	5 (15%)	45,52,52	1.18	4 (8%)
5	ANP	2-A	1511	6	33,33,33	1.59	6 (18%)	45,52,52	1.38	4 (8%)
5	ANP	1-F	1478	6	33,33,33	1.55	7 (21%)	45,52,52	1.51	5 (11%)
5	ANP	2-B	1511	6	33,33,33	1.35	4 (12%)	45,52,52	1.07	3 (6%)
5	ANP	2-F	1478	6	33,33,33	1.70	8 (24%)	45,52,52	1.46	5 (11%)
5	ANP	2-D	1478	6	33,33,33	1.53	6 (18%)	45,52,52	1.64	7 (15%)
5	ANP	1-B	1511	6	33,33,33	1.49	6 (18%)	45,52,52	1.35	4 (8%)
5	ANP	1-C	1511	6	33,33,33	1.34	5 (15%)	45,52,52	1.18	2 (4%)
5	ANP	2-C	1511	6	33,33,33	1.56	6 (18%)	45,52,52	1.37	3 (6%)
5	ANP	1-D	1478	6	33,33,33	1.82	9 (27%)	45,52,52	1.55	8 (17%)

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
5	ANP	1-A	1511	6	-	7/18/38/38	0/3/3/3
5	ANP	2-A	1511	6	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	1-F	1478	6	-	9/18/38/38	0/3/3/3
5	ANP	2-B	1511	6	-	7/18/38/38	0/3/3/3
5	ANP	2-F	1478	6	-	9/18/38/38	0/3/3/3
5	ANP	2-D	1478	6	-	8/18/38/38	0/3/3/3
5	ANP	1-B	1511	6	-	7/18/38/38	0/3/3/3
5	ANP	1-C	1511	6	-	7/18/38/38	0/3/3/3
5	ANP	2-C	1511	6	-	7/18/38/38	0/3/3/3
5	ANP	1-D	1478	6	-	9/18/38/38	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-F	1478	ANP	PG-O2G	-5.42	1.42	1.56
5	1-D	1478	ANP	PG-O2G	-5.14	1.43	1.56
5	2-A	1511	ANP	PG-O2G	-4.56	1.44	1.56
5	2-C	1511	ANP	PG-O1G	4.43	1.52	1.46
5	1-C	1511	ANP	PG-O2G	-4.34	1.45	1.56
5	1-F	1478	ANP	PG-O2G	-4.24	1.45	1.56
5	2-B	1511	ANP	PG-O2G	-4.12	1.45	1.56
5	2-D	1478	ANP	PG-O2G	-3.89	1.46	1.56
5	2-A	1511	ANP	PB-O2B	-3.86	1.46	1.56
5	1-B	1511	ANP	PG-O2G	-3.83	1.46	1.56
5	1-A	1511	ANP	PB-O2B	-3.80	1.46	1.56
5	2-C	1511	ANP	PG-O2G	-3.68	1.47	1.56
5	1-A	1511	ANP	PG-O2G	-3.68	1.47	1.56
5	1-D	1478	ANP	PB-O3A	-3.40	1.54	1.59
5	1-D	1478	ANP	PG-O1G	3.35	1.51	1.46
5	1-F	1478	ANP	PG-O1G	3.24	1.51	1.46
5	1-D	1478	ANP	PA-O3A	-3.19	1.56	1.59
5	1-A	1511	ANP	PG-O1G	3.19	1.51	1.46
5	2-A	1511	ANP	PG-O1G	3.12	1.50	1.46
5	2-F	1478	ANP	PG-O1G	3.08	1.50	1.46
5	1-B	1511	ANP	C4-N3	3.04	1.40	1.34
5	1-D	1478	ANP	PG-N3B	-2.91	1.55	1.63
5	1-B	1511	ANP	PG-O1G	2.90	1.50	1.46
5	2-C	1511	ANP	PB-O2B	-2.90	1.49	1.56
5	2-D	1478	ANP	C2-N1	2.84	1.39	1.33
5	1-F	1478	ANP	PB-O2B	-2.75	1.49	1.56
5	2-F	1478	ANP	PG-O3G	-2.70	1.49	1.56
5	1-B	1511	ANP	PB-O2B	-2.67	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-D	1478	ANP	PG-O1G	2.59	1.50	1.46
5	2-F	1478	ANP	C2-N1	2.59	1.38	1.33
5	2-D	1478	ANP	PG-O3G	-2.56	1.50	1.56
5	1-C	1511	ANP	PB-O2B	-2.56	1.50	1.56
5	2-F	1478	ANP	PB-O2B	-2.56	1.50	1.56
5	2-B	1511	ANP	C4-N3	2.55	1.39	1.34
5	2-D	1478	ANP	C4-N3	2.52	1.39	1.34
5	2-C	1511	ANP	C2-N1	2.52	1.38	1.33
5	2-B	1511	ANP	C2-N1	2.47	1.38	1.33
5	2-F	1478	ANP	PG-N3B	-2.46	1.56	1.63
5	2-D	1478	ANP	PB-O2B	-2.45	1.50	1.56
5	2-A	1511	ANP	C4-N3	2.42	1.38	1.34
5	2-F	1478	ANP	C4-N3	2.33	1.38	1.34
5	2-C	1511	ANP	PG-O3G	-2.27	1.50	1.56
5	2-F	1478	ANP	PB-O3A	-2.26	1.56	1.59
5	1-B	1511	ANP	C2-N1	2.24	1.37	1.33
5	1-F	1478	ANP	C2-N1	2.20	1.37	1.33
5	1-F	1478	ANP	PG-N3B	-2.20	1.57	1.63
5	1-D	1478	ANP	C4-N3	2.18	1.38	1.34
5	2-C	1511	ANP	C4-N3	2.18	1.38	1.34
5	2-B	1511	ANP	PG-O3G	-2.14	1.51	1.56
5	2-A	1511	ANP	C5'-C4'	-2.13	1.45	1.51
5	1-C	1511	ANP	C4-N3	2.12	1.38	1.34
5	1-A	1511	ANP	C2-N1	2.10	1.37	1.33
5	1-F	1478	ANP	C4-N3	2.09	1.38	1.34
5	1-F	1478	ANP	C2'-C3'	-2.09	1.47	1.53
5	1-C	1511	ANP	PG-O3G	-2.09	1.51	1.56
5	1-D	1478	ANP	C3'-C4'	-2.08	1.47	1.53
5	2-A	1511	ANP	C2-N1	2.07	1.37	1.33
5	1-D	1478	ANP	PG-O3G	-2.07	1.51	1.56
5	1-A	1511	ANP	C5'-C4'	-2.03	1.45	1.51
5	1-C	1511	ANP	C2-N1	2.01	1.37	1.33
5	1-B	1511	ANP	PG-O3G	-2.01	1.51	1.56
5	1-D	1478	ANP	C8-N7	2.00	1.35	1.31

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2-D	1478	ANP	O1G-PG-N3B	-6.80	101.76	111.77
5	2-F	1478	ANP	O1G-PG-N3B	-6.45	102.27	111.77
5	1-F	1478	ANP	O1G-PG-N3B	-5.65	103.45	111.77
5	2-C	1511	ANP	O1G-PG-N3B	-5.49	103.68	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2-A	1511	ANP	O1G-PG-N3B	-5.34	103.91	111.77
5	1-B	1511	ANP	O1G-PG-N3B	-5.23	104.07	111.77
5	1-C	1511	ANP	O1G-PG-N3B	-5.02	104.38	111.77
5	1-D	1478	ANP	O1G-PG-N3B	-4.96	104.47	111.77
5	1-A	1511	ANP	O1G-PG-N3B	-4.67	104.90	111.77
5	2-D	1478	ANP	O1B-PB-N3B	-4.28	105.47	111.77
5	1-B	1511	ANP	O4'-C1'-N9	3.53	114.88	108.09
5	1-D	1478	ANP	O1B-PB-N3B	-3.41	106.75	111.77
5	2-F	1478	ANP	O1B-PB-N3B	-3.30	106.91	111.77
5	1-F	1478	ANP	O1B-PB-N3B	-3.29	106.92	111.77
5	2-B	1511	ANP	O4'-C1'-N9	3.24	114.32	108.09
5	1-D	1478	ANP	O4'-C1'-N9	3.22	114.27	108.09
5	2-C	1511	ANP	O1B-PB-N3B	-3.14	107.14	111.77
5	1-D	1478	ANP	O4'-C4'-C5'	3.13	119.35	109.33
5	1-D	1478	ANP	O2B-PB-O3A	3.03	114.74	104.64
5	1-F	1478	ANP	O4'-C1'-N9	3.01	113.88	108.09
5	2-D	1478	ANP	O4'-C4'-C5'	2.98	118.88	109.33
5	2-D	1478	ANP	O4'-C1'-N9	2.91	113.68	108.09
5	1-F	1478	ANP	O4'-C4'-C5'	2.88	118.57	109.33
5	2-B	1511	ANP	O1G-PG-N3B	-2.88	107.53	111.77
5	2-F	1478	ANP	O4'-C1'-N9	2.84	113.55	108.09
5	1-A	1511	ANP	O5'-C5'-C4'	2.71	118.21	108.99
5	1-B	1511	ANP	O4'-C4'-C5'	2.67	117.89	109.33
5	1-D	1478	ANP	O2G-PG-O3G	2.55	114.44	107.59
5	2-A	1511	ANP	O3A-PA-O1A	2.49	118.19	110.70
5	2-D	1478	ANP	O2B-PB-O3A	2.49	112.94	104.64
5	1-A	1511	ANP	O3A-PA-O1A	2.40	117.93	110.70
5	1-F	1478	ANP	O2B-PB-O3A	2.39	112.63	104.64
5	1-A	1511	ANP	O4'-C1'-N9	2.35	112.59	108.09
5	2-D	1478	ANP	O3G-PG-O1G	-2.20	107.94	113.45
5	2-C	1511	ANP	O3A-PA-O1A	2.16	117.19	110.70
5	2-F	1478	ANP	O2B-PB-O3A	2.16	111.84	104.64
5	1-C	1511	ANP	O2G-PG-O1G	-2.12	108.14	113.45
5	1-B	1511	ANP	C2'-C3'-C4'	2.10	106.66	102.61
5	2-A	1511	ANP	C2'-C3'-C4'	2.09	106.66	102.61
5	2-F	1478	ANP	O4'-C4'-C5'	2.09	116.04	109.33
5	2-B	1511	ANP	O2B-PB-O3A	2.09	111.62	104.64
5	1-D	1478	ANP	C1'-N9-C8	2.07	131.70	127.09
5	1-D	1478	ANP	O2G-PG-O1G	-2.02	108.39	113.45
5	2-D	1478	ANP	O5'-C5'-C4'	2.00	115.82	108.99
5	2-A	1511	ANP	O4'-C1'-N9	2.00	111.93	108.09

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1-A	1511	ANP	PB-N3B-PG-O1G
5	1-A	1511	ANP	PG-N3B-PB-O1B
5	1-A	1511	ANP	C5'-O5'-PA-O1A
5	1-A	1511	ANP	C5'-O5'-PA-O2A
5	1-A	1511	ANP	C5'-O5'-PA-O3A
5	2-A	1511	ANP	PB-N3B-PG-O1G
5	2-A	1511	ANP	PG-N3B-PB-O1B
5	2-A	1511	ANP	C5'-O5'-PA-O1A
5	2-A	1511	ANP	C5'-O5'-PA-O2A
5	2-A	1511	ANP	C5'-O5'-PA-O3A
5	1-B	1511	ANP	PB-N3B-PG-O1G
5	1-B	1511	ANP	PG-N3B-PB-O1B
5	1-B	1511	ANP	C5'-O5'-PA-O1A
5	1-B	1511	ANP	C5'-O5'-PA-O2A
5	1-B	1511	ANP	C5'-O5'-PA-O3A
5	2-B	1511	ANP	PB-N3B-PG-O1G
5	2-B	1511	ANP	PG-N3B-PB-O1B
5	2-B	1511	ANP	C5'-O5'-PA-O1A
5	2-B	1511	ANP	C5'-O5'-PA-O2A
5	2-B	1511	ANP	C5'-O5'-PA-O3A
5	2-B	1511	ANP	O4'-C4'-C5'-O5'
5	1-C	1511	ANP	PB-N3B-PG-O1G
5	1-C	1511	ANP	PG-N3B-PB-O1B
5	1-C	1511	ANP	C5'-O5'-PA-O1A
5	1-C	1511	ANP	C5'-O5'-PA-O2A
5	1-C	1511	ANP	C5'-O5'-PA-O3A
5	1-C	1511	ANP	O4'-C4'-C5'-O5'
5	2-C	1511	ANP	PB-N3B-PG-O1G
5	2-C	1511	ANP	PG-N3B-PB-O1B
5	2-C	1511	ANP	C5'-O5'-PA-O1A
5	2-C	1511	ANP	C5'-O5'-PA-O2A
5	2-C	1511	ANP	C5'-O5'-PA-O3A
5	2-C	1511	ANP	O4'-C4'-C5'-O5'
5	1-D	1478	ANP	PB-N3B-PG-O1G
5	1-D	1478	ANP	PG-N3B-PB-O1B
5	1-D	1478	ANP	PA-O3A-PB-O2B
5	1-D	1478	ANP	C5'-O5'-PA-O1A
5	1-D	1478	ANP	C5'-O5'-PA-O2A
5	1-D	1478	ANP	C5'-O5'-PA-O3A
5	1-D	1478	ANP	O4'-C4'-C5'-O5'
5	2-D	1478	ANP	PB-N3B-PG-O1G
5	2-D	1478	ANP	PG-N3B-PB-O1B

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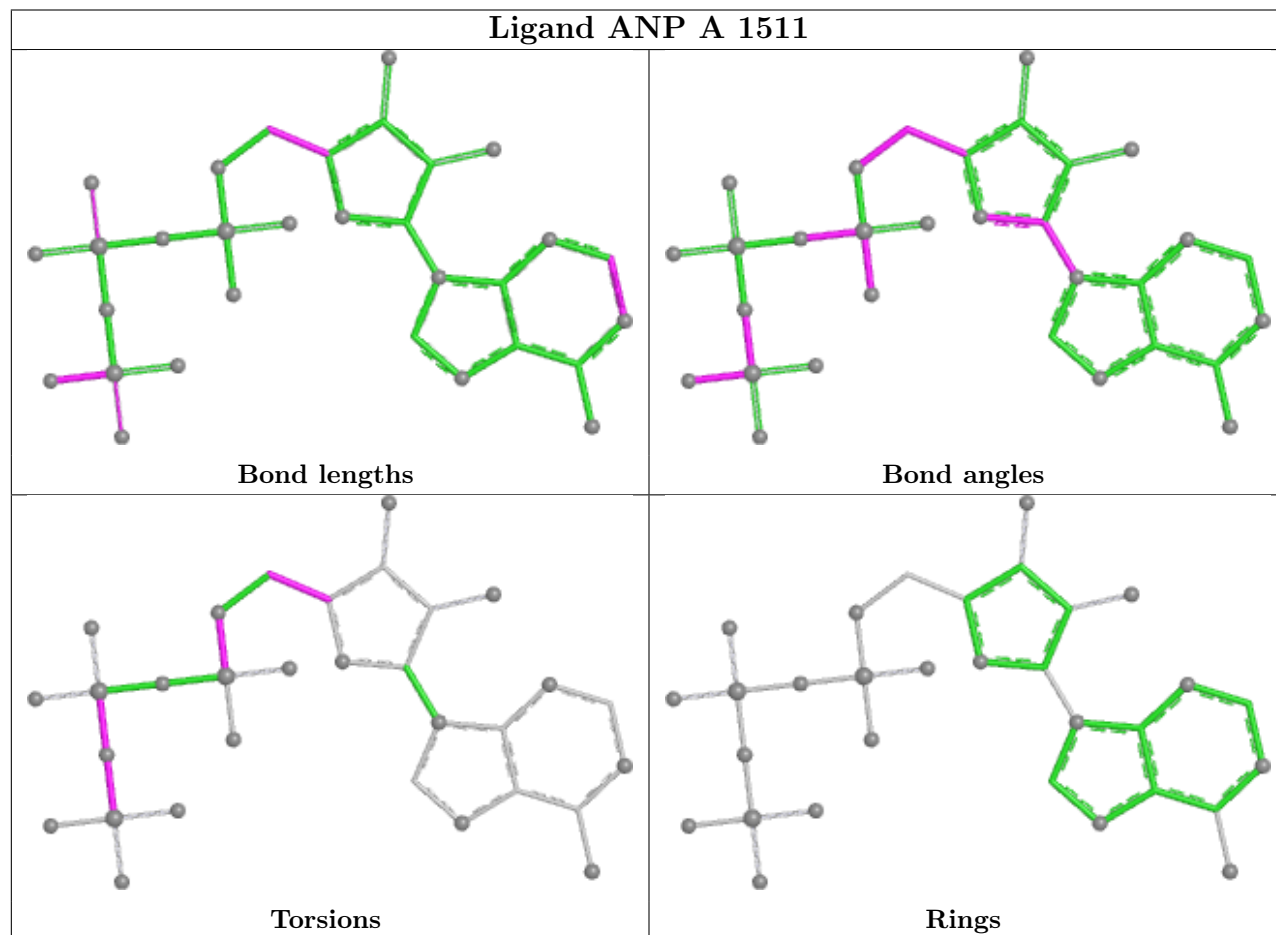
Mol	Chain	Res	Type	Atoms
5	2-D	1478	ANP	C5'-O5'-PA-O1A
5	2-D	1478	ANP	C5'-O5'-PA-O2A
5	2-D	1478	ANP	C5'-O5'-PA-O3A
5	1-F	1478	ANP	PB-N3B-PG-O1G
5	1-F	1478	ANP	PG-N3B-PB-O1B
5	1-F	1478	ANP	PA-O3A-PB-O2B
5	1-F	1478	ANP	C5'-O5'-PA-O1A
5	1-F	1478	ANP	C5'-O5'-PA-O2A
5	1-F	1478	ANP	C5'-O5'-PA-O3A
5	2-F	1478	ANP	PB-N3B-PG-O1G
5	2-F	1478	ANP	PG-N3B-PB-O1B
5	2-F	1478	ANP	PA-O3A-PB-O2B
5	2-F	1478	ANP	C5'-O5'-PA-O1A
5	2-F	1478	ANP	C5'-O5'-PA-O2A
5	2-F	1478	ANP	C5'-O5'-PA-O3A
5	2-F	1478	ANP	O4'-C4'-C5'-O5'
5	2-A	1511	ANP	O4'-C4'-C5'-O5'
5	1-B	1511	ANP	O4'-C4'-C5'-O5'
5	1-F	1478	ANP	O4'-C4'-C5'-O5'
5	2-F	1478	ANP	C3'-C4'-C5'-O5'
5	1-C	1511	ANP	C3'-C4'-C5'-O5'
5	2-A	1511	ANP	C3'-C4'-C5'-O5'
5	1-B	1511	ANP	C3'-C4'-C5'-O5'
5	2-B	1511	ANP	C3'-C4'-C5'-O5'
5	2-C	1511	ANP	C3'-C4'-C5'-O5'
5	1-D	1478	ANP	C3'-C4'-C5'-O5'
5	1-F	1478	ANP	C3'-C4'-C5'-O5'
5	2-D	1478	ANP	C3'-C4'-C5'-O5'
5	2-D	1478	ANP	O4'-C4'-C5'-O5'
5	1-A	1511	ANP	C3'-C4'-C5'-O5'
5	1-A	1511	ANP	O4'-C4'-C5'-O5'
5	1-D	1478	ANP	PA-O3A-PB-O1B
5	2-D	1478	ANP	PA-O3A-PB-O1B
5	1-F	1478	ANP	PA-O3A-PB-O1B
5	2-F	1478	ANP	PA-O3A-PB-O1B

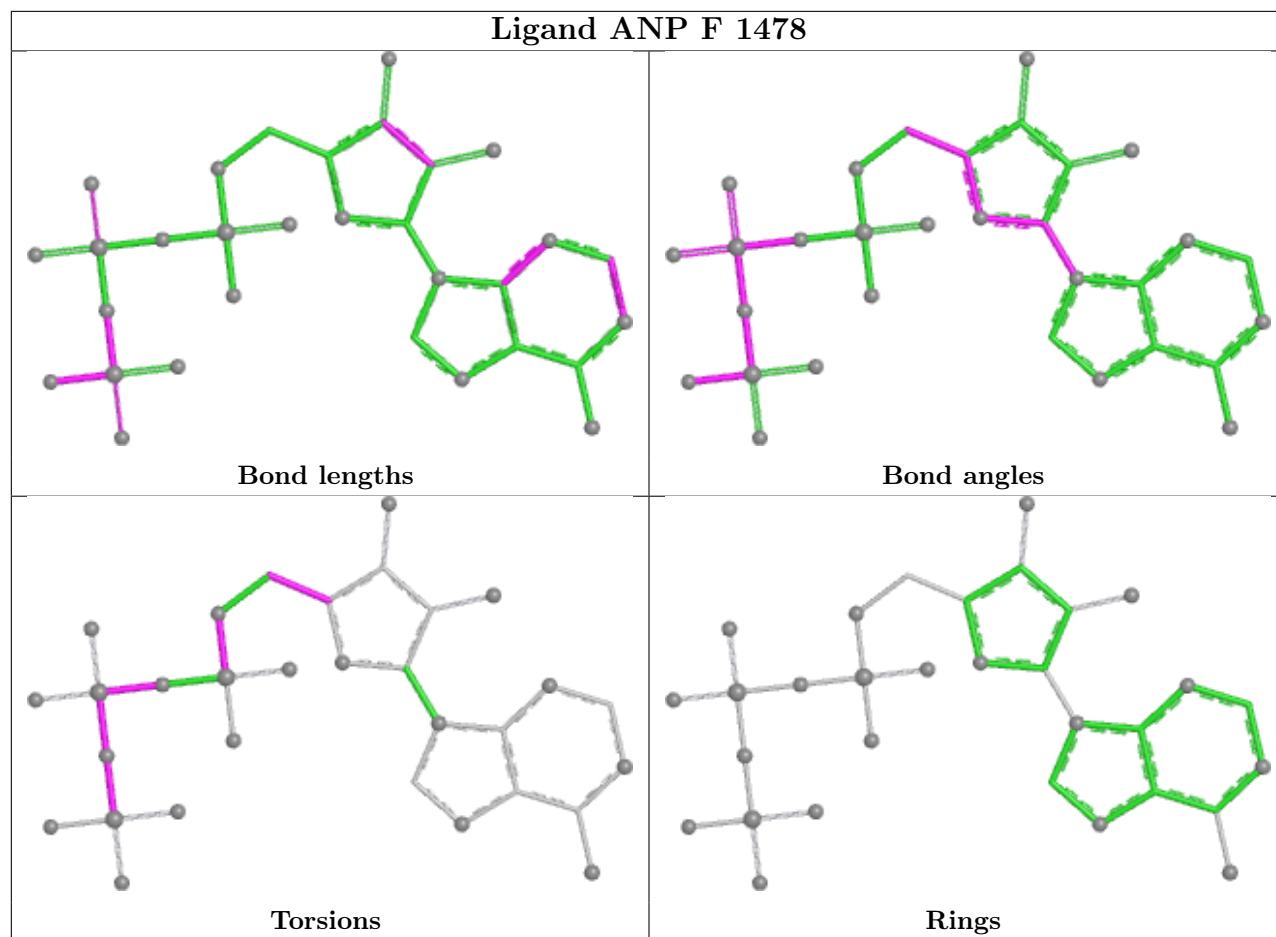
There are no ring outliers.

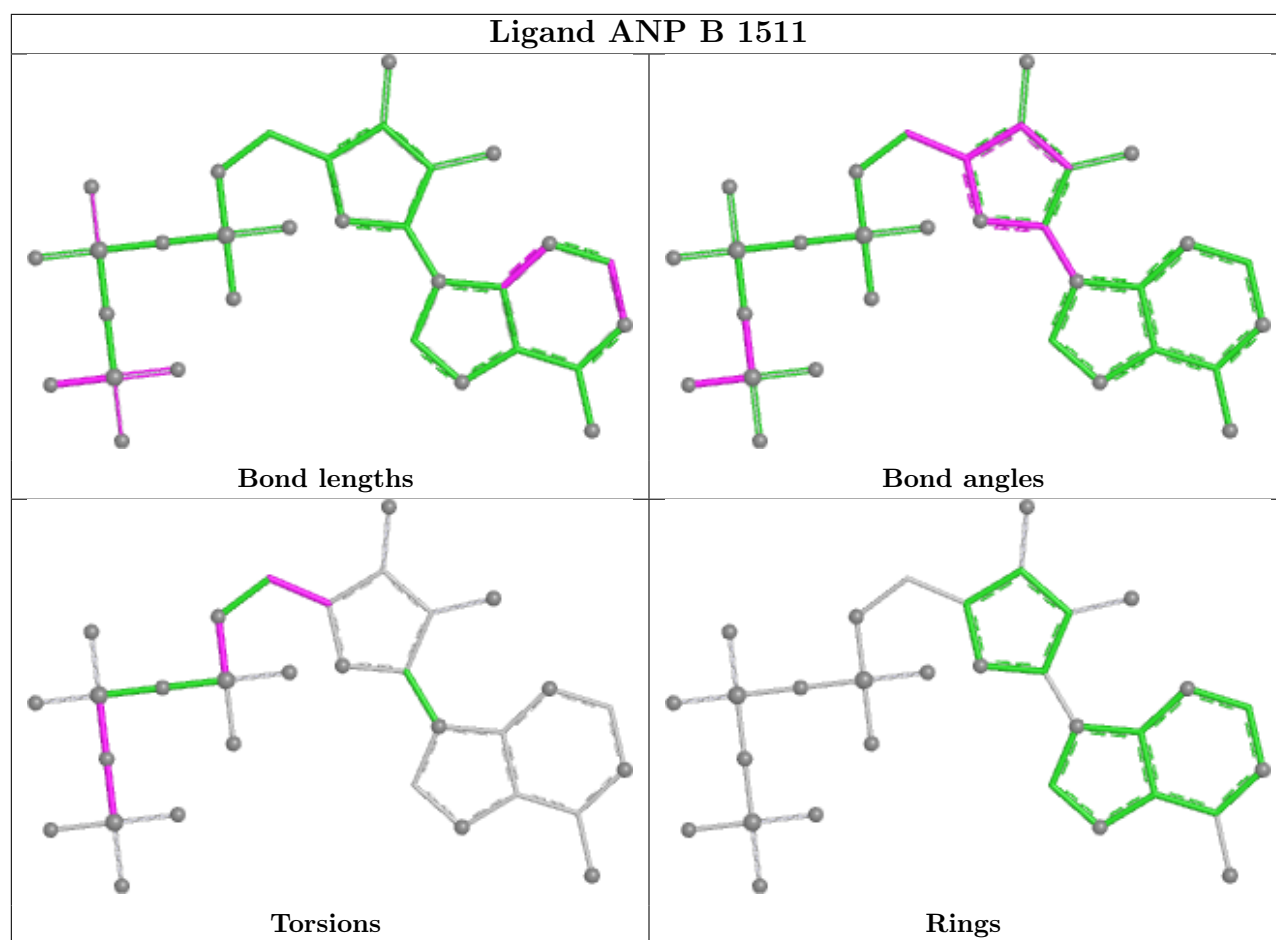
No monomer is involved in short contacts.

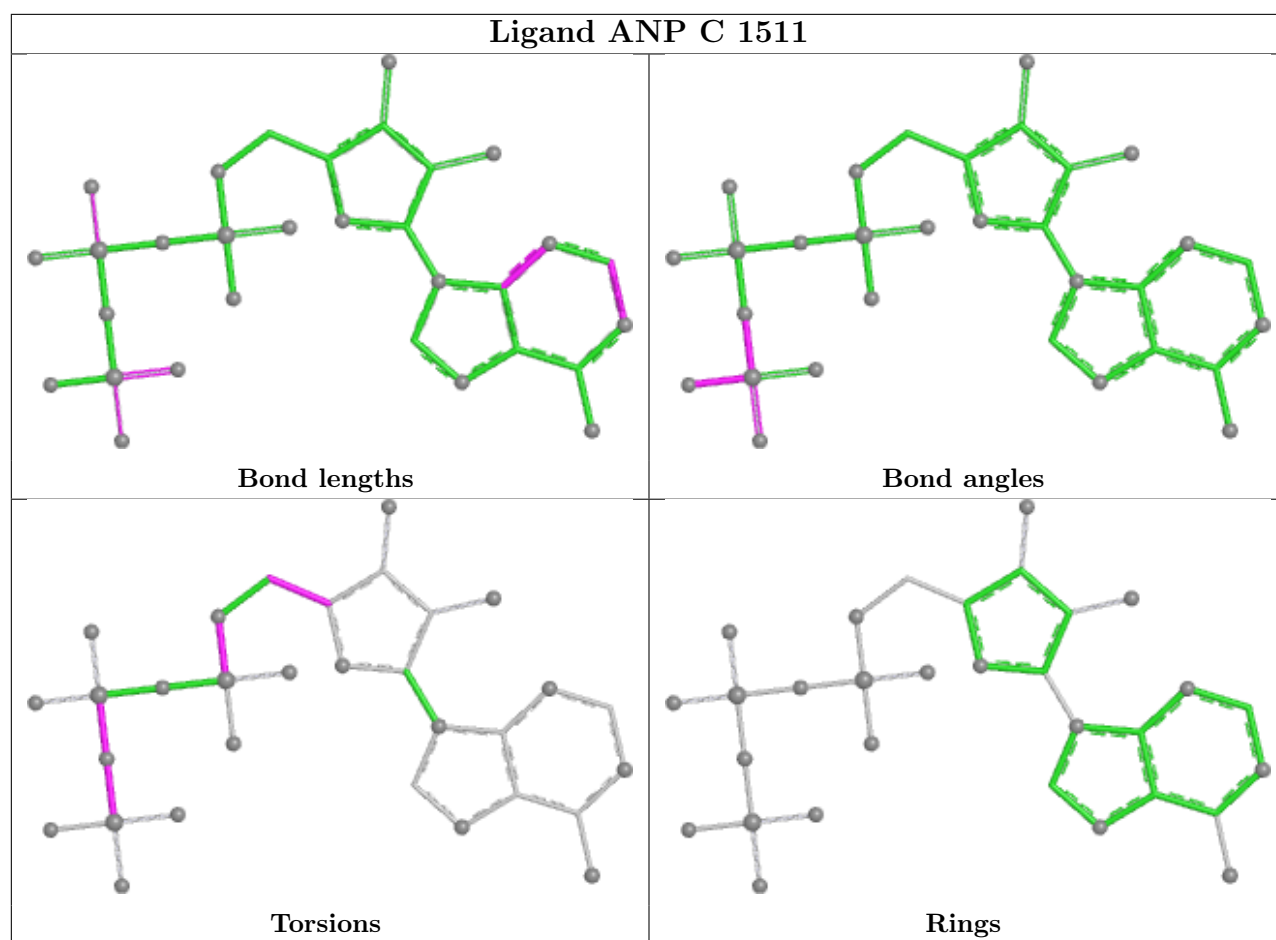
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

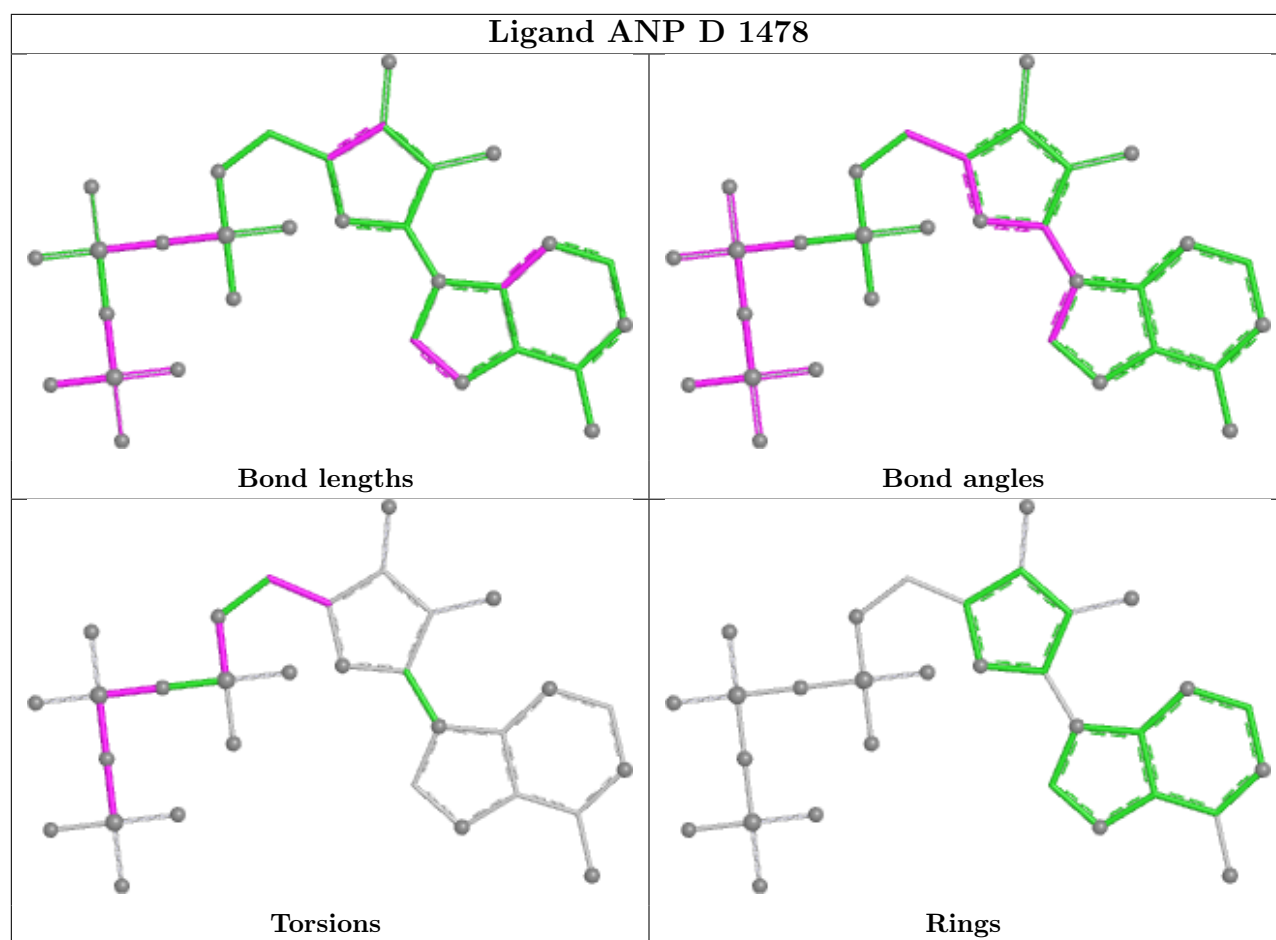
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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	1-A	487/510 (95%)	2.28	262 (53%)  	16, 32, 47, 57	487 (100%)
1	1-B	479/510 (93%)	2.13	228 (47%)  	16, 27, 49, 59	479 (100%)
1	1-C	488/510 (95%)	1.99	213 (43%)  	14, 27, 42, 74	488 (100%)
1	2-A	0/510	-	-	-	-
1	2-B	0/510	-	-	-	-
1	2-C	0/510	-	-	-	-
2	1-D	469/482 (97%)	2.52	296 (63%)  	18, 30, 46, 62	469 (100%)
2	1-E	466/482 (96%)	2.79	322 (69%)  	17, 34, 55, 74	466 (100%)
2	1-F	466/482 (96%)	1.87	188 (40%)  	12, 24, 41, 51	466 (100%)
2	2-D	0/482	-	-	-	-
2	2-E	0/482	-	-	-	-
2	2-F	0/482	-	-	-	-
3	1-G	94/272 (34%)	2.47	53 (56%)  	15, 35, 56, 61	94 (100%)
3	2-G	0/272	-	-	-	-
4	1-H	37/84 (44%)	2.91	24 (64%)  	26, 39, 52, 56	37 (100%)
4	2-H	0/84	-	-	-	-
All	All	2986/6664 (44%)	2.28	1586 (53%)  	12, 30, 49, 74	2986 (100%)

All (1586) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-C	443	ALA	9.5
2	1-E	351	LEU	8.5
1	1-B	400	VAL	8.4
2	1-E	374	VAL	8.2
2	1-E	354	THR	8.2
2	1-E	161	GLY	7.5
2	1-F	433	PRO	7.5
1	1-C	207	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	180	ILE	7.4
2	1-E	164	VAL	7.4
1	1-C	297	ASP	7.4
1	1-A	321	LEU	7.2
2	1-E	390	ILE	7.1
2	1-E	154	LEU	7.0
2	1-E	387	ILE	6.7
2	1-F	434	LEU	6.7
2	1-E	389	ALA	6.7
2	1-E	474	ALA	6.7
1	1-A	203	TYR	6.6
2	1-D	208	LEU	6.6
1	1-B	74	VAL	6.5
2	1-E	142	LEU	6.5
2	1-D	424	PHE	6.5
1	1-C	392	LEU	6.3
2	1-D	9	THR	6.2
2	1-E	215	VAL	6.2
3	1-G	237	LYS	6.2
4	1-H	30	GLU	6.1
2	1-E	331	ALA	6.1
2	1-F	450	ASP	6.1
1	1-B	57	SER	6.0
2	1-E	56	SER	6.0
2	1-E	380	ASP	6.0
2	1-F	144	ALA	6.0
2	1-F	147	ALA	6.0
1	1-B	82	ILE	6.0
1	1-A	354	THR	5.9
1	1-C	293	ALA	5.9
2	1-E	382	LYS	5.9
2	1-D	327	ALA	5.9
1	1-B	471	HIS	5.9
1	1-A	406	PHE	5.9
1	1-A	95	VAL	5.9
2	1-F	280	GLY	5.8
2	1-E	254	PHE	5.8
1	1-A	94	ILE	5.8
2	1-E	211	ALA	5.8
2	1-E	384	LEU	5.8
4	1-H	33	TYR	5.8
3	1-G	26	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
4	1-H	34	PHE	5.7
2	1-D	396	LEU	5.7
1	1-C	152	ALA	5.7
2	1-E	333	THR	5.7
1	1-B	276	VAL	5.7
1	1-B	413	ALA	5.7
2	1-E	356	ARG	5.7
2	1-E	297	THR	5.7
1	1-B	401	ALA	5.7
1	1-B	59	LEU	5.7
1	1-A	133	ALA	5.7
1	1-A	211	SER	5.6
2	1-F	389	ALA	5.6
1	1-C	156	LEU	5.6
2	1-E	375	GLN	5.6
2	1-F	469	LYS	5.6
2	1-F	465	GLU	5.5
2	1-F	320	PRO	5.5
2	1-D	473	LEU	5.5
2	1-F	268	VAL	5.4
1	1-C	391	LYS	5.4
1	1-B	351	PHE	5.4
2	1-E	132	ILE	5.3
1	1-A	220	LEU	5.3
2	1-D	315	ASP	5.3
2	1-E	376	LYS	5.3
1	1-A	88	VAL	5.3
2	1-D	173	VAL	5.3
2	1-E	432	VAL	5.2
2	1-D	28	GLY	5.2
2	1-D	255	ILE	5.2
2	1-E	240	ALA	5.2
2	1-D	385	GLN	5.2
1	1-B	87	ILE	5.2
1	1-C	447	ALA	5.2
3	1-G	21	LYS	5.2
2	1-D	142	LEU	5.2
2	1-D	206	ILE	5.2
2	1-E	473	LEU	5.2
4	1-H	14	ALA	5.1
2	1-E	452	LEU	5.1
3	1-G	1	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	89	LYS	5.0
2	1-D	392	GLY	5.0
1	1-A	130	GLY	5.0
1	1-B	358	TYR	5.0
2	1-E	434	LEU	5.0
1	1-A	167	ILE	5.0
2	1-D	96	ASN	5.0
2	1-D	174	ALA	5.0
2	1-E	233	ALA	5.0
1	1-A	177	SER	5.0
2	1-E	214	LYS	5.0
1	1-C	281	MET	4.9
1	1-A	165	GLU	4.9
2	1-F	363	VAL	4.9
1	1-A	135	GLY	4.9
2	1-F	172	ASN	4.9
1	1-C	427	LEU	4.9
2	1-E	158	ALA	4.9
2	1-E	391	LEU	4.9
2	1-F	410	ILE	4.9
2	1-F	407	ALA	4.9
2	1-D	169	LEU	4.9
1	1-B	235	THR	4.8
2	1-F	452	LEU	4.8
1	1-C	371	VAL	4.8
1	1-A	489	ILE	4.8
4	1-H	15	VAL	4.8
2	1-E	412	ARG	4.8
2	1-D	381	TYR	4.8
2	1-E	256	ASP	4.8
2	1-F	398	GLU	4.8
2	1-D	139	VAL	4.8
1	1-B	55	PHE	4.8
2	1-D	249	GLN	4.8
1	1-C	375	GLY	4.8
1	1-A	352	LEU	4.7
1	1-A	342	VAL	4.7
1	1-A	446	TYR	4.7
3	1-G	4	LYS	4.7
2	1-E	160	VAL	4.7
1	1-B	469	LEU	4.7
2	1-D	233	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
2	1-E	453	PRO	4.7
2	1-F	445	LEU	4.7
1	1-B	473	ILE	4.7
1	1-C	361	ILE	4.7
2	1-E	83	ARG	4.7
2	1-F	390	ILE	4.7
2	1-D	67	GLU	4.7
1	1-C	400	VAL	4.7
1	1-B	212	THR	4.6
1	1-B	76	PHE	4.6
1	1-C	226	MET	4.6
2	1-E	393	MET	4.6
1	1-A	100	GLY	4.6
1	1-B	207	GLY	4.6
1	1-B	412	ALA	4.6
2	1-D	309	ALA	4.6
2	1-F	179	GLY	4.6
1	1-B	396	GLN	4.6
2	1-D	239	VAL	4.6
1	1-B	77	GLY	4.6
2	1-D	411	GLN	4.6
2	1-D	427	HIS	4.6
1	1-B	410	LEU	4.6
2	1-E	378	LEU	4.6
1	1-A	93	ALA	4.6
2	1-E	377	ILE	4.6
2	1-E	349	ASP	4.5
2	1-F	137	ILE	4.5
1	1-A	458	PRO	4.5
2	1-D	397	SER	4.5
3	1-G	238	ASN	4.5
3	1-G	25	MET	4.5
1	1-C	369	LEU	4.5
2	1-E	444	ILE	4.5
2	1-E	90	THR	4.5
1	1-C	350	ILE	4.5
2	1-E	373	GLY	4.5
2	1-E	104	GLU	4.5
1	1-B	394	LEU	4.5
2	1-F	165	LEU	4.5
2	1-E	166	ILE	4.5
1	1-A	337	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
2	1-E	180	TYR	4.4
1	1-B	204	VAL	4.4
1	1-B	428	LEU	4.4
2	1-E	258	ILE	4.4
2	1-E	410	ILE	4.4
1	1-A	264	ALA	4.4
1	1-A	50	GLU	4.4
2	1-F	133	LEU	4.4
1	1-B	459	SER	4.4
1	1-A	447	ALA	4.4
1	1-B	110	ALA	4.4
2	1-D	432	VAL	4.4
1	1-B	172	GLN	4.4
1	1-B	79	ASP	4.4
2	1-D	386	ASP	4.4
2	1-D	348	VAL	4.4
2	1-D	460	VAL	4.4
2	1-E	329	LEU	4.4
2	1-E	344	ILE	4.4
2	1-D	121	PRO	4.4
2	1-E	350	PRO	4.4
2	1-E	370	VAL	4.3
2	1-D	146	TYR	4.3
3	1-G	87	LYS	4.3
2	1-D	254	PHE	4.3
2	1-E	28	GLY	4.3
2	1-E	169	LEU	4.3
2	1-E	355	SER	4.3
2	1-D	384	LEU	4.3
2	1-E	385	GLN	4.3
4	1-H	4	SER	4.3
1	1-B	268	TYR	4.3
1	1-B	461	ILE	4.3
1	1-A	194	ASP	4.3
2	1-E	40	GLY	4.3
2	1-E	136	GLY	4.3
2	1-E	149	GLY	4.3
2	1-E	257	ASN	4.2
2	1-E	379	GLN	4.2
2	1-D	388	ILE	4.2
2	1-E	94	ILE	4.2
1	1-C	395	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
4	1-H	28	ALA	4.2
1	1-A	25	LEU	4.2
2	1-D	252	LEU	4.2
2	1-F	169	LEU	4.2
2	1-E	419	GLN	4.2
2	1-F	272	LEU	4.2
2	1-E	437	THR	4.2
2	1-D	209	LYS	4.2
1	1-A	64	LEU	4.2
2	1-D	37	GLU	4.2
2	1-D	143	LEU	4.2
2	1-E	220	GLY	4.2
1	1-B	270	ASP	4.2
1	1-C	347	ASP	4.2
2	1-E	25	PHE	4.2
1	1-A	308	ARG	4.1
2	1-F	435	LYS	4.1
1	1-B	30	ARG	4.1
2	1-F	139	VAL	4.1
2	1-F	417	PRO	4.1
1	1-A	110	ALA	4.1
4	1-H	18	ALA	4.1
1	1-B	349	GLN	4.1
2	1-D	117	HIS	4.1
2	1-E	134	VAL	4.1
2	1-D	417	PRO	4.1
1	1-A	121	ILE	4.1
2	1-E	352	ASP	4.1
3	1-G	2	THR	4.1
2	1-D	253	LEU	4.1
2	1-F	311	TYR	4.1
1	1-A	253	MET	4.1
1	1-C	345	ILE	4.1
1	1-B	354	THR	4.0
1	1-B	472	VAL	4.0
1	1-C	430	GLN	4.0
2	1-E	10	THR	4.0
2	1-E	251	VAL	4.0
2	1-E	162	LYS	4.0
1	1-A	136	ILE	4.0
1	1-A	35	GLY	4.0
1	1-C	85	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	1-E	326	PHE	4.0
1	1-B	75	VAL	4.0
2	1-F	403	THR	4.0
4	1-H	36	ALA	4.0
2	1-F	388	ILE	4.0
2	1-D	413	PHE	4.0
2	1-E	424	PHE	4.0
1	1-C	157	VAL	4.0
2	1-E	435	LYS	4.0
1	1-A	364	ALA	4.0
1	1-A	382	ALA	4.0
1	1-C	171	ARG	4.0
1	1-C	268	TYR	4.0
1	1-A	266	ILE	3.9
1	1-A	443	ALA	3.9
3	1-G	29	ALA	3.9
2	1-E	22	ASP	3.9
2	1-E	72	GLY	3.9
1	1-A	410	LEU	3.9
2	1-E	148	LYS	3.9
2	1-D	200	MET	3.9
2	1-F	367	HIS	3.9
1	1-B	380	THR	3.9
1	1-C	69	ASP	3.9
2	1-E	259	PHE	3.9
2	1-E	253	LEU	3.9
2	1-F	391	LEU	3.9
1	1-C	334	VAL	3.9
2	1-D	181	SER	3.9
2	1-D	90	THR	3.9
2	1-D	110	THR	3.9
2	1-E	184	ALA	3.9
2	1-E	299	THR	3.9
2	1-F	153	GLY	3.9
1	1-A	265	LEU	3.9
2	1-E	188	GLU	3.9
1	1-A	300	TYR	3.9
2	1-D	219	TYR	3.9
2	1-D	345	TYR	3.9
2	1-D	404	VAL	3.9
2	1-E	82	ILE	3.9
1	1-A	304	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
3	1-G	236	SER	3.9
2	1-E	305	THR	3.9
2	1-E	332	THR	3.9
2	1-E	403	THR	3.9
1	1-B	37	GLY	3.9
2	1-D	196	LEU	3.9
1	1-B	53	VAL	3.9
1	1-B	475	GLN	3.9
2	1-E	221	GLN	3.9
1	1-A	323	ALA	3.9
1	1-A	408	SER	3.9
2	1-F	261	PHE	3.8
1	1-C	409	ASP	3.8
2	1-D	24	GLN	3.8
1	1-A	346	THR	3.8
1	1-B	346	THR	3.8
1	1-C	429	LYS	3.8
2	1-D	163	THR	3.8
2	1-E	266	SER	3.8
2	1-E	353	SER	3.8
2	1-F	440	GLY	3.8
2	1-E	131	GLU	3.8
2	1-E	443	GLN	3.8
1	1-B	256	TYR	3.8
1	1-A	49	ALA	3.8
1	1-A	467	ALA	3.8
2	1-E	9	THR	3.8
3	1-G	3	LEU	3.8
1	1-A	290	GLY	3.8
1	1-B	327	ILE	3.8
1	1-C	483	ILE	3.8
2	1-D	296	ILE	3.8
2	1-D	444	ILE	3.8
1	1-B	391	LYS	3.8
1	1-C	278	TYR	3.8
1	1-C	378	ALA	3.8
2	1-D	182	VAL	3.8
2	1-D	229	ARG	3.8
2	1-E	239	VAL	3.8
2	1-E	420	VAL	3.8
1	1-B	438	ILE	3.8
1	1-A	201	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	1-C	79	ASP	3.8
2	1-E	146	TYR	3.8
2	1-E	126	MET	3.8
3	1-G	79	GLY	3.8
1	1-B	468	PHE	3.8
1	1-C	403	PHE	3.8
2	1-D	43	THR	3.8
1	1-A	233	SER	3.7
2	1-D	232	VAL	3.7
2	1-D	132	ILE	3.7
2	1-F	174	ALA	3.7
3	1-G	231	ALA	3.7
2	1-D	207	ASN	3.7
1	1-A	92	GLY	3.7
1	1-A	403	PHE	3.7
2	1-D	215	VAL	3.7
1	1-A	230	ILE	3.7
1	1-A	350	ILE	3.7
4	1-H	17	ASP	3.7
1	1-B	285	LEU	3.7
2	1-E	216	ALA	3.7
1	1-B	286	ARG	3.7
4	1-H	37	ARG	3.7
2	1-E	346	PRO	3.7
1	1-A	240	ALA	3.7
2	1-F	474	ALA	3.7
2	1-D	395	GLU	3.7
1	1-C	502	THR	3.7
3	1-G	221	THR	3.7
2	1-E	357	ILE	3.7
1	1-C	376	SER	3.7
2	1-E	383	SER	3.7
1	1-A	131	LEU	3.7
1	1-A	315	ALA	3.7
2	1-D	222	MET	3.7
2	1-E	12	ARG	3.7
3	1-G	268	GLY	3.7
1	1-A	414	THR	3.7
1	1-C	221	THR	3.7
1	1-C	329	THR	3.7
1	1-C	389	THR	3.7
2	1-E	298	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	163	GLN	3.6
1	1-B	427	LEU	3.6
1	1-C	469	LEU	3.6
2	1-E	217	LEU	3.6
2	1-E	237	LEU	3.6
1	1-B	448	GLY	3.6
3	1-G	18	LYS	3.6
1	1-C	74	VAL	3.6
1	1-C	367	VAL	3.6
1	1-A	103	LEU	3.6
2	1-D	342	LEU	3.6
1	1-A	243	GLN	3.6
1	1-B	470	SER	3.6
2	1-D	19	ALA	3.6
1	1-B	398	ARG	3.6
2	1-F	136	GLY	3.6
2	1-F	400	ASP	3.6
3	1-G	244	ASP	3.6
2	1-D	241	GLU	3.6
2	1-E	152	ILE	3.6
1	1-A	444	VAL	3.6
2	1-D	218	VAL	3.6
2	1-E	381	TYR	3.6
1	1-C	131	LEU	3.6
2	1-E	36	LEU	3.6
1	1-A	239	ALA	3.6
1	1-A	310	ALA	3.6
1	1-C	147	GLN	3.6
2	1-E	421	ALA	3.6
1	1-A	202	ILE	3.6
2	1-F	258	ILE	3.6
2	1-F	386	ASP	3.6
2	1-D	104	GLU	3.6
2	1-E	449	TYR	3.6
2	1-D	452	LEU	3.6
2	1-F	414	LEU	3.6
2	1-F	148	LYS	3.6
2	1-D	294	GLU	3.6
1	1-A	200	TYR	3.6
1	1-B	389	THR	3.6
2	1-E	416	GLN	3.5
1	1-A	504	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	1-D	183	PHE	3.5
2	1-E	155	PHE	3.5
2	1-F	155	PHE	3.5
1	1-C	438	ILE	3.5
2	1-D	303	SER	3.5
2	1-D	387	ILE	3.5
2	1-F	127	SER	3.5
3	1-G	16	ILE	3.5
2	1-D	199	GLU	3.5
2	1-D	103	ASP	3.5
1	1-B	216	LEU	3.5
1	1-B	480	LEU	3.5
2	1-E	342	LEU	3.5
2	1-F	143	LEU	3.5
1	1-B	363	PRO	3.5
2	1-D	111	LYS	3.5
2	1-D	238	THR	3.5
1	1-A	114	ALA	3.5
1	1-A	510	ALA	3.5
2	1-E	338	ALA	3.5
2	1-E	470	ALA	3.5
2	1-D	220	GLY	3.5
2	1-D	440	GLY	3.5
1	1-B	195	GLU	3.5
2	1-D	305	THR	3.5
1	1-C	331	ALA	3.5
1	1-C	506	ALA	3.5
2	1-F	331	ALA	3.5
1	1-B	500	ILE	3.5
2	1-D	362	ILE	3.5
2	1-E	348	VAL	3.5
1	1-A	292	GLU	3.5
2	1-D	341	GLU	3.5
1	1-A	369	LEU	3.5
2	1-E	428	LEU	3.5
1	1-B	275	ALA	3.5
2	1-D	184	ALA	3.5
1	1-C	396	GLN	3.5
1	1-C	487	GLY	3.5
2	1-D	106	GLY	3.5
2	1-D	136	GLY	3.5
1	1-B	393	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	1-B	479	LEU	3.5
1	1-C	64	LEU	3.5
2	1-F	138	LYS	3.5
3	1-G	30	LYS	3.5
1	1-C	370	SER	3.5
2	1-E	213	SER	3.5
1	1-A	291	ARG	3.5
3	1-G	230	THR	3.5
1	1-B	510	ALA	3.5
1	1-C	404	ALA	3.5
3	1-G	19	ILE	3.4
1	1-A	129	VAL	3.4
2	1-E	218	VAL	3.4
2	1-F	154	LEU	3.4
1	1-B	248	TYR	3.4
1	1-B	329	THR	3.4
2	1-D	50	ALA	3.4
2	1-E	137	ILE	3.4
1	1-A	231	VAL	3.4
2	1-D	46	VAL	3.4
2	1-D	86	VAL	3.4
2	1-D	160	VAL	3.4
1	1-A	506	ALA	3.4
2	1-F	176	ALA	3.4
4	1-H	38	ALA	3.4
1	1-C	193	THR	3.4
2	1-E	291	THR	3.4
1	1-C	330	GLN	3.4
2	1-D	438	ILE	3.4
1	1-A	132	LYS	3.4
2	1-D	11	GLY	3.4
2	1-E	414	LEU	3.4
1	1-C	399	GLU	3.4
2	1-F	360	PRO	3.4
1	1-A	249	SER	3.4
1	1-C	225	ALA	3.4
1	1-C	412	ALA	3.4
2	1-D	120	ALA	3.4
2	1-E	176	ALA	3.4
4	1-H	21	ALA	3.4
2	1-D	344	ILE	3.4
2	1-E	102	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	1-C	208	GLN	3.4
2	1-E	386	ASP	3.4
2	1-E	450	ASP	3.4
1	1-C	47	VAL	3.4
2	1-D	133	LEU	3.4
2	1-E	139	VAL	3.4
2	1-E	285	LEU	3.4
4	1-H	8	VAL	3.4
1	1-C	436	MET	3.4
1	1-C	349	GLN	3.4
2	1-D	400	ASP	3.4
2	1-E	330	ASP	3.4
1	1-B	505	LEU	3.3
2	1-D	414	LEU	3.3
2	1-E	205	VAL	3.3
4	1-H	13	GLY	3.3
1	1-A	225	ALA	3.3
1	1-A	246	ALA	3.3
1	1-B	377	ALA	3.3
1	1-B	463	LYS	3.3
2	1-D	331	ALA	3.3
2	1-D	469	LYS	3.3
2	1-D	472	LYS	3.3
2	1-E	95	MET	3.3
1	1-B	474	SER	3.3
2	1-E	455	GLN	3.3
1	1-B	32	LEU	3.3
2	1-E	208	LEU	3.3
1	1-A	41	VAL	3.3
1	1-C	386	VAL	3.3
2	1-F	141	ASP	3.3
1	1-B	160	GLY	3.3
2	1-D	398	GLU	3.3
1	1-A	159	ILE	3.3
2	1-D	102	ILE	3.3
2	1-E	32	ILE	3.3
2	1-F	198	HIS	3.3
3	1-G	229	MET	3.3
2	1-D	308	GLN	3.3
2	1-E	47	LEU	3.3
1	1-B	340	THR	3.3
1	1-C	63	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	1-E	127	SER	3.3
2	1-E	467	VAL	3.3
2	1-F	423	VAL	3.3
1	1-B	162	GLY	3.3
2	1-F	461	GLY	3.3
2	1-E	225	PRO	3.3
1	1-A	345	ILE	3.3
1	1-C	365	ILE	3.3
2	1-E	84	ILE	3.3
2	1-E	113	PHE	3.3
2	1-E	445	LEU	3.3
2	1-D	406	ARG	3.3
2	1-E	411	GLN	3.3
1	1-B	41	VAL	3.3
2	1-E	46	VAL	3.3
1	1-B	360	GLY	3.3
1	1-C	130	GLY	3.3
3	1-G	84	SER	3.3
1	1-C	433	TYR	3.3
2	1-D	197	TYR	3.3
1	1-B	230	ILE	3.3
2	1-F	470	ALA	3.3
1	1-C	417	LEU	3.3
2	1-D	235	THR	3.3
2	1-F	426	GLY	3.3
1	1-B	434	SER	3.3
2	1-D	458	TYR	3.2
2	1-D	433	PRO	3.2
1	1-A	508	PHE	3.2
2	1-F	130	GLN	3.2
2	1-F	291	THR	3.2
1	1-A	344	SER	3.2
2	1-E	197	TYR	3.2
1	1-B	269	ASP	3.2
1	1-A	402	ALA	3.2
1	1-A	497	LEU	3.2
2	1-D	335	LEU	3.2
1	1-A	257	PHE	3.2
1	1-A	232	VAL	3.2
1	1-A	472	VAL	3.2
1	1-B	157	VAL	3.2
2	1-E	75	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	1-E	404	VAL	3.2
2	1-F	370	VAL	3.2
1	1-B	60	LYS	3.2
1	1-B	209	LYS	3.2
2	1-D	425	THR	3.2
2	1-F	178	GLY	3.2
2	1-F	167	MET	3.2
2	1-F	281	TYR	3.2
1	1-B	365	ILE	3.2
2	1-D	141	ASP	3.2
2	1-E	255	ILE	3.2
2	1-F	387	ILE	3.2
2	1-F	444	ILE	3.2
1	1-A	245	LEU	3.2
1	1-A	309	ALA	3.2
1	1-B	369	LEU	3.2
2	1-D	391	LEU	3.2
3	1-G	77	LEU	3.2
1	1-C	351	PHE	3.2
2	1-E	409	LYS	3.2
1	1-A	439	GLU	3.2
1	1-B	440	GLU	3.2
1	1-A	158	PRO	3.2
1	1-B	452	TYR	3.2
1	1-C	167	ILE	3.2
2	1-D	180	TYR	3.2
2	1-D	405	SER	3.2
2	1-E	304	ILE	3.2
2	1-E	322	PRO	3.2
2	1-E	397	SER	3.2
2	1-E	431	LEU	3.2
2	1-D	228	ALA	3.2
2	1-D	328	HIS	3.2
1	1-A	97	VAL	3.2
2	1-E	460	VAL	3.2
2	1-D	99	GLY	3.2
1	1-C	235	THR	3.2
1	1-A	353	GLU	3.2
2	1-D	454	GLU	3.2
2	1-E	129	GLU	3.2
1	1-A	138	PRO	3.2
3	1-G	81	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-B	103	LEU	3.1
2	1-F	473	LEU	3.1
1	1-A	377	ALA	3.1
2	1-D	474	ALA	3.1
2	1-E	174	ALA	3.1
2	1-F	118	ALA	3.1
2	1-F	175	LYS	3.1
1	1-A	367	VAL	3.1
1	1-B	353	GLU	3.1
1	1-A	134	PRO	3.1
1	1-C	435	PRO	3.1
2	1-D	258	ILE	3.1
2	1-F	296	ILE	3.1
2	1-F	438	ILE	3.1
2	1-F	271	LEU	3.1
1	1-A	256	TYR	3.1
1	1-A	214	ALA	3.1
2	1-D	314	ALA	3.1
3	1-G	22	SER	3.1
1	1-A	351	PHE	3.1
2	1-E	442	GLN	3.1
2	1-E	11	GLY	3.1
1	1-B	339	PRO	3.1
1	1-C	288	PRO	3.1
2	1-D	298	THR	3.1
2	1-E	133	LEU	3.1
1	1-A	196	LYS	3.1
1	1-C	239	ALA	3.1
2	1-D	211	ALA	3.1
2	1-D	216	ALA	3.1
2	1-D	466	ALA	3.1
2	1-E	219	TYR	3.1
1	1-A	42	HIS	3.1
1	1-A	56	SER	3.1
1	1-B	201	CYS	3.1
2	1-E	14	VAL	3.1
1	1-C	477	GLN	3.1
2	1-E	159	GLY	3.1
2	1-D	377	ILE	3.1
2	1-E	388	ILE	3.1
2	1-E	398	GLU	3.1
1	1-B	325	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	1-D	29	LEU	3.1
1	1-C	197	LYS	3.1
1	1-B	125	ALA	3.1
2	1-D	114	ALA	3.1
3	1-G	27	ALA	3.1
1	1-B	203	TYR	3.1
1	1-A	24	ASP	3.1
2	1-D	415	SER	3.1
2	1-E	181	SER	3.1
2	1-D	172	ASN	3.1
2	1-F	250	ASP	3.1
2	1-D	227	GLY	3.1
2	1-D	61	ILE	3.1
2	1-E	310	ILE	3.1
2	1-F	275	ILE	3.1
1	1-B	289	PRO	3.1
2	1-F	431	LEU	3.1
1	1-A	173	THR	3.1
2	1-F	135	THR	3.1
2	1-E	286	ALA	3.0
2	1-E	311	TYR	3.0
2	1-F	432	VAL	3.0
1	1-A	252	SER	3.0
1	1-B	56	SER	3.0
1	1-C	372	SER	3.0
2	1-D	306	SER	3.0
1	1-A	507	GLY	3.0
1	1-B	431	GLY	3.0
1	1-A	87	ILE	3.0
2	1-E	362	ILE	3.0
1	1-C	394	LEU	3.0
2	1-D	192	GLU	3.0
1	1-A	464	PHE	3.0
1	1-B	446	TYR	3.0
2	1-D	242	TYR	3.0
1	1-A	169	GLY	3.0
2	1-D	51	GLN	3.0
2	1-D	463	ILE	3.0
2	1-E	244	ARG	3.0
2	1-F	310	ILE	3.0
3	1-G	78	CYS	3.0
2	1-D	351	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	1-D	402	LEU	3.0
1	1-A	386	VAL	3.0
1	1-A	261	GLY	3.0
1	1-A	482	LYS	3.0
1	1-B	167	ILE	3.0
1	1-B	227	LYS	3.0
1	1-C	150	ILE	3.0
1	1-C	206	ILE	3.0
1	1-A	341	ASN	3.0
2	1-D	455	GLN	3.0
1	1-B	166	LEU	3.0
2	1-E	316	ASP	3.0
2	1-F	267	GLU	3.0
1	1-C	485	THR	3.0
1	1-B	437	ALA	3.0
2	1-E	328	HIS	3.0
4	1-H	22	PHE	3.0
2	1-E	300	LYS	3.0
2	1-D	191	ARG	3.0
4	1-H	16	ARG	3.0
1	1-B	352	LEU	3.0
2	1-E	157	GLY	3.0
2	1-F	329	LEU	3.0
2	1-F	428	LEU	3.0
2	1-D	256	ASP	3.0
2	1-E	37	GLU	3.0
1	1-A	52	MET	3.0
1	1-A	223	ALA	3.0
1	1-C	173	THR	3.0
1	1-C	387	ALA	3.0
2	1-D	176	ALA	3.0
2	1-F	240	ALA	3.0
2	1-E	182	VAL	3.0
2	1-F	160	VAL	3.0
1	1-B	175	LYS	2.9
1	1-B	460	LYS	2.9
2	1-E	175	LYS	2.9
3	1-G	14	LYS	2.9
1	1-A	438	ILE	2.9
1	1-B	267	ILE	2.9
2	1-D	357	ILE	2.9
2	1-E	17	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	1-F	252	LEU	2.9
2	1-F	443	GLN	2.9
1	1-C	333	ASP	2.9
2	1-D	31	PRO	2.9
2	1-E	433	PRO	2.9
2	1-D	266	SER	2.9
2	1-F	383	SER	2.9
2	1-D	393	MET	2.9
1	1-C	508	PHE	2.9
2	1-D	251	VAL	2.9
2	1-E	110	THR	2.9
2	1-F	259	PHE	2.9
2	1-E	408	ARG	2.9
1	1-B	150	ILE	2.9
1	1-A	301	LEU	2.9
1	1-B	497	LEU	2.9
2	1-D	281	TYR	2.9
2	1-E	92	GLY	2.9
2	1-E	179	GLY	2.9
1	1-A	465	GLU	2.9
1	1-A	509	GLU	2.9
1	1-B	439	GLU	2.9
1	1-A	63	SER	2.9
1	1-A	141	SER	2.9
1	1-A	269	ASP	2.9
1	1-C	179	ALA	2.9
2	1-D	57	THR	2.9
2	1-D	123	PHE	2.9
2	1-D	140	VAL	2.9
3	1-G	24	LYS	2.9
2	1-D	198	HIS	2.9
1	1-A	242	LEU	2.9
2	1-F	142	LEU	2.9
2	1-F	392	GLY	2.9
1	1-A	186	GLN	2.9
1	1-A	430	GLN	2.9
2	1-F	145	PRO	2.9
2	1-E	168	GLU	2.9
1	1-A	412	ALA	2.9
1	1-A	419	SER	2.9
1	1-B	88	VAL	2.9
1	1-C	298	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	1-E	457	PHE	2.9
1	1-B	485	THR	2.9
1	1-C	362	ARG	2.9
2	1-D	297	THR	2.9
2	1-D	354	THR	2.9
2	1-E	372	ARG	2.9
1	1-B	184	ILE	2.9
2	1-D	152	ILE	2.9
2	1-F	132	ILE	2.9
2	1-D	445	LEU	2.9
1	1-B	147	GLN	2.9
1	1-C	68	PRO	2.9
2	1-D	63	MET	2.9
2	1-D	311	TYR	2.9
2	1-D	462	PRO	2.9
2	1-D	399	GLU	2.9
2	1-E	358	MET	2.9
2	1-D	439	LYS	2.9
1	1-B	181	ASP	2.9
1	1-B	387	ALA	2.9
1	1-C	95	VAL	2.9
1	1-C	411	ASP	2.9
2	1-D	334	VAL	2.9
2	1-D	347	ALA	2.9
2	1-E	363	VAL	2.9
2	1-F	230	ALA	2.9
2	1-F	374	VAL	2.9
1	1-A	357	PHE	2.9
1	1-B	508	PHE	2.9
1	1-C	335	SER	2.9
2	1-D	383	SER	2.9
2	1-D	441	PHE	2.9
2	1-F	418	PHE	2.9
1	1-B	462	THR	2.9
1	1-A	216	LEU	2.9
1	1-A	469	LEU	2.9
1	1-B	361	ILE	2.9
1	1-B	456	LEU	2.9
2	1-D	92	GLY	2.8
2	1-D	280	GLY	2.8
2	1-E	343	GLY	2.8
1	1-C	295	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	1-D	283	PRO	2.8
2	1-E	222	MET	2.8
1	1-C	196	LYS	2.8
2	1-F	209	LYS	2.8
1	1-A	71	VAL	2.8
1	1-A	99	VAL	2.8
2	1-D	307	VAL	2.8
2	1-D	257	ASN	2.8
2	1-E	147	ALA	2.8
1	1-A	44	LEU	2.8
1	1-A	166	LEU	2.8
1	1-B	156	LEU	2.8
1	1-C	87	ILE	2.8
1	1-C	216	LEU	2.8
2	1-D	324	THR	2.8
2	1-E	163	THR	2.8
2	1-E	238	THR	2.8
2	1-E	425	THR	2.8
2	1-F	149	GLY	2.8
2	1-D	30	PRO	2.8
2	1-F	453	PRO	2.8
1	1-C	393	GLU	2.8
1	1-A	268	TYR	2.8
2	1-F	146	TYR	2.8
1	1-B	444	VAL	2.8
2	1-D	240	ALA	2.8
2	1-D	337	ARG	2.8
2	1-F	274	ARG	2.8
2	1-D	457	PHE	2.8
2	1-E	243	PHE	2.8
1	1-C	38	ILE	2.8
1	1-C	159	ILE	2.8
2	1-E	143	LEU	2.8
2	1-F	402	LEU	2.8
1	1-A	322	THR	2.8
1	1-C	272	SER	2.8
2	1-E	262	THR	2.8
2	1-F	157	GLY	2.8
4	1-H	31	GLU	2.8
1	1-B	234	ALA	2.8
1	1-C	133	ALA	2.8
2	1-E	418	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	1-A	267	ILE	2.8
1	1-B	113	ASN	2.8
1	1-B	36	ASP	2.8
2	1-E	306	SER	2.8
1	1-B	383	MET	2.8
2	1-D	65	GLY	2.8
1	1-C	280	GLN	2.8
2	1-F	27	GLU	2.8
3	1-G	254	ARG	2.8
2	1-D	16	VAL	2.8
1	1-B	378	ALA	2.8
2	1-D	321	ALA	2.8
2	1-E	281	TYR	2.8
3	1-G	235	ALA	2.8
1	1-A	453	LEU	2.8
1	1-C	271	LEU	2.8
1	1-B	476	HIS	2.8
1	1-A	28	THR	2.8
1	1-A	96	ASP	2.8
1	1-C	262	LYS	2.8
2	1-E	130	GLN	2.7
1	1-A	307	GLU	2.7
2	1-D	448	GLU	2.7
2	1-F	247	GLU	2.7
1	1-A	298	VAL	2.7
2	1-D	23	VAL	2.7
2	1-E	97	VAL	2.7
2	1-E	140	VAL	2.7
1	1-C	437	ALA	2.7
1	1-B	200	TYR	2.7
2	1-E	201	ILE	2.7
2	1-E	402	LEU	2.7
2	1-F	384	LEU	2.7
2	1-F	117	HIS	2.7
1	1-A	36	ASP	2.7
1	1-B	24	ASP	2.7
1	1-B	176	THR	2.7
2	1-E	26	ASP	2.7
2	1-D	12	ARG	2.7
2	1-D	260	ARG	2.7
1	1-A	355	GLU	2.7
2	1-F	399	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	1-F	464	GLU	2.7
2	1-D	370	VAL	2.7
2	1-E	186	VAL	2.7
2	1-E	423	VAL	2.7
1	1-B	467	ALA	2.7
2	1-D	410	ILE	2.7
2	1-D	459	MET	2.7
1	1-B	35	GLY	2.7
1	1-C	194	ASP	2.7
1	1-C	270	ASP	2.7
1	1-C	247	PRO	2.7
1	1-B	282	SER	2.7
1	1-C	484	ARG	2.7
1	1-C	432	GLN	2.7
1	1-B	465	GLU	2.7
1	1-C	328	GLU	2.7
2	1-F	134	VAL	2.7
1	1-A	277	ALA	2.7
1	1-A	401	ALA	2.7
1	1-B	324	LEU	2.7
1	1-C	205	ALA	2.7
1	1-C	402	ALA	2.7
2	1-D	15	ALA	2.7
2	1-D	418	PHE	2.7
2	1-E	19	ALA	2.7
2	1-E	53	LEU	2.7
1	1-A	209	LYS	2.7
2	1-E	209	LYS	2.7
2	1-D	477	HIS	2.7
2	1-E	289	MET	2.7
1	1-B	46	ASN	2.7
1	1-B	171	ARG	2.7
1	1-B	291	ARG	2.7
2	1-D	18	GLY	2.7
2	1-D	59	ARG	2.7
2	1-D	135	THR	2.7
2	1-E	223	ASN	2.7
1	1-A	224	ASP	2.7
1	1-B	295	PRO	2.7
2	1-E	16	VAL	2.7
2	1-E	70	VAL	2.7
2	1-E	199	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	1-F	308	GLN	2.7
2	1-F	355	SER	2.7
1	1-A	74	VAL	2.7
1	1-A	501	VAL	2.7
2	1-D	75	VAL	2.7
1	1-C	168	ILE	2.7
2	1-E	317	LEU	2.7
1	1-C	264	ALA	2.7
2	1-E	35	ALA	2.7
2	1-F	166	ILE	2.7
2	1-F	270	ALA	2.7
1	1-A	244	TYR	2.7
1	1-C	143	ARG	2.7
2	1-E	44	ARG	2.7
1	1-B	58	GLY	2.7
2	1-D	88	PRO	2.7
2	1-E	320	PRO	2.7
2	1-F	462	PRO	2.7
1	1-A	270	ASP	2.7
2	1-E	394	ASP	2.7
1	1-A	195	GLU	2.7
1	1-A	334	VAL	2.7
1	1-A	440	GLU	2.7
1	1-B	231	VAL	2.7
1	1-C	355	GLU	2.7
1	1-C	457	GLU	2.7
1	1-C	509	GLU	2.7
2	1-F	419	GLN	2.7
3	1-G	255	GLN	2.7
3	1-G	85	VAL	2.7
1	1-B	370	SER	2.7
1	1-A	89	LYS	2.6
1	1-A	429	LYS	2.6
1	1-B	124	LYS	2.6
1	1-C	82	ILE	2.6
2	1-E	396	LEU	2.7
2	1-F	362	ILE	2.6
1	1-B	495	ALA	2.6
1	1-C	504	PHE	2.6
2	1-D	243	PHE	2.6
2	1-D	389	ALA	2.6
2	1-D	468	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	1-G	86	ALA	2.6
2	1-E	458	TYR	2.6
1	1-A	164	ARG	2.6
1	1-C	149	GLY	2.6
2	1-D	453	PRO	2.6
1	1-A	142	VAL	2.6
1	1-A	259	ASP	2.6
1	1-A	324	LEU	2.6
2	1-D	14	VAL	2.6
2	1-D	366	GLU	2.6
2	1-F	128	VAL	2.6
1	1-C	180	ILE	2.6
2	1-D	108	ILE	2.6
2	1-D	390	ILE	2.6
1	1-A	226	MET	2.6
1	1-B	364	ALA	2.6
1	1-C	233	SER	2.6
2	1-E	62	ALA	2.6
2	1-E	405	SER	2.6
1	1-B	40	ARG	2.6
1	1-C	291	ARG	2.6
2	1-E	295	ARG	2.6
1	1-C	363	PRO	2.6
2	1-D	10	THR	2.6
1	1-C	410	LEU	2.6
2	1-D	217	LEU	2.6
2	1-F	207	ASN	2.6
1	1-A	415	GLN	2.6
1	1-B	280	GLN	2.6
2	1-F	404	VAL	2.6
2	1-E	170	ILE	2.6
2	1-E	275	ILE	2.6
1	1-B	264	ALA	2.6
1	1-A	33	SER	2.6
1	1-B	376	SER	2.6
2	1-F	328	HIS	2.6
1	1-A	262	LYS	2.6
1	1-C	166	LEU	2.6
2	1-D	170	ILE	2.6
1	1-B	330	GLN	2.6
2	1-D	188	GLU	2.6
1	1-A	409	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	1-C	476	HIS	2.6
2	1-F	269	SER	2.6
2	1-F	356	ARG	2.6
2	1-D	214	LYS	2.6
2	1-D	225	PRO	2.6
2	1-E	138	LYS	2.6
1	1-A	360	GLY	2.6
2	1-E	302	GLY	2.6
2	1-E	313	PRO	2.6
2	1-D	21	VAL	2.6
2	1-D	166	ILE	2.6
2	1-E	124	VAL	2.6
2	1-F	108	ILE	2.6
1	1-C	165	GLU	2.6
1	1-C	236	ALA	2.6
3	1-G	28	ALA	2.6
2	1-F	451	HIS	2.5
3	1-G	252	ARG	2.5
1	1-A	57	SER	2.5
1	1-B	155	SER	2.5
1	1-A	197	LYS	2.5
2	1-E	401	LYS	2.5
2	1-E	273	GLY	2.5
2	1-F	107	PRO	2.5
2	1-D	47	LEU	2.5
1	1-C	178	ILE	2.5
2	1-D	205	VAL	2.5
2	1-D	312	VAL	2.5
2	1-F	357	ILE	2.5
2	1-E	294	GLU	2.5
1	1-A	189	PHE	2.5
3	1-G	270	ALA	2.5
1	1-A	219	ARG	2.5
2	1-D	349	ASP	2.5
1	1-A	488	LYS	2.5
1	1-C	488	LYS	2.5
2	1-D	382	LYS	2.5
4	1-H	39	LYS	2.5
1	1-A	120	PRO	2.5
1	1-A	431	GLY	2.5
2	1-D	461	GLY	2.5
3	1-G	10	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-B	206	ILE	2.5
1	1-B	445	ILE	2.5
2	1-D	126	MET	2.5
2	1-E	268	VAL	2.5
2	1-E	339	ILE	2.5
1	1-A	278	TYR	2.5
1	1-B	294	TYR	2.5
2	1-D	202	GLU	2.5
2	1-E	247	GLU	2.5
4	1-H	40	GLU	2.5
2	1-D	112	GLN	2.5
3	1-G	240	SER	2.5
1	1-B	146	MET	2.5
1	1-B	392	LEU	2.5
2	1-D	95	MET	2.5
2	1-D	378	LEU	2.5
2	1-E	107	PRO	2.5
2	1-E	145	PRO	2.5
2	1-E	459	MET	2.5
2	1-F	317	LEU	2.5
1	1-B	38	ILE	2.5
2	1-E	206	ILE	2.5
2	1-F	343	GLY	2.5
1	1-A	422	VAL	2.5
1	1-C	97	VAL	2.5
2	1-F	449	TYR	2.5
1	1-A	101	GLU	2.5
1	1-B	464	PHE	2.5
1	1-B	504	PHE	2.5
2	1-D	27	GLU	2.5
1	1-A	179	ALA	2.5
1	1-A	215	GLN	2.5
2	1-E	123	PHE	2.5
2	1-E	413	PHE	2.5
2	1-F	51	GLN	2.5
1	1-A	463	LYS	2.5
2	1-E	361	ASN	2.5
2	1-F	257	ASN	2.5
2	1-E	64	ASP	2.5
1	1-A	66	LEU	2.5
1	1-C	324	LEU	2.5
1	1-A	325	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	77	GLY	2.5
1	1-A	343	ILE	2.5
1	1-A	407	GLY	2.5
1	1-B	320	SER	2.5
1	1-C	211	SER	2.5
2	1-D	101	PRO	2.5
1	1-C	348	GLY	2.5
1	1-C	434	SER	2.5
2	1-F	373	GLY	2.5
4	1-H	19	GLY	2.5
2	1-D	49	VAL	2.5
1	1-A	328	GLU	2.5
1	1-C	203	TYR	2.5
1	1-A	188	ARG	2.5
1	1-B	287	ARG	2.5
1	1-B	148	THR	2.5
1	1-C	148	THR	2.5
2	1-E	278	ALA	2.5
2	1-F	9	THR	2.5
3	1-G	249	THR	2.5
1	1-A	62	MET	2.4
1	1-A	306	LEU	2.4
2	1-D	319	ASP	2.4
2	1-D	339	ILE	2.4
1	1-A	157	VAL	2.4
2	1-E	128	VAL	2.4
1	1-A	393	GLU	2.4
1	1-C	101	GLU	2.4
2	1-E	441	PHE	2.4
1	1-A	118	LYS	2.4
1	1-B	293	ALA	2.4
1	1-C	132	LYS	2.4
1	1-C	382	ALA	2.4
2	1-F	430	LYS	2.4
1	1-C	81	LEU	2.4
1	1-B	247	PRO	2.4
1	1-A	204	VAL	2.4
1	1-C	360	GLY	2.4
1	1-A	362	ARG	2.4
1	1-B	219	ARG	2.4
1	1-B	420	ARG	2.4
1	1-C	56	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	1-D	175	LYS	2.4
2	1-E	301	LYS	2.4
1	1-B	208	GLN	2.4
1	1-B	240	ALA	2.4
1	1-C	172	GLN	2.4
1	1-C	413	ALA	2.4
1	1-A	485	THR	2.4
2	1-E	325	THR	2.4
1	1-C	305	LEU	2.4
1	1-C	356	LEU	2.4
2	1-E	272	LEU	2.4
1	1-B	120	PRO	2.4
1	1-C	105	GLY	2.4
2	1-D	20	VAL	2.4
2	1-D	87	GLY	2.4
2	1-E	307	VAL	2.4
1	1-B	482	LYS	2.4
1	1-C	151	LYS	2.4
1	1-C	463	LYS	2.4
2	1-D	109	LYS	2.4
1	1-A	372	SER	2.4
1	1-A	399	GLU	2.4
1	1-B	54	GLU	2.4
1	1-C	440	GLU	2.4
2	1-F	123	PHE	2.4
3	1-G	223	SER	2.4
4	1-H	26	GLU	2.4
1	1-C	467	ALA	2.4
1	1-C	478	ALA	2.4
4	1-H	12	ALA	2.4
2	1-E	263	GLN	2.4
1	1-A	248	TYR	2.4
1	1-C	414	THR	2.4
2	1-E	324	THR	2.4
2	1-F	29	LEU	2.4
1	1-B	168	ILE	2.4
1	1-A	98	PRO	2.4
1	1-C	313	ASN	2.4
1	1-A	213	VAL	2.4
1	1-C	296	GLY	2.4
2	1-D	426	GLY	2.4
2	1-E	150	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	1-E	204	GLY	2.4
2	1-F	173	VAL	2.4
2	1-F	232	VAL	2.4
2	1-F	429	GLY	2.4
1	1-B	491	GLU	2.4
3	1-G	264	GLU	2.4
2	1-D	167	MET	2.4
2	1-F	292	MET	2.4
2	1-F	332	THR	2.4
2	1-E	29	LEU	2.4
1	1-A	445	ILE	2.4
2	1-D	360	PRO	2.4
1	1-A	190	ASN	2.3
1	1-B	362	ARG	2.3
1	1-C	374	VAL	2.3
2	1-D	97	VAL	2.3
2	1-E	173	VAL	2.3
2	1-F	215	VAL	2.3
1	1-A	454	ASP	2.3
1	1-B	69	ASP	2.3
2	1-D	259	PHE	2.3
2	1-E	359	ASP	2.3
1	1-B	179	ALA	2.3
1	1-B	205	ALA	2.3
1	1-B	163	GLN	2.3
1	1-B	432	GLN	2.3
1	1-C	475	GLN	2.3
2	1-D	379	GLN	2.3
2	1-E	282	GLN	2.3
1	1-B	226	MET	2.3
1	1-B	390	MET	2.3
2	1-D	358	MET	2.3
2	1-F	306	SER	2.3
1	1-B	173	THR	2.3
2	1-D	234	LEU	2.3
2	1-D	318	THR	2.3
1	1-B	180	ILE	2.3
2	1-D	82	ILE	2.3
1	1-B	442	VAL	2.3
1	1-C	444	VAL	2.3
1	1-C	472	VAL	2.3
2	1-D	44	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	1-D	412	ARG	2.3
2	1-F	279	VAL	2.3
1	1-C	388	GLY	2.3
1	1-B	333	ASP	2.3
2	1-E	67	GLU	2.3
2	1-E	103	ASP	2.3
2	1-E	454	GLU	2.3
2	1-F	394	ASP	2.3
1	1-B	506	ALA	2.3
2	1-D	446	ALA	2.3
2	1-F	233	ALA	2.3
2	1-D	263	GLN	2.3
1	1-A	356	LEU	2.3
2	1-D	262	THR	2.3
2	1-D	325	THR	2.3
2	1-E	296	ILE	2.3
1	1-A	80	LYS	2.3
1	1-A	484	ARG	2.3
1	1-B	373	ARG	2.3
2	1-F	101	PRO	2.3
1	1-B	334	VAL	2.3
2	1-E	280	GLY	2.3
2	1-F	364	GLY	2.3
2	1-E	34	ASN	2.3
2	1-D	278	ALA	2.3
2	1-E	267	GLU	2.3
2	1-F	100	GLU	2.3
1	1-C	390	MET	2.3
2	1-E	77	ASP	2.3
1	1-B	64	LEU	2.3
2	1-E	45	LEU	2.3
2	1-E	117	HIS	2.3
2	1-E	451	HIS	2.3
2	1-D	336	SER	2.3
2	1-E	203	SER	2.3
2	1-F	181	SER	2.3
2	1-F	397	SER	2.3
2	1-F	10	THR	2.3
1	1-C	99	VAL	2.3
1	1-C	501	VAL	2.3
1	1-B	290	GLY	2.3
2	1-E	63	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	1-E	125	GLU	2.3
2	1-E	192	GLU	2.3
2	1-E	422	GLU	2.3
1	1-A	32	LEU	2.3
1	1-A	199	LEU	2.3
1	1-A	379	GLN	2.3
1	1-C	505	LEU	2.3
1	1-B	198	LYS	2.3
1	1-A	137	ILE	2.3
1	1-A	140	ILE	2.3
1	1-A	193	THR	2.3
1	1-B	28	THR	2.3
1	1-C	188	ARG	2.3
1	1-A	31	VAL	2.3
1	1-C	142	VAL	2.3
2	1-D	423	VAL	2.3
2	1-D	236	GLY	2.3
2	1-E	99	GLY	2.3
2	1-F	326	PHE	2.2
1	1-B	478	ALA	2.2
1	1-C	65	ASN	2.2
1	1-C	78	ASN	2.2
2	1-D	89	GLU	2.2
1	1-A	305	LEU	2.2
1	1-B	453	LEU	2.2
1	1-C	497	LEU	2.2
1	1-A	349	GLN	2.2
1	1-B	384	LYS	2.2
2	1-D	73	GLN	2.2
2	1-F	246	GLN	2.2
2	1-D	471	ASP	2.2
1	1-A	178	ILE	2.2
1	1-B	34	ILE	2.2
2	1-E	61	ILE	2.2
2	1-E	438	ILE	2.2
2	1-F	170	ILE	2.2
3	1-G	263	ILE	2.2
1	1-A	263	HIS	2.2
1	1-B	188	ARG	2.2
2	1-D	403	THR	2.2
1	1-C	177	SER	2.2
1	1-C	337	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	105	GLY	2.2
1	1-A	122	GLY	2.2
1	1-A	348	GLY	2.2
1	1-C	332	GLY	2.2
2	1-D	150	GLY	2.2
1	1-A	404	ALA	2.2
1	1-B	283	LEU	2.2
2	1-D	69	LEU	2.2
2	1-D	129	GLU	2.2
2	1-D	428	LEU	2.2
2	1-E	89	GLU	2.2
2	1-E	109	LYS	2.2
1	1-B	441	GLN	2.2
1	1-C	338	ILE	2.2
2	1-D	26	ASP	2.2
2	1-E	250	ASP	2.2
2	1-F	315	ASP	2.2
1	1-A	380	THR	2.2
1	1-C	153	VAL	2.2
1	1-C	182	THR	2.2
2	1-D	186	VAL	2.2
2	1-D	291	THR	2.2
2	1-D	313	PRO	2.2
2	1-F	283	PRO	2.2
1	1-A	452	TYR	2.2
1	1-A	470	SER	2.2
1	1-A	296	GLY	2.2
2	1-E	193	GLY	2.2
2	1-F	28	GLY	2.2
2	1-F	161	GLY	2.2
2	1-D	155	PHE	2.2
2	1-E	261	PHE	2.2
1	1-B	66	LEU	2.2
1	1-C	275	ALA	2.2
1	1-C	284	LEU	2.2
2	1-D	62	ALA	2.2
2	1-D	421	ALA	2.2
2	1-E	196	LEU	2.2
2	1-E	264	ALA	2.2
2	1-F	396	LEU	2.2
1	1-A	405	GLN	2.2
2	1-D	93	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	1-E	274	ARG	2.2
2	1-F	339	ILE	2.2
1	1-B	411	ASP	2.2
1	1-C	442	VAL	2.2
2	1-D	226	PRO	2.2
1	1-C	462	THR	2.2
2	1-D	332	THR	2.2
1	1-C	317	GLY	2.2
2	1-E	185	GLY	2.2
1	1-A	299	PHE	2.2
2	1-E	151	LYS	2.2
2	1-E	183	PHE	2.2
1	1-B	492	GLU	2.2
2	1-E	50	ALA	2.2
1	1-C	30	ARG	2.2
2	1-E	198	HIS	2.2
1	1-B	326	VAL	2.2
2	1-D	276	PRO	2.2
1	1-B	281	MET	2.2
2	1-D	60	THR	2.2
2	1-E	200	MET	2.2
2	1-D	74	LYS	2.2
1	1-A	358	TYR	2.2
1	1-B	278	TYR	2.2
1	1-C	155	SER	2.2
1	1-C	352	LEU	2.2
1	1-B	152	ALA	2.2
1	1-B	509	GLU	2.2
2	1-E	241	GLU	2.2
2	1-F	131	GLU	2.2
2	1-F	436	GLU	2.2
1	1-A	40	ARG	2.1
1	1-B	266	ILE	2.1
1	1-C	127	ARG	2.1
2	1-D	451	HIS	2.1
2	1-F	177	HIS	2.1
3	1-G	234	ASN	2.1
2	1-D	145	PRO	2.1
2	1-F	307	VAL	2.1
2	1-F	420	VAL	2.1
1	1-A	181	ASP	2.1
1	1-C	146	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	1-D	77	ASP	2.1
2	1-D	330	ASP	2.1
1	1-A	43	GLY	2.1
1	1-A	502	THR	2.1
1	1-C	176	THR	2.1
2	1-E	76	LEU	2.1
2	1-D	470	ALA	2.1
2	1-E	202	GLU	2.1
2	1-E	395	GLU	2.1
2	1-E	108	ILE	2.1
2	1-F	152	ILE	2.1
1	1-A	441	GLN	2.1
1	1-B	430	GLN	2.1
1	1-A	260	ASN	2.1
1	1-B	78	ASN	2.1
2	1-D	128	VAL	2.1
2	1-E	30	PRO	2.1
2	1-F	348	VAL	2.1
1	1-A	273	LYS	2.1
1	1-A	170	ASP	2.1
2	1-D	210	ASP	2.1
2	1-D	288	ASP	2.1
2	1-D	352	ASP	2.1
2	1-D	394	ASP	2.1
1	1-C	174	GLY	2.1
2	1-E	156	GLY	2.1
2	1-F	156	GLY	2.1
2	1-F	284	THR	2.1
2	1-F	425	THR	2.1
2	1-F	437	THR	2.1
1	1-A	128	ARG	2.1
1	1-C	373	ARG	2.1
2	1-E	345	TYR	2.1
1	1-A	320	SER	2.1
1	1-B	237	SER	2.1
1	1-C	195	GLU	2.1
2	1-E	119	GLU	2.1
2	1-F	102	ILE	2.1
2	1-F	168	GLU	2.1
2	1-F	405	SER	2.1
3	1-G	12	SER	2.1
1	1-B	107	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	298	VAL	2.1
1	1-B	498	LYS	2.1
1	1-C	449	VAL	2.1
2	1-D	223	ASN	2.1
2	1-E	334	VAL	2.1
1	1-C	134	PRO	2.1
2	1-E	472	LYS	2.1
3	1-G	245	LYS	2.1
1	1-A	81	LEU	2.1
1	1-A	222	ASP	2.1
1	1-B	149	GLY	2.1
1	1-C	181	ASP	2.1
2	1-D	237	LEU	2.1
2	1-F	236	GLY	2.1
1	1-C	229	THR	2.1
2	1-D	25	PHE	2.1
2	1-E	43	THR	2.1
2	1-F	352	ASP	2.1
3	1-G	5	ASP	2.1
1	1-C	304	ARG	2.1
2	1-D	408	ARG	2.1
1	1-A	150	ILE	2.1
1	1-C	114	ALA	2.1
1	1-C	125	ALA	2.1
1	1-C	50	GLU	2.1
1	1-C	183	ILE	2.1
1	1-C	401	ALA	2.1
2	1-D	323	ALA	2.1
1	1-C	426	GLU	2.1
1	1-C	123	SER	2.1
2	1-E	112	GLN	2.1
2	1-E	308	GLN	2.1
2	1-F	112	GLN	2.1
2	1-E	292	MET	2.1
1	1-A	53	VAL	2.1
1	1-B	232	VAL	2.1
2	1-E	279	VAL	2.1
2	1-F	182	VAL	2.1
2	1-E	88	PRO	2.1
2	1-E	101	PRO	2.1
1	1-B	131	LEU	2.1
1	1-A	192	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-C	61	GLY	2.1
2	1-F	113	PHE	2.1
1	1-B	154	ASP	2.1
1	1-B	182	THR	2.1
2	1-F	210	ASP	2.1
2	1-F	238	THR	2.1
4	1-H	35	ARG	2.1
1	1-A	183	ILE	2.1
1	1-B	350	ILE	2.1
1	1-C	234	ALA	2.1
1	1-C	343	ILE	2.1
2	1-D	340	ALA	2.1
2	1-E	347	ALA	2.1
2	1-E	446	ALA	2.1
2	1-E	456	ALA	2.1
1	1-A	457	GLU	2.1
1	1-B	355	GLU	2.1
1	1-A	376	SER	2.0
1	1-B	196	LYS	2.0
1	1-B	416	GLN	2.0
1	1-C	201	CYS	2.0
2	1-E	469	LYS	2.0
1	1-A	442	VAL	2.0
1	1-B	501	VAL	2.0
2	1-E	121	PRO	2.0
1	1-A	318	GLY	2.0
2	1-E	153	GLY	2.0
2	1-F	457	PHE	2.0
1	1-A	115	ILE	2.0
1	1-A	461	ILE	2.0
1	1-B	502	THR	2.0
1	1-C	246	ALA	2.0
2	1-D	456	ALA	2.0
2	1-E	369	ASP	2.0
2	1-F	380	ASP	2.0
3	1-G	80	ALA	2.0
1	1-A	255	GLU	2.0
2	1-D	100	GLU	2.0
2	1-F	199	GLU	2.0
2	1-F	109	LYS	2.0
2	1-F	458	TYR	2.0
2	1-D	289	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	471	HIS	2.0
2	1-D	58	VAL	2.0
2	1-F	442	GLN	2.0
3	1-G	83	SER	2.0
1	1-A	288	PRO	2.0
1	1-C	480	LEU	2.0
2	1-D	295	ARG	2.0
2	1-D	68	GLY	2.0
2	1-E	236	GLY	2.0
2	1-F	447	GLY	2.0
1	1-A	184	ILE	2.0
2	1-D	13	ILE	2.0
1	1-B	414	THR	2.0
1	1-C	323	ALA	2.0
3	1-G	7	THR	2.0
1	1-A	83	LYS	2.0
1	1-A	84	GLU	2.0
1	1-B	86	ASP	2.0
2	1-E	315	ASP	2.0
1	1-A	496	LYS	2.0
3	1-G	224	GLU	2.0
1	1-C	383	MET	2.0
1	1-B	397	TYR	2.0
2	1-D	70	VAL	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](#)

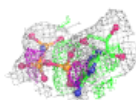
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	MG	1-B	1512	1/1	0.38	0.22	57,57,57,57	1
5	ANP	2-A	1511	31/31	-	-	40,59,70,76	31
6	MG	1-C	1512	1/1	0.72	0.17	46,46,46,46	1
5	ANP	2-B	1511	31/31	-	-	40,54,61,67	31
6	MG	1-A	1512	1/1	0.76	0.10	39,39,39,39	1
5	ANP	2-C	1511	31/31	-	-	36,64,75,78	31
5	ANP	1-C	1511	31/31	0.76	0.20	29,44,58,62	31
5	ANP	2-D	1478	31/31	-	-	39,48,56,58	31
5	ANP	1-D	1478	31/31	0.76	0.18	40,54,62,62	31
5	ANP	2-F	1478	31/31	-	-	49,69,75,79	31
5	ANP	1-B	1511	31/31	0.81	0.17	41,68,80,81	31
6	MG	2-A	1512	1/1	-	-	41,41,41,41	1
5	ANP	1-A	1511	31/31	0.82	0.15	39,57,65,70	31
6	MG	2-B	1512	1/1	-	-	45,45,45,45	1
6	MG	1-D	1479	1/1	0.83	0.20	60,60,60,60	1
6	MG	2-C	1512	1/1	-	-	44,44,44,44	1
5	ANP	1-F	1478	31/31	0.85	0.13	33,52,59,61	31
6	MG	2-D	1479	1/1	-	-	47,47,47,47	1
6	MG	1-F	1479	1/1	0.85	0.12	44,44,44,44	1
6	MG	2-F	1479	1/1	-	-	62,62,62,62	1

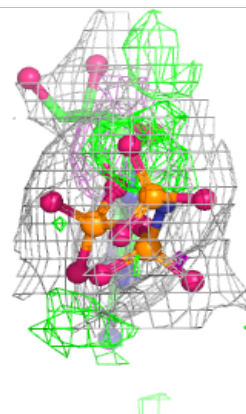
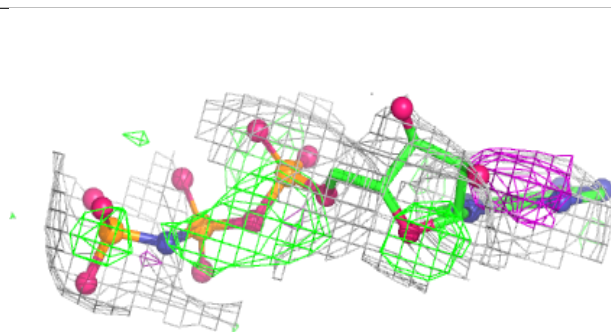
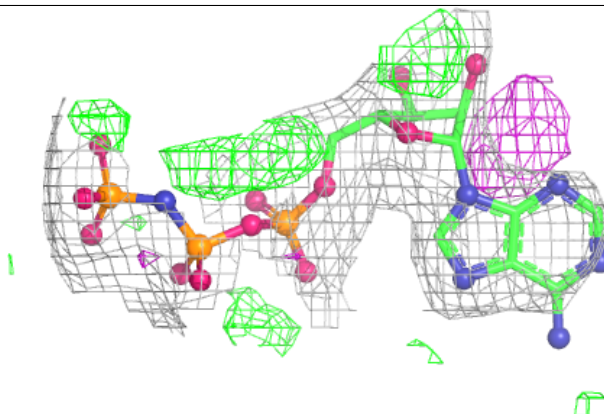
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP 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)

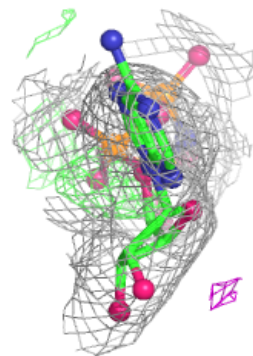
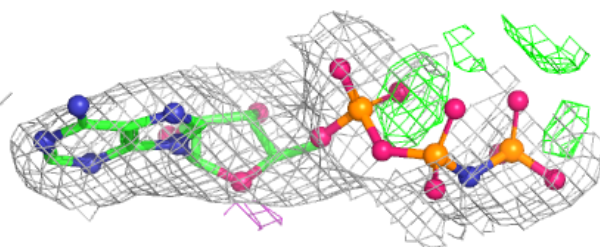
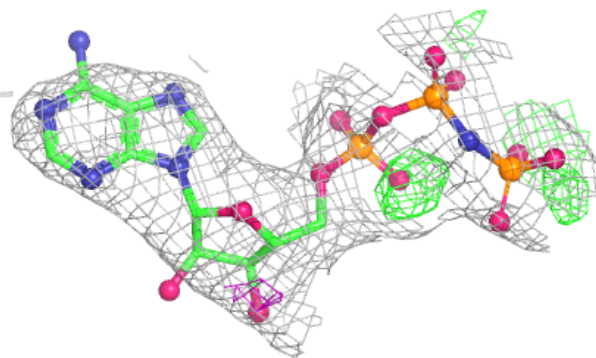
**Electron density around ANP D 1478:**

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

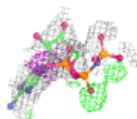
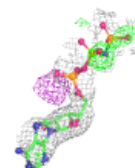


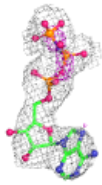
Electron density around ANP B 1511:

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

**Electron density around ANP A 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 1478: 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.