



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 AM UTC

PDB ID : 3B5Y / pdb_00003b5y
Title : Crystal Structure of MsbA from Salmonella typhimurium with AMPPNP
Authors : Ward, A.; Reyes, C.L.; Yu, J.; Roth, C.B.; Chang, G.
Deposited on : 2007-10-26
Resolution : 4.50 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

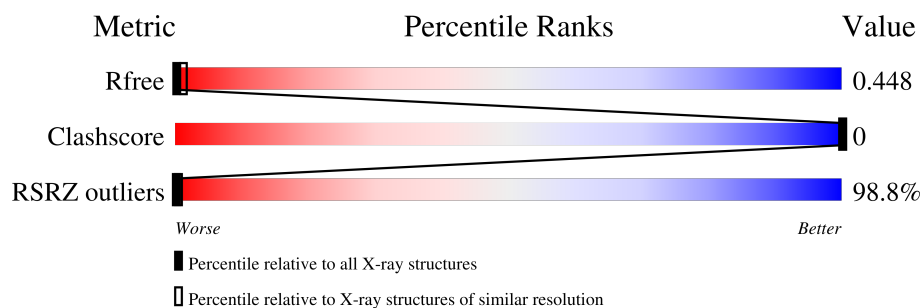
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
RSRZ outliers	180081	1122 (5.10-3.90)

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	582	97%  98%
1	B	582	97%  98%
1	C	582	97%  98%
1	D	582	97%  98%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ANP	A	5002	-	-	-	X
2	ANP	B	5001	-	-	-	X
2	ANP	D	5003	-	-	-	X

2 Entry composition ⓘ

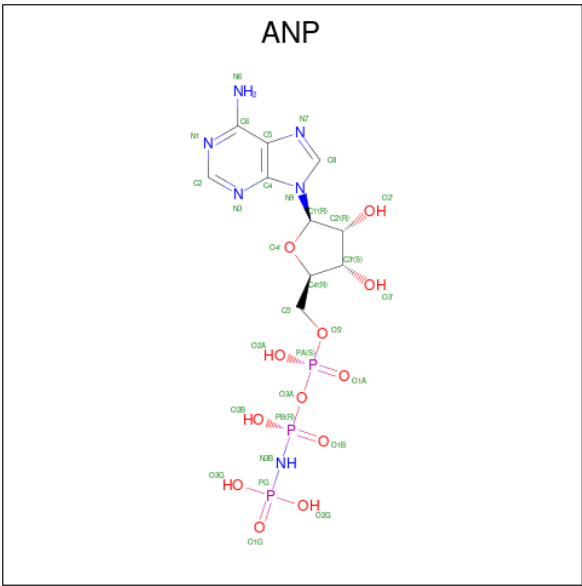
There are 2 unique types of molecules in this entry. The entry contains 2412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lipid A export ATP-binding/permease protein msbA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	572	Total	C	0	0	572
			572	572			
1	B	572	Total	C	0	0	572
			572	572			
1	C	572	Total	C	0	0	572
			572	572			
1	D	572	Total	C	0	0	572
			572	572			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

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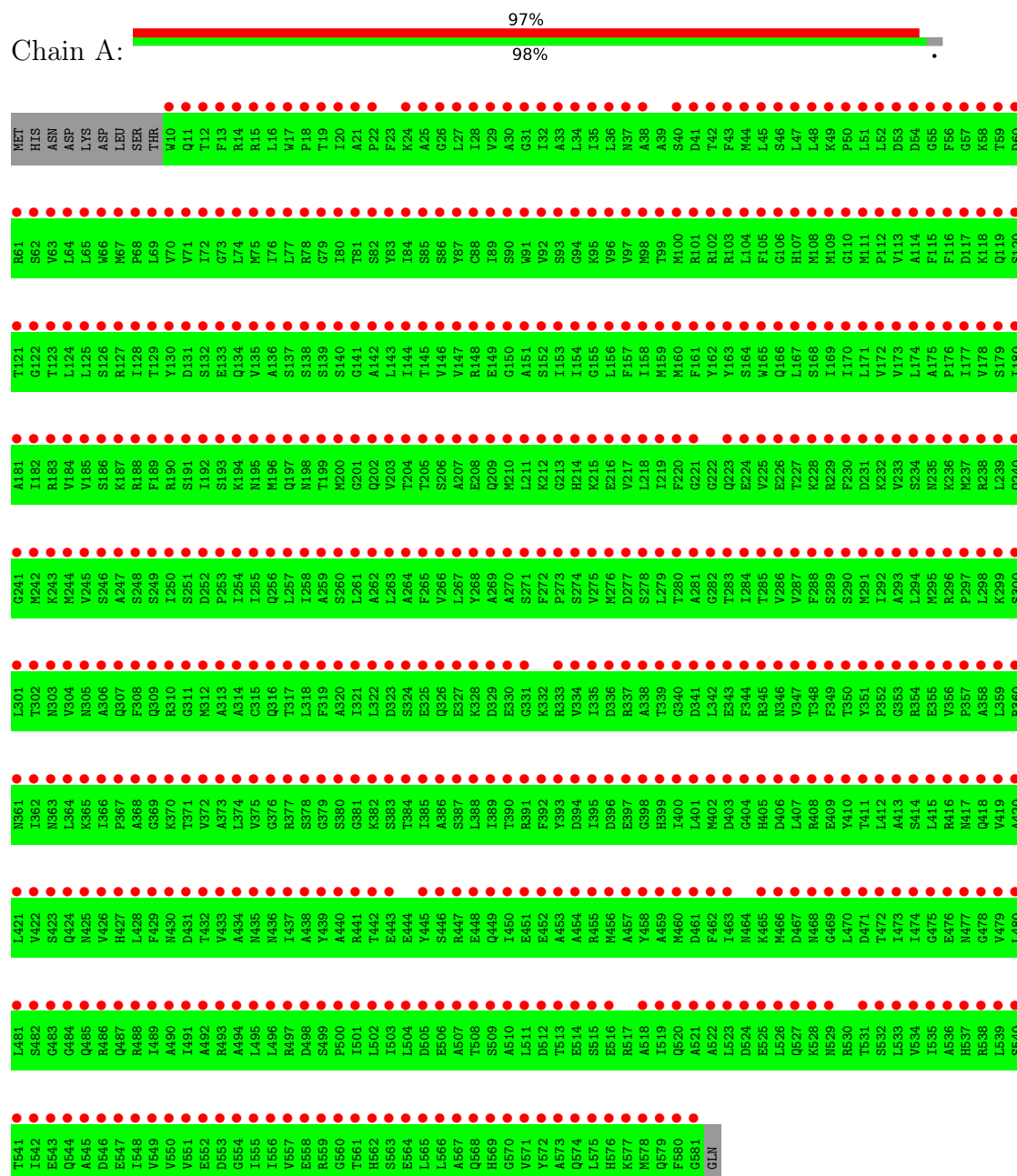
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

3 Residue-property plots

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

- Molecule 1: Lipid A export ATP-binding/permease protein msbA



● Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain B:



T541	I542	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	D498	S499	P500	I501	L502	S503	E504	L505	D506	E507	T508	S509	A510	L511	D512	T513	E514	S515	E516	R517	A518	I519	Q520	A521	A522	L523	D524	E525	L526	Q527	K528	N529	R530	T531	S532	L533	V534	I535	A536	H537	R538	L539	S540
I541	L542	S482	S483	G483	G484	Q485	R486	Q487	R488	I489	A490	I491	A492	R493	A494	L495	L496	R497	D498	S499	P500	I501	L502	S503	E504	L505	D506	E507	T508	S509	A510	L511	D512	T513	E514	S515	E516	R517	A518	I519	Q520	A521	A522	L523	D524	E525	L526	Q527	K528	N529	R530	T531	S532	L533	V534	I535	A536	H537	R538	L539	S540
V421	V422	S423	Q424	Q425	V426	H427	L428	F429	M430	D431	T432	V433	A434	M435	M436	I437	A438	Y439	A440	R441	T442	E443	E444	Y445	S446	R447	E448	Q449	I450	E451	E452	A453	A454	R455	M456	A457	Y458	A459	M460	D461	F462	I463	M464	K465	M466	D467	M468	G469	L470	D471	T472	I473	I474	G475	E476	M477	G478	V479	A480		
N361	I362	R363	L364	K365	I366	P367	A368	G369	K370	T371	V372	A373	L374	V375	G376	R377	S378	G379	S380	G381	K382	S383	T384	I385	A386	S387	L388	I389	T390	R391	P392	Y393	D394	I395	D396	E397	G398	H399	I400	L401	M402	P403	D404	H405	D406	L407	R408	E409	Y410	T411	L412	A413	S414	L415	R416	M417	Q418	V419	A420		
L301	T302	R303	V304	R305	A306	Q307	F308	Q309	R310	G311	M312	A313	A314	C315	Q316	T317	L318	F319	A320	I321	L322	D323	S324	E325	Q326	E327	K328	D329	E330	G331	K332	R333	V334	I335	D336	R337	A338	T339	G340	D341	L342	E343	F344	R345	R346	V347	T348	F349	T350	Y351	P352	G353	R354	E355	V356	P357	A358	L359	R360		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.93Å 121.24Å 173.12Å 90.00° 121.89° 90.00°	Depositor
Resolution (Å)	19.98 – 4.50 19.98 – 4.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (19.98-4.50) 93.8 (19.98-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 4.54Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.295 , 0.343 0.447 , 0.448	Depositor DCC
R_{free} test set	2606 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	184.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	170.07 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	2412	wwPDB-VP
Average B, all atoms (Å ²)	219.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	572	0	0	0	0
1	B	572	0	0	0	0
1	C	572	0	0	0	0
1	D	572	0	0	0	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
All	All	2412	0	52	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 [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ANP	C	5004	-	33,33,33	1.53	5 (15%)	45,52,52	1.84	10 (22%)
2	ANP	D	5003	-	33,33,33	1.53	5 (15%)	45,52,52	1.83	10 (22%)
2	ANP	A	5002	-	33,33,33	1.52	5 (15%)	45,52,52	1.83	10 (22%)
2	ANP	B	5001	-	33,33,33	2.67	15 (45%)	45,52,52	2.10	10 (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
2	ANP	C	5004	-	-	3/18/38/38	0/3/3/3
2	ANP	D	5003	-	-	3/18/38/38	0/3/3/3
2	ANP	A	5002	-	-	3/18/38/38	0/3/3/3
2	ANP	B	5001	-	-	3/18/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	PA-O3A	7.55	1.67	1.59
2	B	5001	ANP	PB-O1B	-5.13	1.38	1.46
2	B	5001	ANP	PB-O2B	-4.49	1.44	1.56
2	B	5001	ANP	PA-O1A	-4.48	1.35	1.50
2	C	5004	ANP	PB-O2B	-4.04	1.46	1.56
2	A	5002	ANP	PB-O2B	-3.98	1.46	1.56
2	B	5001	ANP	C4-N9	3.96	1.45	1.37
2	D	5003	ANP	PB-O2B	-3.96	1.46	1.56
2	C	5004	ANP	PG-O2G	-3.68	1.47	1.56
2	D	5003	ANP	PG-O2G	-3.64	1.47	1.56
2	A	5002	ANP	PG-O2G	-3.63	1.47	1.56
2	B	5001	ANP	C3'-C4'	-3.50	1.44	1.53
2	B	5001	ANP	C8-N9	3.37	1.43	1.37
2	B	5001	ANP	C1'-N9	3.34	1.55	1.46
2	B	5001	ANP	C8-N7	3.16	1.37	1.31
2	D	5003	ANP	PA-O3A	3.10	1.62	1.59
2	A	5002	ANP	PA-O3A	3.07	1.62	1.59
2	C	5004	ANP	C1'-N9	2.97	1.54	1.46
2	B	5001	ANP	O3'-C3'	2.94	1.50	1.43
2	D	5003	ANP	C1'-N9	2.93	1.54	1.46
2	C	5004	ANP	PA-O3A	2.91	1.62	1.59
2	A	5002	ANP	C1'-N9	2.87	1.54	1.46
2	B	5001	ANP	PG-O2G	-2.76	1.49	1.56
2	B	5001	ANP	PB-N3B	2.39	1.69	1.63
2	B	5001	ANP	O4'-C1'	-2.27	1.36	1.42
2	B	5001	ANP	PG-N3B	2.03	1.68	1.63
2	B	5001	ANP	C5-N7	-2.03	1.35	1.39
2	C	5004	ANP	PG-O3G	-2.02	1.51	1.56
2	D	5003	ANP	PG-O3G	-2.01	1.51	1.56
2	A	5002	ANP	PG-O3G	-2.01	1.51	1.56

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	ANP	C4-N9-C8	-4.91	100.58	105.74
2	B	5001	ANP	O2B-PB-O1B	4.83	120.24	109.87
2	B	5001	ANP	O4'-C1'-C2'	-4.73	96.50	106.62
2	C	5004	ANP	O1B-PB-N3B	-4.69	104.87	111.77
2	A	5002	ANP	O1B-PB-N3B	-4.65	104.92	111.77
2	D	5003	ANP	O1B-PB-N3B	-4.64	104.94	111.77
2	A	5002	ANP	C2'-C1'-N9	4.59	124.70	113.30
2	D	5003	ANP	C2'-C1'-N9	4.57	124.67	113.30
2	B	5001	ANP	C4'-O4'-C1'	-4.51	99.50	109.47
2	C	5004	ANP	C2'-C1'-N9	4.50	124.49	113.30
2	C	5004	ANP	O4'-C1'-C2'	-4.41	97.18	106.62
2	A	5002	ANP	O4'-C1'-C2'	-4.38	97.24	106.62
2	D	5003	ANP	O4'-C1'-C2'	-4.38	97.24	106.62
2	C	5004	ANP	O1G-PG-N3B	-4.36	105.34	111.77
2	A	5002	ANP	O1G-PG-N3B	-4.34	105.37	111.77
2	D	5003	ANP	O1G-PG-N3B	-4.34	105.38	111.77
2	B	5001	ANP	C2'-C1'-N9	4.30	123.99	113.30
2	B	5001	ANP	O1B-PB-N3B	-4.02	105.85	111.77
2	C	5004	ANP	O2B-PB-O1B	3.67	117.74	109.87
2	D	5003	ANP	O2B-PB-O1B	3.67	117.74	109.87
2	A	5002	ANP	O2B-PB-O1B	3.64	117.67	109.87
2	B	5001	ANP	C4-C5-N7	3.08	114.10	110.58
2	D	5003	ANP	C4'-O4'-C1'	-2.93	102.99	109.47
2	B	5001	ANP	O3G-PG-O1G	-2.93	106.10	113.45
2	A	5002	ANP	C4'-O4'-C1'	-2.91	103.04	109.47
2	C	5004	ANP	C4'-O4'-C1'	-2.90	103.07	109.47
2	D	5003	ANP	O2G-PG-O3G	2.56	114.47	107.59
2	C	5004	ANP	O2G-PG-O3G	2.56	114.46	107.59
2	A	5002	ANP	O2G-PG-O3G	2.54	114.41	107.59
2	B	5001	ANP	C4-N9-C1'	2.44	132.33	126.63
2	C	5004	ANP	O2B-PB-O3A	2.35	112.49	104.64
2	A	5002	ANP	O2B-PB-O3A	2.34	112.44	104.64
2	D	5003	ANP	O2B-PB-O3A	2.33	112.40	104.64
2	A	5002	ANP	O2A-PA-O3A	2.31	113.53	107.27
2	C	5004	ANP	O2A-PA-O3A	2.30	113.49	107.27
2	D	5003	ANP	O2A-PA-O3A	2.27	113.40	107.27
2	C	5004	ANP	C4-N9-C8	-2.27	103.36	105.74
2	A	5002	ANP	C4-N9-C8	-2.25	103.37	105.74
2	D	5003	ANP	C4-N9-C8	-2.23	103.39	105.74
2	B	5001	ANP	C3'-C2'-C1'	-2.06	97.56	101.46

There are no chirality outliers.

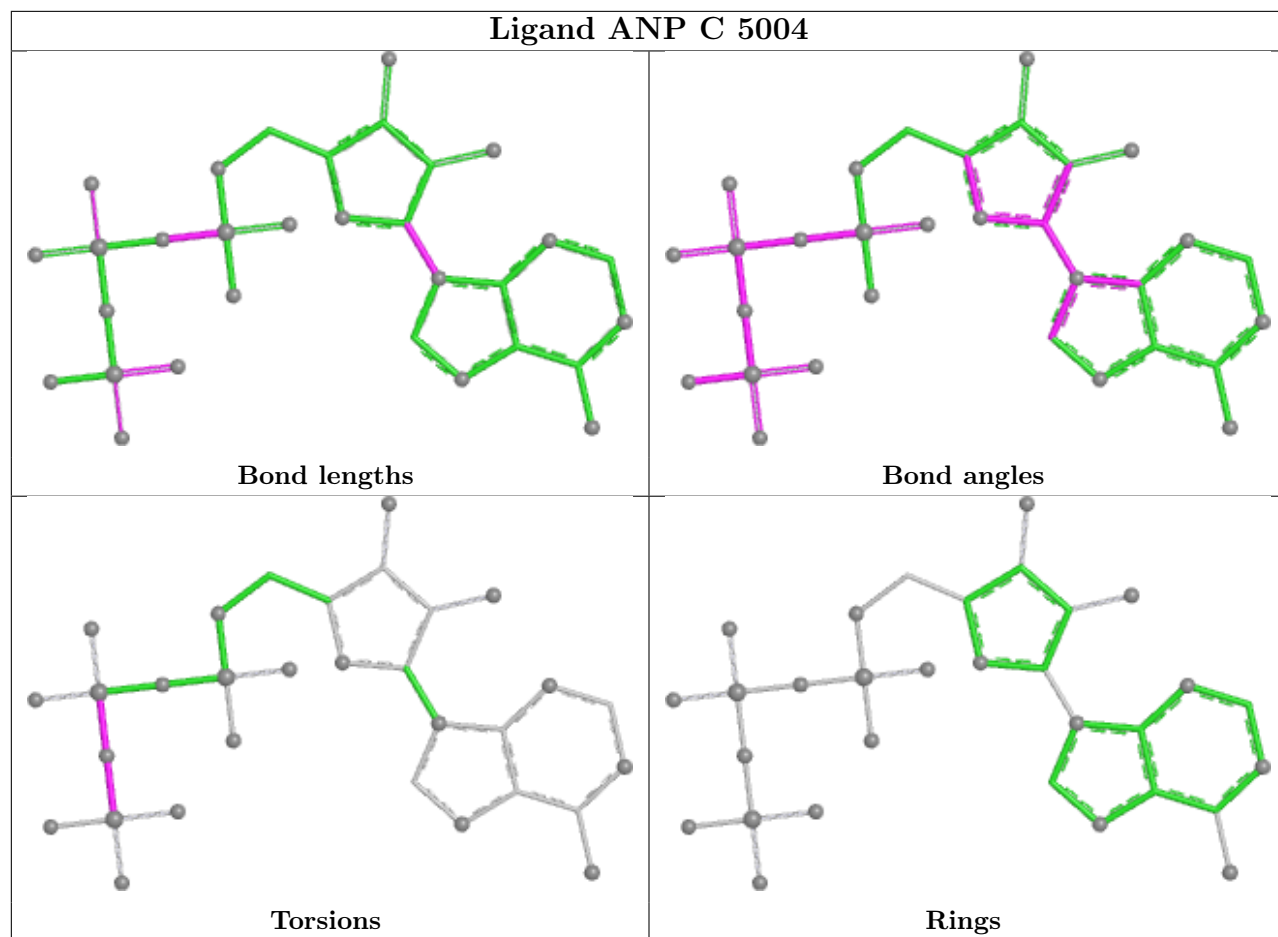
All (12) torsion outliers are listed below:

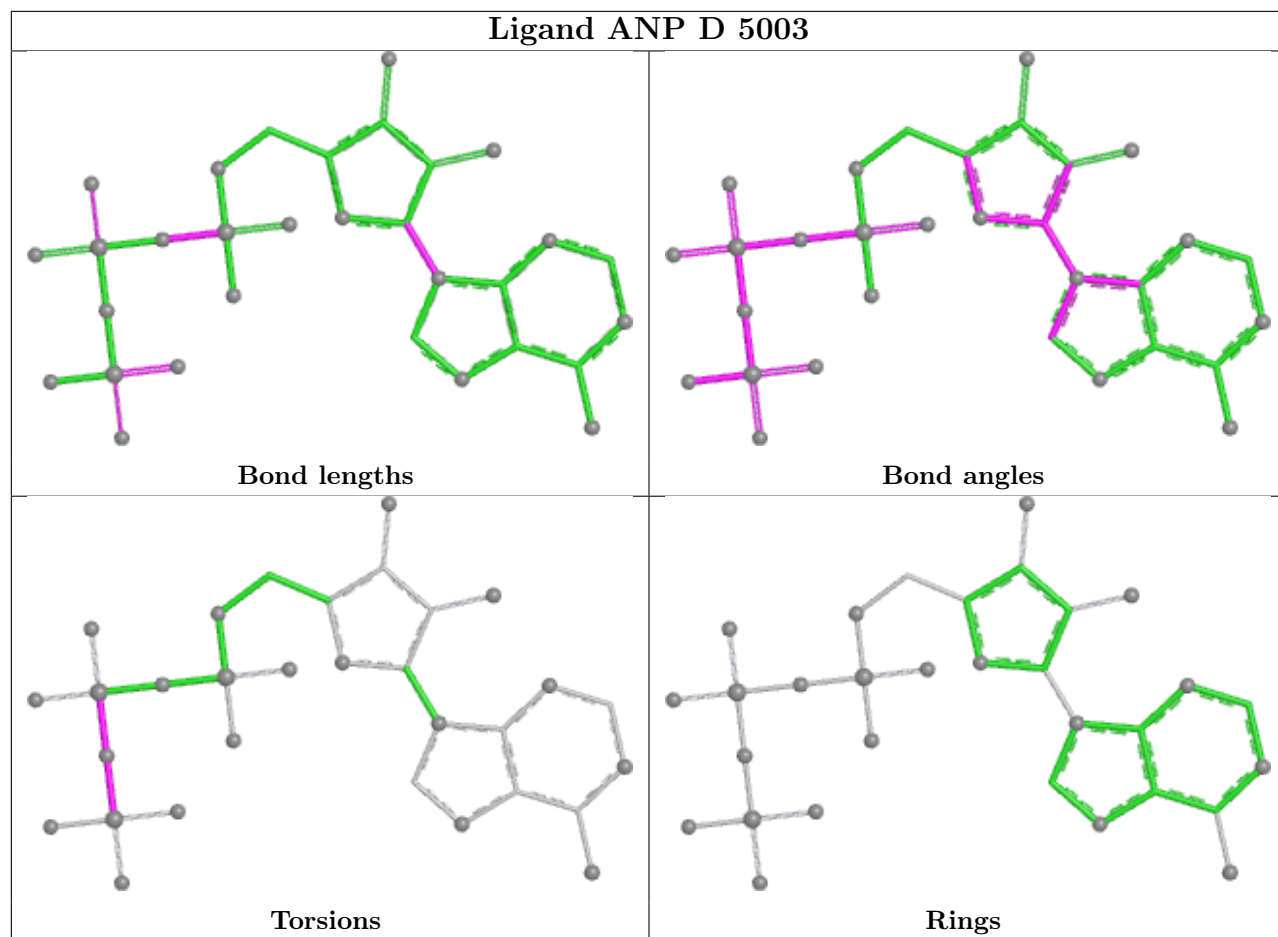
Mol	Chain	Res	Type	Atoms
2	A	5002	ANP	PB-N3B-PG-O1G
2	A	5002	ANP	PG-N3B-PB-O1B
2	A	5002	ANP	PG-N3B-PB-O3A
2	B	5001	ANP	PB-N3B-PG-O1G
2	B	5001	ANP	PG-N3B-PB-O1B
2	B	5001	ANP	PG-N3B-PB-O3A
2	C	5004	ANP	PB-N3B-PG-O1G
2	C	5004	ANP	PG-N3B-PB-O1B
2	C	5004	ANP	PG-N3B-PB-O3A
2	D	5003	ANP	PB-N3B-PG-O1G
2	D	5003	ANP	PG-N3B-PB-O1B
2	D	5003	ANP	PG-N3B-PB-O3A

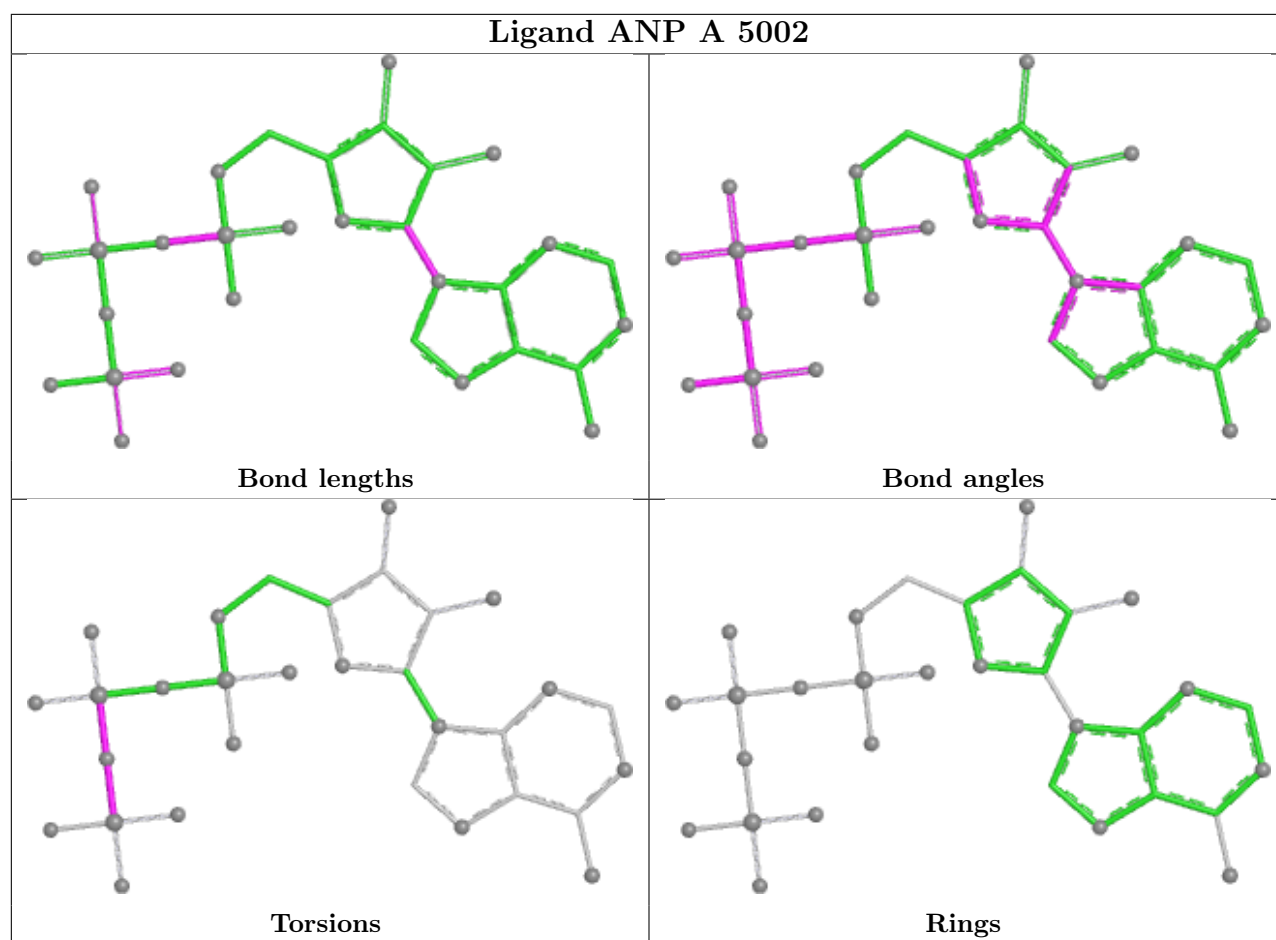
There are no ring outliers.

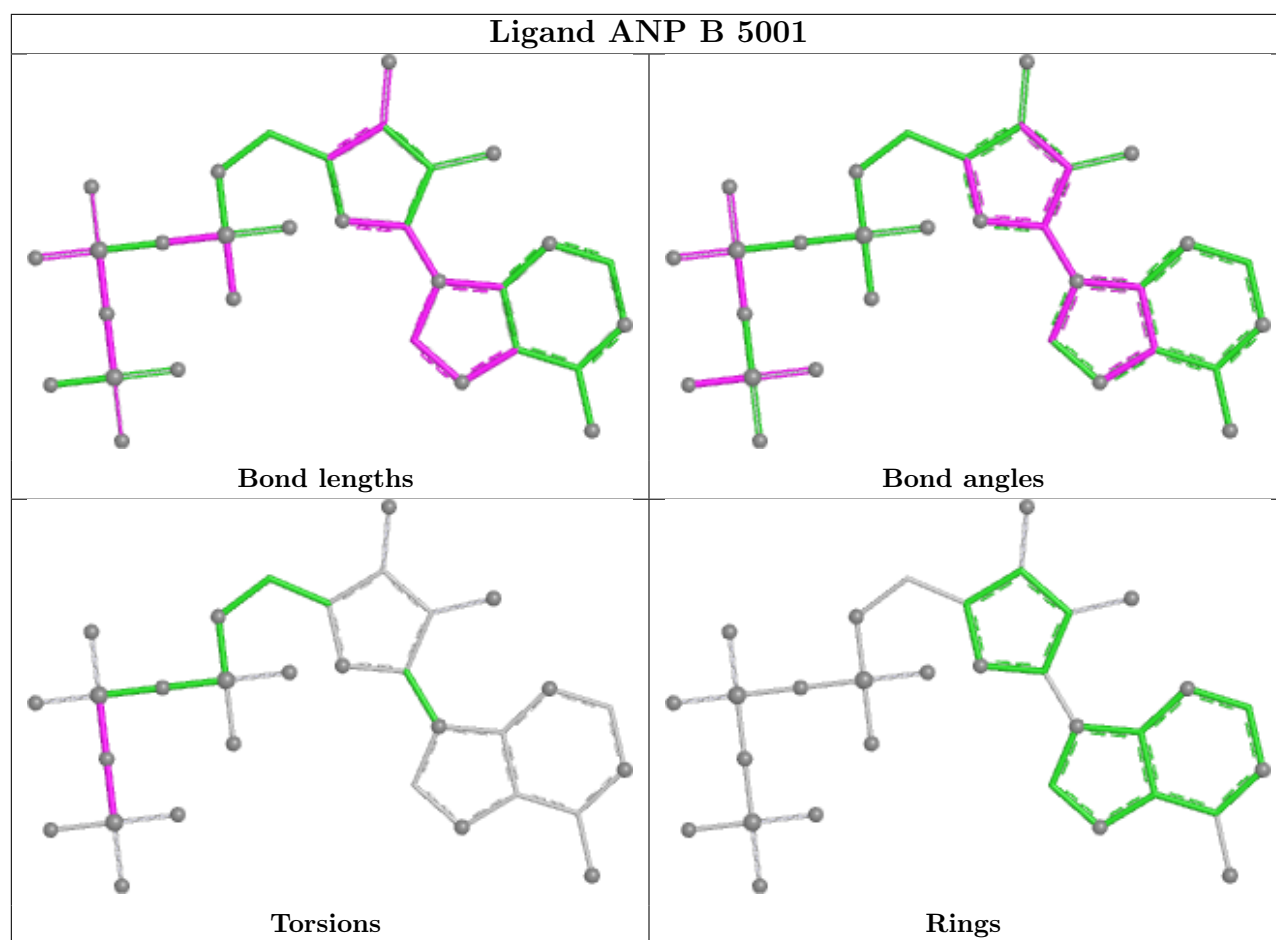
No monomer is involved in short contacts.

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	A	572/582 (98%)	10.66	564 (98%) 0 0	142, 225, 277, 312	0
1	B	572/582 (98%)	10.59	566 (98%) 0 0	112, 212, 274, 321	0
1	C	572/582 (98%)	11.16	564 (98%) 0 0	130, 218, 271, 309	0
1	D	572/582 (98%)	10.16	566 (98%) 0 0	132, 220, 271, 314	0
All	All	2288/2328 (98%)	10.64	2260 (98%) 0 0	112, 219, 274, 321	0

All (2260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	TRP	87.7
1	C	134	GLN	65.9
1	D	246	SER	59.1
1	A	417	ASN	56.0
1	A	414	SER	51.9
1	B	383	SER	50.4
1	C	253	PRO	48.9
1	A	162	TYR	48.6
1	D	113	VAL	45.3
1	D	264	ALA	43.7
1	C	336	ASP	43.5
1	D	149	GLU	43.4
1	A	274	SER	42.4
1	B	11	GLN	41.1
1	A	160	MET	39.8
1	A	163	TYR	39.6
1	C	242	MET	39.6
1	D	213	GLY	39.3
1	B	561	THR	39.1
1	D	569	HIS	38.5
1	C	257	LEU	37.6

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Mol	Chain	Res	Type	RSRZ
1	C	444	GLU	37.3
1	D	371	THR	36.2
1	A	398	GLY	36.0
1	B	399	HIS	36.0
1	C	137	SER	35.9
1	A	396	ASP	35.9
1	B	345	ARG	35.3
1	C	561	THR	34.8
1	A	446	SER	34.7
1	C	398	GLY	34.6
1	C	560	GLY	34.5
1	C	314	ALA	34.4
1	C	131	ASP	34.2
1	C	274	SER	34.0
1	A	161	PHE	33.8
1	C	246	SER	33.7
1	A	56	PHE	33.3
1	A	276	MET	32.7
1	C	258	ILE	32.5
1	C	329	ASP	32.3
1	D	552	GLU	32.1
1	A	293	ALA	32.1
1	B	314	ALA	32.0
1	C	149	GLU	31.8
1	B	280	THR	31.5
1	A	46	SER	31.5
1	A	289	SER	31.4
1	B	286	VAL	31.2
1	A	399	HIS	31.0
1	C	427	HIS	30.8
1	B	336	ASP	30.7
1	D	249	SER	30.5
1	D	242	MET	30.3
1	A	159	MET	30.3
1	B	560	GLY	29.9
1	A	345	ARG	29.8
1	A	45	LEU	29.8
1	A	41	ASP	29.6
1	A	397	GLU	29.3
1	B	327	GLU	29.2
1	C	135	VAL	28.7
1	D	396	ASP	28.5

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Mol	Chain	Res	Type	RSRZ
1	D	546	ASP	28.5
1	D	250	ILE	28.3
1	C	136	ALA	28.2
1	B	335	ILE	28.2
1	A	54	ASP	28.1
1	D	214	HIS	27.9
1	D	335	ILE	27.9
1	A	53	ASP	27.7
1	A	387	SER	27.7
1	C	252	ASP	27.6
1	C	156	LEU	27.5
1	B	334	VAL	27.4
1	D	216	GLU	27.3
1	A	344	PHE	27.2
1	D	199	THR	27.2
1	B	344	PHE	27.2
1	C	56	PHE	27.2
1	D	53	ASP	26.9
1	D	261	LEU	26.9
1	A	334	VAL	26.9
1	C	249	SER	26.9
1	C	261	LEU	26.9
1	D	336	ASP	26.8
1	B	41	ASP	26.8
1	B	113	VAL	26.7
1	B	430	ASN	26.6
1	C	140	SER	26.6
1	B	59	THR	26.5
1	D	253	PRO	26.5
1	A	431	ASP	26.4
1	C	399	HIS	26.2
1	D	217	VAL	26.1
1	C	260	SER	26.1
1	C	239	LEU	26.0
1	A	107	HIS	26.0
1	C	271	SER	25.9
1	A	363	ASN	25.9
1	C	426	VAL	25.8
1	C	256	GLN	25.5
1	B	431	ASP	25.4
1	B	338	ALA	25.3
1	B	527	GLN	25.1

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Mol	Chain	Res	Type	RSRZ
1	C	275	VAL	25.0
1	A	330	GLU	25.0
1	D	453	ALA	24.7
1	C	564	GLU	24.7
1	B	163	TYR	24.4
1	A	103	ARG	24.2
1	A	420	ALA	24.2
1	C	330	GLU	24.1
1	B	529	ASN	24.1
1	C	545	ALA	24.1
1	C	338	ALA	24.0
1	C	238	ARG	24.0
1	B	217	VAL	23.8
1	C	544	GLN	23.7
1	D	540	SER	23.7
1	D	378	SER	23.4
1	A	275	VAL	23.4
1	C	579	GLN	23.4
1	A	532	SER	23.4
1	C	133	GLU	23.3
1	B	278	SER	23.2
1	D	260	SER	23.2
1	D	147	VAL	23.1
1	B	95	LYS	23.0
1	A	335	ILE	22.9
1	C	141	GLY	22.9
1	A	50	PRO	22.9
1	C	456	MET	22.9
1	B	384	THR	22.9
1	C	445	TYR	22.9
1	D	202	GLN	22.8
1	D	240	GLN	22.8
1	D	209	GLN	22.8
1	A	473	ILE	22.8
1	D	362	ILE	22.7
1	C	213	GLY	22.6
1	A	430	ASN	22.5
1	B	281	ALA	22.5
1	C	240	GLN	22.5
1	D	456	MET	22.3
1	B	325	GLU	22.2
1	C	217	VAL	22.2

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Mol	Chain	Res	Type	RSRZ
1	B	164	SER	22.1
1	C	277	ASP	22.1
1	C	403	ASP	22.1
1	A	44	MET	22.0
1	B	528	LYS	21.9
1	A	18	PRO	21.9
1	D	12	THR	21.9
1	D	496	LEU	21.9
1	C	250	ILE	21.9
1	C	132	SER	21.8
1	B	289	SER	21.8
1	C	272	PHE	21.7
1	C	280	THR	21.6
1	A	290	SER	21.6
1	C	532	SER	21.5
1	B	563	SER	21.3
1	C	236	LYS	21.3
1	D	573	ALA	21.3
1	A	567	ALA	21.2
1	B	354	ARG	21.2
1	D	148	ARG	21.2
1	C	251	SER	21.1
1	B	285	THR	21.1
1	C	565	LEU	21.1
1	B	93	SER	21.0
1	D	140	SER	21.0
1	C	548	ILE	21.0
1	D	570	GLY	21.0
1	C	214	HIS	20.9
1	B	313	ALA	20.9
1	C	563	SER	20.9
1	B	339	THR	20.9
1	D	405	HIS	20.9
1	B	303	ASN	20.9
1	A	132	SER	20.8
1	D	553	ASP	20.8
1	B	363	ASN	20.8
1	B	317	THR	20.8
1	B	112	PRO	20.7
1	B	160	MET	20.6
1	D	136	ALA	20.6
1	D	132	SER	20.6

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Mol	Chain	Res	Type	RSRZ
1	D	243	LYS	20.6
1	D	112	PRO	20.5
1	C	446	SER	20.5
1	A	392	PHE	20.5
1	C	559	ARG	20.5
1	C	237	MET	20.5
1	B	38	ALA	20.5
1	C	313	ALA	20.3
1	A	273	PRO	20.3
1	C	458	TYR	20.2
1	D	265	PHE	20.2
1	D	532	SER	20.2
1	A	194	LYS	20.1
1	B	421	LEU	20.1
1	B	398	GLY	20.0
1	B	473	ILE	20.0
1	C	335	ILE	19.9
1	A	394	ASP	19.9
1	C	540	SER	19.9
1	C	158	ILE	19.8
1	A	93	SER	19.8
1	C	247	ALA	19.8
1	C	373	ALA	19.8
1	C	425	ASN	19.7
1	B	219	ILE	19.7
1	A	68	PRO	19.7
1	B	57	GLY	19.6
1	C	243	LYS	19.6
1	D	97	VAL	19.6
1	C	248	SER	19.6
1	C	420	ALA	19.6
1	B	564	GLU	19.5
1	A	193	SER	19.5
1	A	17	TRP	19.5
1	C	153	ILE	19.4
1	A	418	GLN	19.4
1	A	286	VAL	19.3
1	A	339	THR	19.3
1	B	94	GLY	19.2
1	D	551	VAL	19.2
1	B	97	VAL	19.2
1	A	190	ARG	19.2

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Mol	Chain	Res	Type	RSRZ
1	A	558	GLU	19.2
1	C	273	PRO	19.1
1	B	54	ASP	19.1
1	C	487	GLN	19.1
1	C	578	MET	19.1
1	C	152	SER	19.0
1	A	445	TYR	19.0
1	A	57	GLY	18.9
1	C	337	ARG	18.8
1	B	395	ILE	18.8
1	D	420	ALA	18.7
1	C	543	GLU	18.7
1	C	317	THR	18.7
1	C	475	GLY	18.7
1	A	563	SER	18.7
1	D	248	SER	18.6
1	A	277	ASP	18.6
1	B	559	ARG	18.6
1	A	309	GLN	18.6
1	D	484	GLY	18.5
1	B	322	LEU	18.5
1	D	404	GLY	18.5
1	B	547	GLU	18.5
1	C	553	ASP	18.3
1	C	159	MET	18.3
1	D	387	SER	18.3
1	D	257	LEU	18.3
1	C	510	ALA	18.2
1	D	338	ALA	18.2
1	C	577	LYS	18.2
1	A	102	ARG	18.2
1	D	252	ASP	18.1
1	C	554	GLY	18.1
1	C	339	THR	18.1
1	C	404	GLY	18.1
1	C	268	TYR	18.1
1	C	315	CYS	18.1
1	B	197	GLN	18.0
1	B	337	ARG	18.0
1	C	443	GLU	18.0
1	D	435	ASN	18.0
1	B	140	SER	18.0

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Mol	Chain	Res	Type	RSRZ
1	C	562	HIS	17.9
1	C	400	ILE	17.9
1	B	510	ALA	17.9
1	A	136	ALA	17.9
1	C	483	GLY	17.9
1	D	571	VAL	17.8
1	C	254	ILE	17.8
1	A	508	THR	17.8
1	B	530	ARG	17.8
1	B	12	THR	17.8
1	B	562	HIS	17.8
1	C	378	SER	17.7
1	A	522	ALA	17.7
1	D	93	SER	17.7
1	A	519	ILE	17.7
1	C	22	PRO	17.7
1	B	355	GLU	17.6
1	C	233	VAL	17.6
1	A	404	GLY	17.5
1	C	121	THR	17.5
1	B	420	ALA	17.4
1	D	251	SER	17.4
1	A	355	GLU	17.4
1	B	548	ILE	17.4
1	C	155	GLY	17.4
1	D	372	VAL	17.4
1	D	196	MET	17.4
1	A	393	TYR	17.3
1	D	223	GLN	17.3
1	C	474	ILE	17.3
1	D	457	ALA	17.3
1	A	566	LEU	17.3
1	C	219	ILE	17.3
1	C	347	VAL	17.2
1	D	502	LEU	17.2
1	A	106	GLY	17.2
1	A	403	ASP	17.1
1	D	494	ALA	17.1
1	D	436	ASN	17.1
1	C	457	ALA	17.1
1	D	397	GLU	17.0
1	A	270	ALA	17.0

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Mol	Chain	Res	Type	RSRZ
1	B	553	ASP	17.0
1	D	339	THR	17.0
1	D	205	THR	17.0
1	D	503	ILE	16.9
1	B	425	ASN	16.9
1	D	56	PHE	16.9
1	B	509	SER	16.9
1	A	333	ARG	16.9
1	A	313	ALA	16.9
1	A	388	LEU	16.7
1	B	305	ASN	16.7
1	B	306	ALA	16.7
1	D	334	VAL	16.7
1	C	57	GLY	16.7
1	A	510	ALA	16.7
1	B	321	ILE	16.7
1	A	278	SER	16.6
1	D	294	LEU	16.6
1	A	299	LYS	16.6
1	A	133	GLU	16.6
1	D	328	LYS	16.6
1	B	447	ARG	16.6
1	B	457	ALA	16.5
1	C	244	MET	16.5
1	C	55	GLY	16.5
1	A	140	SER	16.4
1	D	454	ALA	16.4
1	A	540	SER	16.4
1	D	512	ASP	16.4
1	B	37	ASN	16.4
1	D	204	THR	16.4
1	A	395	ILE	16.4
1	B	44	MET	16.3
1	D	510	ALA	16.3
1	D	212	LYS	16.3
1	C	255	ILE	16.3
1	D	509	SER	16.2
1	A	419	VAL	16.2
1	D	377	ARG	16.2
1	B	494	ALA	16.2
1	A	425	ASN	16.2
1	A	383	SER	16.1

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Mol	Chain	Res	Type	RSRZ
1	D	581	GLY	16.1
1	B	492	ALA	16.1
1	C	549	VAL	16.1
1	C	241	GLY	16.1
1	D	421	LEU	16.1
1	A	518	ALA	16.1
1	A	110	GLY	16.1
1	D	493	ARG	16.1
1	B	302	THR	16.0
1	C	312	MET	16.0
1	D	162	TYR	16.0
1	D	337	ARG	16.0
1	C	478	GLY	15.9
1	C	502	LEU	15.9
1	C	547	GLU	15.9
1	A	19	THR	15.9
1	A	436	ASN	15.9
1	D	218	LEU	15.8
1	D	329	ASP	15.8
1	B	474	ILE	15.8
1	A	386	ALA	15.8
1	C	234	SER	15.7
1	D	492	ALA	15.7
1	A	302	THR	15.6
1	C	542	ILE	15.6
1	B	519	ILE	15.6
1	D	513	THR	15.6
1	C	270	ALA	15.6
1	C	421	LEU	15.6
1	D	247	ALA	15.6
1	B	299	LYS	15.6
1	B	193	SER	15.5
1	B	450	ILE	15.5
1	A	310	ARG	15.5
1	B	424	GLN	15.5
1	B	40	SER	15.5
1	C	541	THR	15.5
1	D	115	PHE	15.5
1	A	559	ARG	15.4
1	D	185	VAL	15.4
1	A	474	ILE	15.4
1	A	48	LEU	15.4

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Mol	Chain	Res	Type	RSRZ
1	B	121	THR	15.4
1	A	494	ALA	15.4
1	D	315	CYS	15.3
1	A	413	ALA	15.3
1	D	60	ASP	15.3
1	A	295	MET	15.3
1	C	259	ALA	15.3
1	A	416	ARG	15.2
1	B	279	LEU	15.1
1	B	31	GLY	15.1
1	A	315	CYS	15.1
1	A	97	VAL	15.1
1	B	96	VAL	15.0
1	A	294	LEU	15.0
1	A	269	ALA	15.0
1	B	127	ARG	14.9
1	D	275	VAL	14.9
1	C	127	ARG	14.9
1	C	422	VAL	14.9
1	D	203	VAL	14.9
1	D	429	PHE	14.8
1	D	497	ARG	14.8
1	B	48	LEU	14.8
1	B	352	PRO	14.8
1	C	82	SER	14.8
1	A	442	THR	14.8
1	B	19	THR	14.8
1	B	283	THR	14.7
1	C	269	ALA	14.7
1	A	509	SER	14.7
1	D	244	MET	14.7
1	B	218	LEU	14.7
1	D	237	MET	14.7
1	D	241	GLY	14.7
1	B	382	LYS	14.7
1	B	194	LYS	14.6
1	C	480	LEU	14.6
1	D	139	SER	14.6
1	B	369	GLY	14.6
1	C	113	VAL	14.6
1	B	365	LYS	14.6
1	C	44	MET	14.6

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Mol	Chain	Res	Type	RSRZ
1	D	297	PRO	14.6
1	D	188	ARG	14.5
1	B	318	LEU	14.5
1	C	148	ARG	14.5
1	C	379	GLY	14.5
1	D	179	SER	14.5
1	B	106	GLY	14.5
1	C	19	THR	14.5
1	A	447	ARG	14.4
1	D	474	ILE	14.4
1	A	466	MET	14.4
1	C	265	PHE	14.4
1	C	529	ASN	14.4
1	D	568	GLN	14.3
1	B	541	THR	14.2
1	B	20	ILE	14.2
1	D	206	SER	14.2
1	C	157	PHE	14.2
1	C	552	GLU	14.2
1	C	484	GLY	14.2
1	B	400	ILE	14.2
1	D	208	GLU	14.1
1	B	298	LEU	14.1
1	B	55	GLY	14.1
1	B	356	VAL	14.1
1	B	295	MET	14.1
1	A	251	SER	14.1
1	C	316	GLN	14.1
1	A	457	ALA	14.0
1	A	527	GLN	14.0
1	B	310	ARG	14.0
1	A	287	VAL	14.0
1	D	269	ALA	13.9
1	C	328	LYS	13.9
1	C	498	ASP	13.9
1	A	356	VAL	13.9
1	D	379	GLY	13.8
1	A	579	GLN	13.8
1	A	553	ASP	13.8
1	B	454	ALA	13.8
1	C	442	THR	13.8
1	D	176	PRO	13.8

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Mol	Chain	Res	Type	RSRZ
1	B	204	THR	13.8
1	A	47	LEU	13.7
1	B	390	THR	13.7
1	A	264	ALA	13.7
1	D	262	ALA	13.7
1	D	86	SER	13.7
1	A	43	PHE	13.7
1	D	498	ASP	13.7
1	A	548	ILE	13.7
1	C	139	SER	13.7
1	C	245	VAL	13.7
1	B	549	VAL	13.7
1	A	65	LEU	13.6
1	A	104	LEU	13.6
1	A	551	VAL	13.6
1	B	136	ALA	13.6
1	A	550	VAL	13.6
1	B	482	SER	13.6
1	B	98	MET	13.6
1	D	356	VAL	13.5
1	B	309	GLN	13.5
1	C	278	SER	13.5
1	C	144	ILE	13.5
1	D	215	LYS	13.5
1	B	251	SER	13.5
1	D	376	GLY	13.4
1	A	298	LEU	13.4
1	A	285	THR	13.4
1	A	306	ALA	13.4
1	D	175	ALA	13.4
1	D	572	TYR	13.4
1	A	549	VAL	13.4
1	C	369	GLY	13.4
1	A	20	ILE	13.4
1	B	315	CYS	13.4
1	D	101	ARG	13.4
1	A	462	PHE	13.3
1	A	101	ARG	13.3
1	B	99	THR	13.3
1	B	429	PHE	13.3
1	A	376	GLY	13.3
1	D	200	MET	13.3

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Mol	Chain	Res	Type	RSRZ
1	C	362	ILE	13.3
1	C	377	ARG	13.3
1	C	215	LYS	13.3
1	B	458	TYR	13.3
1	B	508	THR	13.3
1	D	144	ILE	13.3
1	C	576	HIS	13.2
1	B	125	LEU	13.2
1	D	533	LEU	13.2
1	D	278	SER	13.2
1	D	403	ASP	13.2
1	D	547	GLU	13.2
1	A	292	ILE	13.2
1	D	163	TYR	13.2
1	B	536	ALA	13.1
1	C	145	THR	13.1
1	D	48	LEU	13.1
1	D	332	LYS	13.1
1	A	238	ARG	13.1
1	C	473	ILE	13.1
1	C	218	LEU	13.1
1	C	281	ALA	13.1
1	A	144	ILE	13.1
1	C	125	LEU	13.0
1	D	390	THR	13.0
1	B	92	VAL	12.9
1	B	166	GLN	12.9
1	B	394	ASP	12.9
1	D	128	ILE	12.9
1	B	248	SER	12.8
1	B	198	ASN	12.8
1	A	137	SER	12.8
1	A	129	THR	12.8
1	B	89	ILE	12.8
1	C	518	ALA	12.7
1	D	511	LEU	12.7
1	C	517	ARG	12.7
1	C	210	MET	12.7
1	A	521	ALA	12.7
1	D	245	VAL	12.7
1	A	303	ASN	12.7
1	B	220	PHE	12.7

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Mol	Chain	Res	Type	RSRZ
1	A	15	ARG	12.7
1	D	418	GLN	12.7
1	D	49	LYS	12.7
1	C	490	ALA	12.6
1	B	498	ASP	12.6
1	D	211	LEU	12.6
1	D	82	SER	12.6
1	C	575	LEU	12.6
1	C	568	GLN	12.6
1	D	355	GLU	12.5
1	B	364	LEU	12.5
1	B	415	LEU	12.5
1	C	47	LEU	12.5
1	A	390	THR	12.5
1	D	135	VAL	12.5
1	A	492	ALA	12.5
1	C	209	GLN	12.5
1	A	483	GLY	12.5
1	B	378	SER	12.5
1	C	512	ASP	12.5
1	D	437	ILE	12.5
1	D	268	TYR	12.5
1	A	16	LEU	12.4
1	A	536	ALA	12.4
1	B	373	ALA	12.4
1	A	209	GLN	12.4
1	A	52	LEU	12.4
1	B	131	ASP	12.4
1	D	109	MET	12.4
1	C	211	LEU	12.4
1	B	252	ASP	12.3
1	A	55	GLY	12.3
1	D	434	ALA	12.3
1	A	412	LEU	12.3
1	B	386	ALA	12.3
1	B	190	ARG	12.3
1	C	284	ILE	12.3
1	A	60	ASP	12.3
1	C	48	LEU	12.3
1	B	393	TYR	12.3
1	B	82	SER	12.3
1	A	252	ASP	12.3

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Mol	Chain	Res	Type	RSRZ
1	B	208	GLU	12.3
1	B	483	GLY	12.2
1	C	128	ILE	12.2
1	C	318	LEU	12.2
1	C	492	ALA	12.2
1	D	576	HIS	12.2
1	C	393	TYR	12.2
1	A	109	MET	12.2
1	A	465	LYS	12.2
1	C	124	LEU	12.2
1	C	129	THR	12.2
1	C	138	SER	12.2
1	B	475	GLY	12.1
1	C	567	ALA	12.1
1	D	487	GLN	12.1
1	A	88	CYS	12.1
1	A	415	LEU	12.1
1	D	495	LEU	12.1
1	D	579	GLN	12.1
1	D	210	MET	12.1
1	D	143	LEU	12.0
1	D	428	LEU	12.0
1	B	480	LEU	12.0
1	A	262	ALA	12.0
1	A	467	ASP	12.0
1	D	152	SER	12.0
1	C	496	LEU	12.0
1	B	129	THR	12.0
1	D	94	GLY	11.9
1	A	382	LYS	11.9
1	C	495	LEU	11.9
1	B	207	ALA	11.9
1	B	215	LYS	11.9
1	A	477	ASN	11.9
1	B	301	LEU	11.9
1	D	98	MET	11.9
1	D	121	THR	11.9
1	B	567	ALA	11.9
1	C	212	LYS	11.8
1	B	436	ASN	11.8
1	A	179	SER	11.8
1	A	482	SER	11.8

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Mol	Chain	Res	Type	RSRZ
1	A	541	THR	11.8
1	A	248	SER	11.8
1	B	416	ARG	11.8
1	B	124	LEU	11.7
1	C	449	GLN	11.7
1	A	265	PHE	11.7
1	C	208	GLU	11.7
1	D	293	ALA	11.7
1	A	208	GLU	11.7
1	B	357	PRO	11.7
1	D	413	ALA	11.7
1	D	499	SER	11.7
1	B	47	LEU	11.6
1	B	300	SER	11.6
1	C	198	ASN	11.6
1	A	191	SER	11.6
1	A	206	SER	11.6
1	B	100	MET	11.6
1	D	52	LEU	11.5
1	A	125	LEU	11.5
1	A	223	GLN	11.5
1	B	459	ALA	11.5
1	A	85	SER	11.5
1	D	417	ASN	11.5
1	A	347	VAL	11.5
1	D	550	VAL	11.5
1	D	366	ILE	11.5
1	C	479	VAL	11.5
1	C	488	ARG	11.5
1	B	116	PHE	11.5
1	A	108	MET	11.4
1	A	456	MET	11.4
1	C	195	ASN	11.4
1	B	249	SER	11.4
1	C	493	ARG	11.4
1	B	462	PHE	11.4
1	A	214	HIS	11.4
1	B	532	SER	11.4
1	C	509	SER	11.4
1	A	377	ARG	11.4
1	B	486	ARG	11.4
1	C	494	ALA	11.4

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Mol	Chain	Res	Type	RSRZ
1	D	467	ASP	11.4
1	B	139	SER	11.4
1	D	44	MET	11.4
1	A	305	ASN	11.4
1	B	161	PHE	11.4
1	A	86	SER	11.4
1	B	101	ARG	11.4
1	A	317	THR	11.3
1	A	429	PHE	11.3
1	B	86	SER	11.3
1	D	430	ASN	11.3
1	D	207	ALA	11.3
1	D	105	PHE	11.3
1	B	34	LEU	11.3
1	A	433	VAL	11.3
1	B	144	ILE	11.3
1	D	486	ARG	11.3
1	B	256	GLN	11.3
1	C	285	THR	11.3
1	C	508	THR	11.3
1	B	326	GLN	11.3
1	A	459	ALA	11.3
1	B	358	ALA	11.3
1	C	412	LEU	11.3
1	D	490	ALA	11.2
1	A	371	THR	11.2
1	B	537	HIS	11.2
1	C	99	THR	11.2
1	D	110	GLY	11.2
1	D	415	LEU	11.2
1	C	519	ILE	11.2
1	C	197	GLN	11.2
1	C	358	ALA	11.2
1	D	361	ASN	11.2
1	C	486	ARG	11.2
1	D	549	VAL	11.2
1	D	19	THR	11.2
1	C	397	GLU	11.2
1	B	284	ILE	11.2
1	A	336	ASP	11.1
1	B	543	GLU	11.1
1	A	69	LEU	11.1

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Mol	Chain	Res	Type	RSRZ
1	C	106	GLY	11.1
1	C	97	VAL	11.1
1	A	291	MET	11.1
1	B	540	SER	11.1
1	A	379	GLY	11.1
1	A	215	LYS	11.0
1	B	216	GLU	11.0
1	C	376	GLY	11.0
1	D	129	THR	11.0
1	A	268	TYR	11.0
1	B	456	MET	11.0
1	B	223	GLN	11.0
1	A	537	HIS	10.9
1	A	458	TYR	10.9
1	B	377	ARG	10.9
1	C	88	CYS	10.9
1	D	536	ALA	10.9
1	D	537	HIS	10.9
1	A	560	GLY	10.9
1	A	105	PHE	10.9
1	C	394	ASP	10.9
1	A	375	VAL	10.9
1	B	181	ALA	10.9
1	B	435	ASN	10.9
1	B	292	ILE	10.9
1	D	419	VAL	10.9
1	C	417	ASN	10.8
1	D	116	PHE	10.8
1	A	249	SER	10.8
1	A	128	ILE	10.8
1	C	334	VAL	10.8
1	B	467	ASP	10.8
1	D	374	LEU	10.8
1	D	348	THR	10.8
1	A	62	SER	10.8
1	B	579	GLN	10.8
1	B	255	ILE	10.8
1	A	100	MET	10.8
1	B	392	PHE	10.8
1	B	102	ARG	10.8
1	A	139	SER	10.8
1	D	59	THR	10.7

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Mol	Chain	Res	Type	RSRZ
1	B	88	CYS	10.7
1	B	573	ALA	10.7
1	D	438	ALA	10.7
1	A	491	ILE	10.7
1	B	85	SER	10.7
1	C	448	GLU	10.7
1	B	21	ALA	10.7
1	B	379	GLY	10.7
1	B	39	ALA	10.7
1	B	328	LYS	10.7
1	C	207	ALA	10.7
1	B	449	GLN	10.7
1	C	61	ARG	10.7
1	A	576	HIS	10.7
1	C	501	ILE	10.6
1	D	309	GLN	10.6
1	A	82	SER	10.6
1	B	376	GLY	10.6
1	B	243	LYS	10.6
1	A	357	PRO	10.6
1	B	488	ARG	10.6
1	B	381	GLY	10.6
1	D	471	ASP	10.6
1	D	491	ILE	10.6
1	D	235	ASN	10.6
1	A	21	ALA	10.6
1	B	287	VAL	10.6
1	C	179	SER	10.5
1	A	580	PHE	10.5
1	A	463	ILE	10.5
1	B	571	VAL	10.5
1	D	146	VAL	10.5
1	B	451	GLU	10.5
1	C	223	GLN	10.5
1	D	519	ILE	10.5
1	A	51	LEU	10.5
1	C	481	LEU	10.5
1	C	566	LEU	10.5
1	B	130	TYR	10.5
1	B	262	ALA	10.5
1	A	211	LEU	10.4
1	D	539	LEU	10.4

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Mol	Chain	Res	Type	RSRZ
1	B	126	SER	10.4
1	B	433	VAL	10.4
1	A	539	LEU	10.4
1	D	305	ASN	10.4
1	D	394	ASP	10.4
1	C	199	THR	10.4
1	A	405	HIS	10.4
1	B	119	GLN	10.4
1	B	487	GLN	10.4
1	A	490	ALA	10.4
1	B	512	ASP	10.4
1	D	323	ASP	10.4
1	B	374	LEU	10.4
1	C	513	THR	10.4
1	D	333	ARG	10.4
1	A	351	TYR	10.4
1	D	389	ILE	10.4
1	B	247	ALA	10.4
1	A	319	PHE	10.4
1	B	244	MET	10.4
1	C	16	LEU	10.4
1	B	491	ILE	10.3
1	C	437	ILE	10.3
1	D	234	SER	10.3
1	B	534	VAL	10.3
1	C	51	LEU	10.3
1	D	263	LEU	10.3
1	A	488	ARG	10.3
1	A	487	GLN	10.3
1	C	580	PHE	10.3
1	D	88	CYS	10.3
1	B	391	ARG	10.3
1	A	164	SER	10.3
1	A	260	SER	10.3
1	B	259	ALA	10.3
1	A	166	GLN	10.3
1	B	56	PHE	10.3
1	B	109	MET	10.3
1	B	385	ILE	10.3
1	B	45	LEU	10.3
1	B	294	LEU	10.3
1	B	414	SER	10.3

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Mol	Chain	Res	Type	RSRZ
1	C	533	LEU	10.3
1	A	197	GLN	10.2
1	B	246	SER	10.2
1	C	86	SER	10.2
1	C	93	SER	10.2
1	C	387	SER	10.2
1	B	122	GLY	10.2
1	A	364	LEU	10.2
1	B	245	VAL	10.2
1	C	262	ALA	10.2
1	B	253	PRO	10.2
1	A	131	ASP	10.2
1	A	316	GLN	10.2
1	A	384	THR	10.2
1	D	25	ALA	10.2
1	B	329	ASP	10.2
1	B	493	ARG	10.2
1	A	329	ASP	10.2
1	A	512	ASP	10.2
1	D	563	SER	10.2
1	C	203	VAL	10.1
1	D	186	SER	10.1
1	D	373	ALA	10.1
1	A	42	THR	10.1
1	A	204	THR	10.1
1	B	478	GLY	10.1
1	B	179	SER	10.1
1	C	191	SER	10.1
1	D	107	HIS	10.1
1	B	523	LEU	10.1
1	A	94	GLY	10.0
1	D	277	ASP	10.0
1	C	365	LYS	10.0
1	C	497	ARG	10.0
1	B	90	SER	10.0
1	B	231	ASP	10.0
1	A	288	PHE	10.0
1	B	375	VAL	10.0
1	C	162	TYR	10.0
1	C	166	GLN	10.0
1	C	537	HIS	10.0
1	A	259	ALA	9.9

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Mol	Chain	Res	Type	RSRZ
1	C	263	LEU	9.9
1	C	364	LEU	9.9
1	D	414	SER	9.9
1	C	366	ILE	9.9
1	B	468	ASN	9.9
1	D	416	ARG	9.9
1	B	568	GLN	9.9
1	D	562	HIS	9.9
1	A	312	MET	9.9
1	C	200	MET	9.9
1	C	193	SER	9.9
1	A	454	ALA	9.9
1	B	440	ALA	9.9
1	C	109	MET	9.9
1	D	195	ASN	9.9
1	C	204	THR	9.9
1	C	507	ALA	9.9
1	B	291	MET	9.9
1	C	196	MET	9.9
1	D	111	MET	9.9
1	B	477	ASN	9.8
1	A	189	PHE	9.8
1	B	448	GLU	9.8
1	C	288	PHE	9.8
1	D	96	VAL	9.8
1	D	482	SER	9.8
1	A	538	ARG	9.8
1	A	374	LEU	9.8
1	D	108	MET	9.8
1	A	373	ALA	9.8
1	C	206	SER	9.8
1	B	105	PHE	9.8
1	A	543	GLU	9.8
1	C	321	ILE	9.8
1	A	207	ALA	9.8
1	A	318	LEU	9.8
1	D	259	ALA	9.8
1	D	538	ARG	9.8
1	B	120	SER	9.8
1	A	89	ILE	9.8
1	B	316	GLN	9.8
1	A	437	ILE	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	261	LEU	9.8
1	B	506	GLU	9.8
1	A	481	LEU	9.8
1	A	557	VAL	9.7
1	A	352	PRO	9.7
1	A	358	ALA	9.7
1	B	60	ASP	9.7
1	D	99	THR	9.7
1	B	572	TYR	9.7
1	A	400	ILE	9.7
1	B	499	SER	9.7
1	D	85	SER	9.7
1	D	446	SER	9.7
1	B	538	ARG	9.7
1	D	488	ARG	9.7
1	D	485	GLN	9.7
1	A	157	PHE	9.7
1	B	361	ASN	9.7
1	A	366	ILE	9.7
1	B	535	ILE	9.7
1	C	363	ASN	9.6
1	A	523	LEU	9.6
1	D	267	LEU	9.6
1	B	225	VAL	9.6
1	C	108	MET	9.6
1	D	472	THR	9.6
1	C	181	ALA	9.6
1	A	245	VAL	9.6
1	B	254	ILE	9.6
1	D	192	ILE	9.6
1	A	98	MET	9.6
1	D	392	PHE	9.6
1	B	175	ALA	9.6
1	C	266	VAL	9.6
1	B	481	LEU	9.5
1	A	210	MET	9.5
1	B	413	ALA	9.5
1	D	358	ALA	9.5
1	D	352	PRO	9.5
1	A	143	LEU	9.5
1	C	511	LEU	9.5
1	D	317	THR	9.5

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Mol	Chain	Res	Type	RSRZ
1	A	556	ILE	9.5
1	B	389	ILE	9.5
1	A	296	ARG	9.5
1	D	104	LEU	9.5
1	D	425	ASN	9.5
1	B	353	GLY	9.5
1	D	130	TYR	9.5
1	C	391	ARG	9.5
1	B	234	SER	9.5
1	A	544	GLN	9.5
1	B	574	GLN	9.5
1	D	266	VAL	9.5
1	A	391	ARG	9.5
1	D	489	ILE	9.5
1	B	265	PHE	9.4
1	C	332	LYS	9.4
1	C	515	SER	9.4
1	B	350	THR	9.4
1	D	124	LEU	9.4
1	A	434	ALA	9.4
1	B	489	ILE	9.4
1	D	501	ILE	9.4
1	A	370	LYS	9.4
1	A	381	GLY	9.4
1	A	87	TYR	9.4
1	C	418	GLN	9.4
1	D	37	ASN	9.4
1	C	390	THR	9.4
1	D	254	ILE	9.4
1	C	279	LEU	9.4
1	B	484	GLY	9.4
1	C	101	ARG	9.4
1	C	558	GLU	9.4
1	C	175	ALA	9.4
1	B	576	HIS	9.4
1	C	468	ASN	9.3
1	A	385	ILE	9.3
1	B	550	VAL	9.3
1	B	341	ASP	9.3
1	D	189	PHE	9.3
1	A	480	LEU	9.3
1	B	87	TYR	9.3

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Mol	Chain	Res	Type	RSRZ
1	C	491	ILE	9.3
1	A	61	ARG	9.3
1	C	436	ASN	9.3
1	A	542	ILE	9.3
1	D	444	GLU	9.3
1	B	347	VAL	9.3
1	A	255	ILE	9.3
1	B	186	SER	9.3
1	D	40	SER	9.3
1	C	569	HIS	9.3
1	B	18	PRO	9.2
1	D	125	LEU	9.2
1	A	63	VAL	9.2
1	A	408	ARG	9.2
1	B	351	TYR	9.2
1	A	212	LYS	9.2
1	B	260	SER	9.2
1	B	367	PRO	9.2
1	B	513	THR	9.2
1	C	31	GLY	9.2
1	C	114	ALA	9.2
1	C	405	HIS	9.2
1	A	279	LEU	9.2
1	C	27	LEU	9.2
1	A	84	ILE	9.2
1	D	433	VAL	9.2
1	A	205	THR	9.2
1	D	91	TRP	9.2
1	B	569	HIS	9.2
1	D	483	GLY	9.1
1	A	31	GLY	9.1
1	A	175	ALA	9.1
1	B	133	GLU	9.1
1	C	53	ASP	9.1
1	B	542	ILE	9.1
1	B	556	ILE	9.1
1	C	267	LEU	9.1
1	A	142	ALA	9.1
1	A	574	GLN	9.1
1	D	102	ARG	9.1
1	D	270	ALA	9.1
1	D	558	GLU	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	407	LEU	9.1
1	B	539	LEU	9.1
1	A	241	GLY	9.1
1	D	349	PHE	9.1
1	B	497	ARG	9.0
1	C	96	VAL	9.0
1	B	17	TRP	9.0
1	C	102	ARG	9.0
1	A	30	ALA	9.0
1	C	306	ALA	9.0
1	B	117	ASP	9.0
1	B	412	LEU	9.0
1	B	258	ILE	9.0
1	C	573	ALA	9.0
1	B	471	ASP	9.0
1	D	100	MET	9.0
1	D	402	MET	9.0
1	C	123	THR	9.0
1	C	35	ILE	9.0
1	B	30	ALA	9.0
1	C	85	SER	9.0
1	B	296	ARG	9.0
1	C	503	ILE	9.0
1	A	440	ALA	9.0
1	D	120	SER	8.9
1	D	412	LEU	8.9
1	B	209	GLN	8.9
1	C	100	MET	8.9
1	C	103	ARG	8.9
1	A	572	TYR	8.9
1	B	143	LEU	8.9
1	D	62	SER	8.9
1	B	465	LYS	8.9
1	A	186	SER	8.9
1	A	246	SER	8.9
1	C	25	ALA	8.9
1	A	486	ARG	8.9
1	A	493	ARG	8.9
1	B	503	ILE	8.9
1	A	471	ASP	8.9
1	D	137	SER	8.9
1	D	529	ASN	8.9

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Mol	Chain	Res	Type	RSRZ
1	C	419	VAL	8.9
1	C	98	MET	8.9
1	A	498	ASP	8.9
1	C	385	ILE	8.9
1	A	79	GLY	8.9
1	B	490	ALA	8.9
1	A	256	GLN	8.8
1	B	485	GLN	8.8
1	B	110	GLY	8.8
1	B	53	ASP	8.8
1	A	258	ILE	8.8
1	B	157	PHE	8.8
1	D	89	ILE	8.8
1	A	81	THR	8.8
1	B	83	TYR	8.8
1	B	502	LEU	8.8
1	B	288	PHE	8.8
1	D	445	TYR	8.8
1	D	106	GLY	8.8
1	A	167	LEU	8.8
1	A	421	LEU	8.8
1	A	489	ILE	8.8
1	B	330	GLU	8.8
1	B	128	ILE	8.8
1	A	511	LEU	8.8
1	B	407	LEU	8.8
1	B	206	SER	8.7
1	B	250	ILE	8.7
1	C	231	ASP	8.7
1	D	508	THR	8.7
1	D	103	ARG	8.7
1	D	238	ARG	8.7
1	A	90	SER	8.7
1	A	495	LEU	8.7
1	C	359	LEU	8.7
1	C	539	LEU	8.7
1	C	95	LYS	8.7
1	C	230	PHE	8.7
1	D	284	ILE	8.7
1	C	164	SER	8.7
1	B	81	THR	8.7
1	C	167	LEU	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	451	GLU	8.7
1	A	34	LEU	8.7
1	C	467	ASP	8.7
1	A	83	TYR	8.7
1	C	489	ILE	8.7
1	D	548	ILE	8.7
1	A	361	ASN	8.7
1	C	355	GLU	8.7
1	A	424	GLN	8.7
1	C	111	MET	8.7
1	C	499	SER	8.7
1	D	500	PRO	8.7
1	A	280	THR	8.7
1	B	437	ILE	8.7
1	A	33	ALA	8.7
1	B	434	ALA	8.7
1	D	31	GLY	8.7
1	A	564	GLU	8.7
1	C	303	ASN	8.7
1	A	497	ARG	8.7
1	C	224	GLU	8.7
1	A	78	ARG	8.6
1	A	372	VAL	8.6
1	C	227	THR	8.6
1	A	479	VAL	8.6
1	D	443	GLU	8.6
1	A	378	SER	8.6
1	B	388	LEU	8.6
1	B	511	LEU	8.6
1	A	534	VAL	8.6
1	C	110	GLY	8.6
1	D	439	TYR	8.6
1	D	271	SER	8.5
1	C	381	GLY	8.5
1	D	351	TYR	8.5
1	C	107	HIS	8.5
1	C	305	ASN	8.5
1	B	469	GLY	8.5
1	A	198	ASN	8.5
1	A	502	LEU	8.5
1	D	327	GLU	8.5
1	B	552	GLU	8.5

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Mol	Chain	Res	Type	RSRZ
1	B	566	LEU	8.5
1	A	546	ASP	8.5
1	C	185	VAL	8.5
1	A	195	ASN	8.5
1	B	312	MET	8.5
1	C	466	MET	8.5
1	C	297	PRO	8.5
1	D	481	LEU	8.5
1	C	32	ILE	8.5
1	C	311	GLY	8.5
1	B	333	ARG	8.5
1	A	507	ALA	8.4
1	D	559	ARG	8.4
1	B	403	ASP	8.4
1	B	428	LEU	8.4
1	D	231	ASP	8.4
1	D	314	ALA	8.4
1	C	26	GLY	8.4
1	C	572	TYR	8.4
1	B	104	LEU	8.4
1	D	41	ASP	8.4
1	B	438	ALA	8.4
1	C	301	LEU	8.4
1	D	480	LEU	8.4
1	B	343	GLU	8.4
1	D	291	MET	8.4
1	D	290	SER	8.4
1	A	118	LYS	8.4
1	B	118	LYS	8.4
1	C	319	PHE	8.4
1	C	384	THR	8.4
1	A	452	GLU	8.4
1	A	178	VAL	8.4
1	D	375	VAL	8.4
1	D	303	ASN	8.4
1	D	13	PHE	8.4
1	A	138	SER	8.4
1	D	73	GLY	8.4
1	A	496	LEU	8.4
1	C	356	VAL	8.3
1	C	375	VAL	8.3
1	C	91	TRP	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	8.3
1	A	453	ALA	8.3
1	C	21	ALA	8.3
1	C	104	LEU	8.3
1	A	282	GLY	8.3
1	B	241	GLY	8.3
1	A	168	SER	8.3
1	D	440	ALA	8.3
1	C	406	ASP	8.3
1	C	30	ALA	8.3
1	C	62	SER	8.3
1	C	33	ALA	8.3
1	C	142	ALA	8.3
1	A	240	GLN	8.3
1	D	363	ASN	8.3
1	B	366	ILE	8.3
1	A	121	THR	8.3
1	A	234	SER	8.3
1	B	479	VAL	8.3
1	D	256	GLN	8.3
1	A	427	HIS	8.3
1	B	27	LEU	8.3
1	C	415	LEU	8.3
1	A	147	VAL	8.2
1	C	386	ALA	8.2
1	C	374	LEU	8.2
1	C	46	SER	8.2
1	D	295	MET	8.2
1	D	466	MET	8.2
1	A	171	LEU	8.2
1	B	360	ARG	8.2
1	B	495	LEU	8.2
1	C	433	VAL	8.2
1	B	205	THR	8.2
1	C	105	PHE	8.2
1	D	432	THR	8.2
1	D	561	THR	8.2
1	D	34	LEU	8.2
1	D	224	GLU	8.2
1	C	287	VAL	8.2
1	A	484	GLY	8.2
1	C	94	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
1	C	469	GLY	8.2
1	C	350	THR	8.2
1	D	341	ASP	8.2
1	D	153	ILE	8.2
1	D	507	ALA	8.2
1	B	551	VAL	8.2
1	C	292	ILE	8.2
1	B	257	LEU	8.1
1	D	385	ILE	8.1
1	B	439	TYR	8.1
1	B	227	THR	8.1
1	C	367	PRO	8.1
1	A	359	LEU	8.1
1	B	267	LEU	8.1
1	D	16	LEU	8.1
1	A	327	GLU	8.1
1	A	360	ARG	8.1
1	A	513	THR	8.1
1	B	570	GLY	8.1
1	C	73	GLY	8.1
1	C	299	LYS	8.1
1	D	22	PRO	8.1
1	D	33	ALA	8.1
1	D	447	ARG	8.1
1	B	146	VAL	8.1
1	B	185	VAL	8.1
1	C	571	VAL	8.0
1	B	230	PHE	8.0
1	A	485	GLN	8.0
1	C	222	GLY	8.0
1	D	560	GLY	8.0
1	B	84	ILE	8.0
1	D	423	SER	8.0
1	D	357	PRO	8.0
1	B	264	ALA	8.0
1	A	35	ILE	8.0
1	B	466	MET	8.0
1	D	119	GLN	8.0
1	B	380	SER	8.0
1	B	577	LYS	8.0
1	D	90	SER	8.0
1	A	218	LEU	8.0

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Mol	Chain	Res	Type	RSRZ
1	B	501	ILE	8.0
1	C	216	GLU	8.0
1	C	307	GLN	8.0
1	A	533	LEU	8.0
1	D	36	LEU	8.0
1	D	534	VAL	8.0
1	D	133	GLU	8.0
1	D	87	TYR	7.9
1	A	12	THR	7.9
1	B	132	SER	7.9
1	D	426	VAL	7.9
1	D	123	THR	7.9
1	B	210	MET	7.9
1	C	89	ILE	7.9
1	C	380	SER	7.9
1	B	235	ASN	7.9
1	D	306	ALA	7.9
1	B	16	LEU	7.9
1	D	81	THR	7.9
1	A	362	ILE	7.9
1	C	70	VAL	7.9
1	C	112	PRO	7.9
1	C	409	GLU	7.9
1	A	174	LEU	7.9
1	B	51	LEU	7.9
1	D	35	ILE	7.9
1	B	240	GLN	7.9
1	A	29	VAL	7.8
1	B	189	PHE	7.8
1	C	352	PRO	7.8
1	C	440	ALA	7.8
1	A	75	MET	7.8
1	C	283	THR	7.8
1	B	533	LEU	7.8
1	C	87	TYR	7.8
1	D	557	VAL	7.8
1	B	13	PHE	7.8
1	C	351	TYR	7.8
1	A	406	ASP	7.7
1	C	29	VAL	7.7
1	B	66	TRP	7.7
1	D	564	GLU	7.7

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Mol	Chain	Res	Type	RSRZ
1	D	442	THR	7.7
1	D	515	SER	7.7
1	A	365	LYS	7.7
1	C	439	TYR	7.7
1	C	18	PRO	7.7
1	B	319	PHE	7.7
1	C	226	GLU	7.7
1	B	142	ALA	7.7
1	B	145	THR	7.7
1	D	386	ALA	7.7
1	A	156	LEU	7.7
1	D	468	ASN	7.7
1	A	176	PRO	7.7
1	C	28	ILE	7.7
1	C	463	ILE	7.7
1	A	581	GLY	7.7
1	C	524	ASP	7.7
1	C	34	LEU	7.7
1	D	458	TYR	7.7
1	B	348	THR	7.7
1	C	357	PRO	7.7
1	A	244	MET	7.7
1	B	269	ALA	7.6
1	A	177	ILE	7.6
1	D	255	ILE	7.6
1	A	91	TRP	7.6
1	B	226	GLU	7.6
1	A	338	ALA	7.6
1	A	130	TYR	7.6
1	A	122	GLY	7.6
1	C	382	LYS	7.6
1	B	154	ILE	7.6
1	B	211	LEU	7.6
1	C	302	THR	7.6
1	D	114	ALA	7.6
1	C	201	GLY	7.6
1	D	77	LEU	7.6
1	D	530	ARG	7.6
1	C	434	ALA	7.6
1	A	243	LYS	7.5
1	D	155	GLY	7.5
1	A	337	ARG	7.5

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Mol	Chain	Res	Type	RSRZ
1	B	362	ILE	7.5
1	D	66	TRP	7.5
1	C	130	TYR	7.5
1	C	423	SER	7.5
1	C	309	GLN	7.5
1	A	170	ILE	7.5
1	D	219	ILE	7.5
1	C	59	THR	7.5
1	C	388	LEU	7.5
1	D	541	THR	7.5
1	C	15	ARG	7.5
1	A	172	VAL	7.5
1	A	323	ASP	7.5
1	C	341	ASP	7.5
1	B	397	GLU	7.5
1	C	534	VAL	7.5
1	A	200	MET	7.5
1	D	298	LEU	7.5
1	A	554	GLY	7.5
1	A	555	ILE	7.5
1	C	186	SER	7.5
1	C	235	ASN	7.5
1	B	520	GLN	7.5
1	A	470	LEU	7.5
1	C	188	ARG	7.5
1	D	117	ASP	7.5
1	D	535	ILE	7.5
1	C	194	LYS	7.5
1	C	471	ASP	7.5
1	B	270	ALA	7.4
1	D	545	ALA	7.4
1	C	192	ILE	7.4
1	D	350	THR	7.4
1	A	38	ALA	7.4
1	B	453	ALA	7.4
1	A	26	GLY	7.4
1	A	141	GLY	7.4
1	D	84	ILE	7.4
1	A	112	PRO	7.4
1	D	92	VAL	7.4
1	C	383	SER	7.4
1	B	115	PHE	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	341	ASP	7.4
1	C	368	ALA	7.4
1	B	558	GLU	7.4
1	D	384	THR	7.4
1	A	535	ILE	7.4
1	B	555	ILE	7.4
1	D	20	ILE	7.4
1	A	37	ASN	7.4
1	C	392	PHE	7.4
1	B	580	PHE	7.4
1	D	273	PRO	7.4
1	D	342	LEU	7.4
1	B	372	VAL	7.3
1	B	581	GLY	7.3
1	D	70	VAL	7.3
1	D	524	ASP	7.3
1	B	46	SER	7.3
1	B	167	LEU	7.3
1	B	516	GLU	7.3
1	D	448	GLU	7.3
1	A	235	ASN	7.3
1	D	67	MET	7.3
1	D	526	LEU	7.3
1	D	230	PHE	7.3
1	C	116	PHE	7.3
1	D	312	MET	7.3
1	A	520	GLN	7.3
1	C	187	LYS	7.3
1	B	103	ARG	7.3
1	C	84	ILE	7.3
1	A	314	ALA	7.3
1	B	147	VAL	7.3
1	C	92	VAL	7.3
1	B	578	MET	7.3
1	C	514	GLU	7.2
1	A	571	VAL	7.2
1	D	479	VAL	7.2
1	C	69	LEU	7.2
1	D	122	GLY	7.2
1	A	72	ILE	7.2
1	C	190	ARG	7.2
1	A	27	LEU	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	263	LEU	7.2
1	B	268	TYR	7.2
1	A	181	ALA	7.2
1	A	569	HIS	7.2
1	D	318	LEU	7.2
1	D	78	ARG	7.2
1	C	90	SER	7.2
1	C	407	LEU	7.2
1	C	205	THR	7.2
1	A	74	LEU	7.2
1	B	526	LEU	7.2
1	C	472	THR	7.2
1	C	461	ASP	7.2
1	B	418	GLN	7.2
1	B	80	ILE	7.2
1	B	148	ARG	7.2
1	B	150	GLY	7.2
1	C	63	VAL	7.2
1	B	174	LEU	7.2
1	D	461	ASP	7.2
1	B	15	ARG	7.2
1	B	73	GLY	7.1
1	C	60	ASP	7.1
1	D	30	ALA	7.1
1	B	472	THR	7.1
1	D	383	SER	7.1
1	B	575	LEU	7.1
1	D	319	PHE	7.1
1	C	459	ALA	7.1
1	C	344	PHE	7.1
1	D	276	MET	7.1
1	D	459	ALA	7.1
1	C	395	ILE	7.1
1	B	371	THR	7.1
1	D	150	GLY	7.1
1	D	157	PHE	7.1
1	C	168	SER	7.1
1	B	417	ASN	7.1
1	D	154	ILE	7.1
1	B	261	LEU	7.1
1	D	316	GLN	7.1
1	D	32	ILE	7.1

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Mol	Chain	Res	Type	RSRZ
1	C	464	ASN	7.0
1	C	17	TRP	7.0
1	A	148	ARG	7.0
1	C	538	ARG	7.0
1	D	29	VAL	7.0
1	B	242	MET	7.0
1	B	214	HIS	7.0
1	A	115	PHE	7.0
1	C	37	ASN	7.0
1	D	308	PHE	7.0
1	A	568	GLN	7.0
1	B	507	ALA	7.0
1	B	514	GLU	7.0
1	C	447	ARG	7.0
1	A	96	VAL	7.0
1	D	23	PHE	7.0
1	A	80	ILE	7.0
1	A	432	THR	7.0
1	C	325	GLU	7.0
1	D	227	THR	7.0
1	A	237	MET	7.0
1	B	155	GLY	7.0
1	B	229	ARG	7.0
1	B	342	LEU	7.0
1	B	470	LEU	7.0
1	D	65	LEU	7.0
1	A	247	ALA	7.0
1	A	307	GLN	7.0
1	D	452	GLU	7.0
1	A	173	VAL	7.0
1	A	180	ILE	7.0
1	D	127	ARG	7.0
1	C	291	MET	7.0
1	A	123	THR	7.0
1	D	63	VAL	6.9
1	B	26	GLY	6.9
1	C	556	ILE	6.9
1	D	126	SER	6.9
1	B	114	ALA	6.9
1	C	326	GLN	6.9
1	C	24	LYS	6.9
1	B	178	VAL	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	419	VAL	6.9
1	C	189	PHE	6.9
1	B	108	MET	6.9
1	C	574	GLN	6.9
1	C	327	GLU	6.9
1	D	450	ILE	6.9
1	B	63	VAL	6.9
1	C	453	ALA	6.9
1	B	212	LYS	6.9
1	C	520	GLN	6.9
1	C	264	ALA	6.9
1	A	380	SER	6.9
1	B	152	SER	6.9
1	D	168	SER	6.9
1	D	272	PHE	6.9
1	D	39	ALA	6.9
1	B	396	ASP	6.9
1	D	422	VAL	6.9
1	A	328	LYS	6.9
1	D	470	LEU	6.9
1	C	408	ARG	6.8
1	D	469	GLY	6.8
1	A	99	THR	6.8
1	A	320	ALA	6.8
1	C	143	LEU	6.8
1	B	24	LYS	6.8
1	C	293	ALA	6.8
1	A	32	ILE	6.8
1	A	219	ILE	6.8
1	B	349	PHE	6.8
1	A	126	SER	6.8
1	B	266	VAL	6.8
1	B	441	ARG	6.8
1	B	213	GLY	6.8
1	D	27	LEU	6.8
1	C	402	MET	6.8
1	C	389	ILE	6.8
1	A	113	VAL	6.8
1	C	178	VAL	6.8
1	B	35	ILE	6.7
1	B	202	GLN	6.7
1	C	220	PHE	6.7

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Mol	Chain	Res	Type	RSRZ
1	D	55	GLY	6.7
1	D	68	PRO	6.7
1	B	170	ILE	6.7
1	D	302	THR	6.7
1	D	313	ALA	6.7
1	D	393	TYR	6.7
1	A	267	LEU	6.7
1	A	573	ALA	6.7
1	D	544	GLN	6.7
1	C	550	VAL	6.7
1	D	449	GLN	6.7
1	B	137	SER	6.7
1	B	191	SER	6.7
1	B	500	PRO	6.7
1	B	496	LEU	6.7
1	D	364	LEU	6.7
1	D	462	PHE	6.7
1	B	557	VAL	6.7
1	C	451	GLU	6.7
1	B	192	ILE	6.7
1	C	182	ILE	6.7
1	C	221	GLY	6.7
1	D	58	LYS	6.7
1	D	283	THR	6.7
1	A	325	GLU	6.7
1	A	124	LEU	6.7
1	C	450	ILE	6.6
1	B	554	GLY	6.6
1	A	127	ARG	6.6
1	B	61	ARG	6.6
1	B	65	LEU	6.6
1	D	38	ALA	6.6
1	D	359	LEU	6.6
1	D	391	ARG	6.6
1	C	126	SER	6.6
1	A	114	ALA	6.6
1	A	545	ALA	6.6
1	C	462	PHE	6.6
1	A	196	MET	6.6
1	B	524	ASP	6.6
1	D	292	ILE	6.6
1	A	468	ASN	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	424	GLN	6.6
1	D	506	GLU	6.6
1	B	515	SER	6.6
1	D	380	SER	6.6
1	B	74	LEU	6.6
1	D	43	PHE	6.6
1	A	284	ILE	6.6
1	A	257	LEU	6.6
1	B	443	GLU	6.6
1	C	551	VAL	6.6
1	C	295	MET	6.6
1	D	75	MET	6.6
1	A	250	ILE	6.6
1	D	72	ILE	6.6
1	D	288	PHE	6.6
1	C	557	VAL	6.6
1	C	435	ASN	6.5
1	A	183	ARG	6.5
1	A	67	MET	6.5
1	B	359	LEU	6.5
1	A	213	GLY	6.5
1	C	428	LEU	6.5
1	D	74	LEU	6.5
1	D	193	SER	6.5
1	D	542	ILE	6.5
1	A	455	ARG	6.5
1	D	287	VAL	6.5
1	A	575	LEU	6.5
1	D	233	VAL	6.5
1	B	171	LEU	6.5
1	B	78	ARG	6.5
1	B	188	ARG	6.5
1	C	298	LEU	6.5
1	A	182	ILE	6.5
1	C	535	ILE	6.5
1	B	71	VAL	6.4
1	B	224	GLU	6.4
1	B	452	GLU	6.4
1	D	61	ARG	6.4
1	B	402	MET	6.4
1	B	107	HIS	6.4
1	B	368	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	475	GLY	6.4
1	B	236	LYS	6.4
1	C	460	MET	6.4
1	C	528	LYS	6.4
1	A	150	GLY	6.4
1	D	523	LEU	6.4
1	D	505	ASP	6.4
1	B	29	VAL	6.4
1	A	28	ILE	6.4
1	B	149	GLU	6.4
1	D	190	ARG	6.4
1	D	310	ARG	6.4
1	D	304	VAL	6.3
1	A	231	ASP	6.3
1	A	311	GLY	6.3
1	C	416	ARG	6.3
1	B	370	LYS	6.3
1	A	242	MET	6.3
1	A	439	TYR	6.3
1	A	411	THR	6.3
1	C	36	LEU	6.3
1	D	69	LEU	6.3
1	D	407	LEU	6.3
1	A	472	THR	6.3
1	D	451	GLU	6.3
1	A	152	SER	6.3
1	A	324	SER	6.3
1	D	580	PHE	6.3
1	B	442	THR	6.3
1	C	289	SER	6.3
1	C	322	LEU	6.3
1	C	470	LEU	6.3
1	C	202	GLN	6.3
1	C	304	VAL	6.3
1	B	273	PRO	6.3
1	B	565	LEU	6.3
1	B	33	ALA	6.2
1	B	182	ILE	6.2
1	B	200	MET	6.2
1	A	283	THR	6.2
1	A	36	LEU	6.2
1	B	68	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	183	ARG	6.2
1	A	135	VAL	6.2
1	C	225	VAL	6.2
1	A	321	ILE	6.2
1	D	463	ILE	6.2
1	C	348	THR	6.2
1	D	399	HIS	6.2
1	A	504	LEU	6.2
1	D	64	LEU	6.2
1	A	66	TRP	6.2
1	A	426	VAL	6.2
1	B	123	THR	6.2
1	C	414	SER	6.2
1	D	236	LYS	6.2
1	B	464	ASN	6.2
1	B	203	VAL	6.1
1	C	74	LEU	6.1
1	A	348	THR	6.1
1	A	169	ILE	6.1
1	B	70	VAL	6.1
1	D	76	ILE	6.1
1	D	57	GLY	6.1
1	B	151	ALA	6.1
1	A	59	THR	6.1
1	B	172	VAL	6.1
1	B	168	SER	6.1
1	C	81	THR	6.1
1	B	340	GLY	6.1
1	A	151	ALA	6.1
1	B	275	VAL	6.1
1	A	528	LYS	6.1
1	C	324	SER	6.1
1	C	115	PHE	6.1
1	C	72	ILE	6.0
1	A	516	GLU	6.0
1	B	183	ARG	6.0
1	D	566	LEU	6.0
1	A	562	HIS	6.0
1	B	404	GLY	6.0
1	C	360	ARG	6.0
1	A	58	LYS	6.0
1	B	195	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	372	VAL	6.0
1	B	237	MET	6.0
1	D	516	GLU	6.0
1	D	26	GLY	6.0
1	C	23	PHE	6.0
1	C	429	PHE	6.0
1	A	254	ILE	6.0
1	D	71	VAL	6.0
1	C	39	ALA	6.0
1	C	12	THR	6.0
1	C	432	THR	6.0
1	A	145	THR	6.0
1	A	308	PHE	6.0
1	C	570	GLY	6.0
1	C	536	ALA	6.0
1	B	67	MET	6.0
1	D	369	GLY	5.9
1	D	473	ILE	5.9
1	A	184	VAL	5.9
1	D	286	VAL	5.9
1	A	301	LEU	5.9
1	A	441	ARG	5.9
1	D	282	GLY	5.9
1	D	395	ILE	5.9
1	C	290	SER	5.9
1	A	342	LEU	5.9
1	C	430	ASN	5.9
1	C	523	LEU	5.9
1	B	222	GLY	5.9
1	A	226	GLU	5.9
1	B	153	ILE	5.9
1	B	159	MET	5.9
1	C	521	ALA	5.9
1	D	167	LEU	5.9
1	D	431	ASP	5.9
1	D	543	GLU	5.9
1	C	118	LYS	5.9
1	B	274	SER	5.9
1	D	182	ILE	5.9
1	D	160	MET	5.9
1	A	116	PHE	5.9
1	C	66	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	221	GLY	5.9
1	B	331	GLY	5.9
1	A	402	MET	5.9
1	D	47	LEU	5.9
1	A	367	PRO	5.8
1	D	18	PRO	5.8
1	B	238	ARG	5.8
1	A	76	ILE	5.8
1	B	72	ILE	5.8
1	D	164	SER	5.8
1	D	575	LEU	5.8
1	A	389	ILE	5.8
1	D	28	ILE	5.8
1	A	349	PHE	5.8
1	C	174	LEU	5.8
1	A	578	MET	5.8
1	B	79	GLY	5.8
1	D	307	GLN	5.8
1	B	233	VAL	5.8
1	C	67	MET	5.8
1	D	565	LEU	5.8
1	D	343	GLU	5.8
1	C	516	GLU	5.8
1	D	478	GLY	5.8
1	B	158	ILE	5.8
1	C	525	GLU	5.7
1	A	526	LEU	5.7
1	B	196	MET	5.7
1	C	282	GLY	5.7
1	D	281	ALA	5.7
1	D	441	ARG	5.7
1	C	485	GLN	5.7
1	D	381	GLY	5.7
1	A	428	LEU	5.7
1	C	146	VAL	5.7
1	C	546	ASP	5.7
1	A	570	GLY	5.7
1	C	13	PHE	5.7
1	C	349	PHE	5.7
1	B	405	HIS	5.7
1	D	42	THR	5.7
1	A	340	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	221	GLY	5.7
1	A	501	ILE	5.7
1	A	409	GLU	5.7
1	D	353	GLY	5.7
1	C	343	GLU	5.6
1	D	232	LYS	5.6
1	B	427	HIS	5.6
1	C	320	ALA	5.6
1	A	423	SER	5.6
1	C	161	PHE	5.6
1	A	503	ILE	5.6
1	A	266	VAL	5.6
1	C	505	ASP	5.6
1	A	369	GLY	5.6
1	C	342	LEU	5.6
1	A	149	GLU	5.6
1	D	464	ASN	5.6
1	A	202	GLN	5.6
1	B	232	LYS	5.6
1	A	120	SER	5.6
1	C	504	LEU	5.6
1	C	371	THR	5.6
1	D	118	LYS	5.5
1	D	411	THR	5.5
1	C	431	ASP	5.5
1	C	78	ARG	5.5
1	A	92	VAL	5.5
1	A	220	PHE	5.5
1	A	435	ASN	5.5
1	C	333	ARG	5.5
1	A	146	VAL	5.5
1	C	50	PRO	5.5
1	D	151	ALA	5.5
1	B	444	GLU	5.5
1	B	272	PHE	5.5
1	C	176	PRO	5.5
1	C	527	GLN	5.5
1	C	68	PRO	5.5
1	D	382	LYS	5.5
1	A	506	GLU	5.5
1	D	46	SER	5.4
1	D	340	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	119	GLN	5.4
1	D	21	ALA	5.4
1	B	432	THR	5.4
1	D	320	ALA	5.4
1	D	567	ALA	5.4
1	D	194	LYS	5.4
1	D	368	ALA	5.4
1	C	165	TRP	5.4
1	B	531	THR	5.4
1	D	522	ALA	5.4
1	D	239	LEU	5.4
1	C	20	ILE	5.4
1	D	158	ILE	5.4
1	D	322	LEU	5.4
1	C	310	ARG	5.4
1	D	408	ARG	5.4
1	C	117	ASP	5.4
1	D	131	ASP	5.4
1	B	141	GLY	5.4
1	D	311	GLY	5.4
1	A	326	GLN	5.3
1	B	271	SER	5.3
1	B	463	ILE	5.3
1	A	410	TYR	5.3
1	B	22	PRO	5.3
1	B	228	LYS	5.3
1	D	300	SER	5.3
1	A	227	THR	5.3
1	B	546	ASP	5.3
1	D	360	ARG	5.3
1	A	322	LEU	5.3
1	A	203	VAL	5.3
1	D	228	LYS	5.3
1	B	134	GLN	5.3
1	B	75	MET	5.3
1	C	184	VAL	5.2
1	D	347	VAL	5.2
1	A	500	PRO	5.2
1	A	577	LYS	5.2
1	C	228	LYS	5.2
1	C	410	TYR	5.2
1	B	177	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	165	TRP	5.2
1	B	411	THR	5.2
1	B	476	GLU	5.2
1	A	401	LEU	5.2
1	D	531	THR	5.2
1	D	330	GLU	5.2
1	A	71	VAL	5.2
1	B	173	VAL	5.2
1	A	469	GLY	5.2
1	C	477	ASN	5.2
1	D	520	GLN	5.2
1	A	304	VAL	5.2
1	D	527	GLN	5.1
1	C	229	ARG	5.1
1	A	343	GLU	5.1
1	C	180	ILE	5.1
1	C	353	GLY	5.1
1	B	277	ASP	5.1
1	B	504	LEU	5.1
1	D	156	LEU	5.1
1	C	163	TYR	5.1
1	B	32	ILE	5.1
1	C	526	LEU	5.1
1	D	197	GLN	5.1
1	D	220	PHE	5.0
1	D	17	TRP	5.0
1	A	253	PRO	5.0
1	B	165	TRP	5.0
1	C	438	ALA	5.0
1	B	50	PRO	5.0
1	C	294	LEU	5.0
1	A	199	THR	5.0
1	D	525	GLU	5.0
1	C	522	ALA	5.0
1	D	400	ILE	4.9
1	C	45	LEU	4.9
1	D	191	SER	4.9
1	B	239	LEU	4.9
1	D	10	TRP	4.9
1	C	396	ASP	4.9
1	A	77	LEU	4.9
1	A	95	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	187	LYS	4.9
1	B	52	LEU	4.9
1	B	69	LEU	4.9
1	A	229	ARG	4.9
1	A	187	LYS	4.9
1	A	368	ALA	4.9
1	B	138	SER	4.9
1	D	15	ARG	4.9
1	B	304	VAL	4.9
1	A	111	MET	4.9
1	B	76	ILE	4.9
1	C	75	MET	4.8
1	C	169	ILE	4.8
1	A	64	LEU	4.8
1	D	80	ILE	4.8
1	B	455	ARG	4.8
1	B	517	ARG	4.8
1	D	401	LEU	4.8
1	C	173	VAL	4.8
1	D	331	GLY	4.8
1	A	185	VAL	4.8
1	B	307	GLN	4.8
1	C	465	LYS	4.8
1	B	408	ARG	4.8
1	C	413	ALA	4.8
1	D	504	LEU	4.8
1	B	461	ASP	4.8
1	D	285	THR	4.8
1	C	71	VAL	4.8
1	D	477	ASN	4.8
1	A	192	ILE	4.7
1	A	422	VAL	4.7
1	A	216	GLU	4.7
1	C	452	GLU	4.7
1	C	38	ALA	4.7
1	D	365	LYS	4.7
1	A	499	SER	4.7
1	C	177	ILE	4.7
1	A	552	GLU	4.7
1	D	577	LYS	4.7
1	D	54	ASP	4.7
1	A	263	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	199	THR	4.7
1	B	525	GLU	4.7
1	A	233	VAL	4.7
1	C	119	GLN	4.7
1	A	449	GLN	4.7
1	B	23	PHE	4.6
1	A	443	GLU	4.6
1	D	556	ILE	4.6
1	D	321	ILE	4.6
1	A	272	PHE	4.6
1	B	42	THR	4.6
1	D	142	ALA	4.6
1	C	147	VAL	4.6
1	C	83	TYR	4.6
1	A	25	ALA	4.6
1	A	232	LYS	4.6
1	D	226	GLU	4.6
1	B	25	ALA	4.6
1	C	41	ASP	4.6
1	A	236	LYS	4.5
1	C	76	ILE	4.5
1	C	482	SER	4.5
1	A	70	VAL	4.5
1	D	24	LYS	4.5
1	D	578	MET	4.5
1	C	500	PRO	4.5
1	A	154	ILE	4.5
1	D	201	GLY	4.5
1	C	77	LEU	4.5
1	D	465	LYS	4.5
1	D	554	GLY	4.5
1	C	401	LEU	4.5
1	C	361	ASN	4.5
1	C	308	PHE	4.5
1	C	64	LEU	4.4
1	D	183	ARG	4.4
1	A	505	ASP	4.4
1	D	51	LEU	4.4
1	B	387	SER	4.4
1	D	406	ASP	4.4
1	A	529	ASN	4.4
1	B	77	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	370	LYS	4.4
1	A	438	ALA	4.4
1	D	229	ARG	4.4
1	D	299	LYS	4.4
1	A	448	GLU	4.4
1	A	134	GLN	4.4
1	D	134	GLN	4.4
1	D	83	TYR	4.4
1	A	524	ASP	4.4
1	A	224	GLU	4.4
1	A	49	LYS	4.4
1	C	454	ALA	4.3
1	D	301	LEU	4.3
1	D	11	GLN	4.3
1	A	165	TRP	4.3
1	D	514	GLU	4.3
1	A	239	LEU	4.3
1	A	476	GLU	4.2
1	A	230	PHE	4.2
1	A	478	GLY	4.2
1	D	574	GLN	4.2
1	D	460	MET	4.2
1	B	91	TRP	4.2
1	D	410	TYR	4.2
1	C	171	LEU	4.2
1	D	367	PRO	4.2
1	B	308	PHE	4.2
1	B	276	MET	4.2
1	B	290	SER	4.2
1	B	406	ASP	4.2
1	B	28	ILE	4.1
1	C	160	MET	4.1
1	A	450	ILE	4.1
1	D	187	LYS	4.1
1	D	198	ASN	4.1
1	A	460	MET	4.1
1	B	58	LYS	4.1
1	B	324	SER	4.1
1	B	505	ASP	4.1
1	C	65	LEU	4.1
1	A	10	TRP	4.1
1	A	221	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	145	THR	4.0
1	C	150	GLY	4.0
1	D	171	LEU	4.0
1	D	326	GLN	4.0
1	A	561	THR	4.0
1	D	79	GLY	4.0
1	A	228	LYS	4.0
1	B	311	GLY	4.0
1	D	95	LYS	4.0
1	D	181	ALA	4.0
1	B	184	VAL	3.9
1	B	176	PRO	3.9
1	B	521	ALA	3.9
1	D	138	SER	3.9
1	A	14	ARG	3.9
1	B	297	PRO	3.9
1	C	331	GLY	3.9
1	C	170	ILE	3.9
1	D	427	HIS	3.9
1	B	522	ALA	3.9
1	A	73	GLY	3.9
1	D	345	ARG	3.8
1	D	258	ILE	3.8
1	C	411	THR	3.8
1	B	446	SER	3.8
1	A	350	THR	3.8
1	C	345	ARG	3.8
1	D	166	GLN	3.8
1	C	172	VAL	3.8
1	B	169	ILE	3.8
1	C	323	ASP	3.7
1	A	188	ARG	3.7
1	A	354	ARG	3.7
1	A	201	GLY	3.7
1	C	79	GLY	3.7
1	D	178	VAL	3.7
1	B	62	SER	3.7
1	A	514	GLU	3.7
1	A	547	GLU	3.7
1	C	506	GLU	3.7
1	A	117	ASP	3.7
1	A	158	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	370	LYS	3.7
1	C	296	ARG	3.7
1	D	528	LYS	3.7
1	C	122	GLY	3.6
1	D	398	GLY	3.6
1	D	344	PHE	3.6
1	C	441	ARG	3.6
1	B	36	LEU	3.6
1	D	45	LEU	3.6
1	A	217	VAL	3.6
1	C	43	PHE	3.6
1	B	346	ASN	3.6
1	B	410	TYR	3.6
1	A	153	ILE	3.6
1	D	177	ILE	3.5
1	D	289	SER	3.5
1	C	232	LYS	3.5
1	D	159	MET	3.5
1	D	184	VAL	3.5
1	D	325	GLU	3.5
1	A	461	ASP	3.4
1	A	565	LEU	3.4
1	A	24	LYS	3.4
1	C	49	LYS	3.4
1	A	225	VAL	3.4
1	B	111	MET	3.4
1	B	332	LYS	3.3
1	B	401	LEU	3.3
1	B	293	ALA	3.3
1	C	286	VAL	3.3
1	D	296	ARG	3.3
1	C	80	ILE	3.3
1	D	555	ILE	3.3
1	B	460	MET	3.3
1	D	161	PHE	3.3
1	D	180	ILE	3.2
1	B	409	GLU	3.2
1	A	300	SER	3.2
1	A	515	SER	3.2
1	D	172	VAL	3.2
1	D	222	GLY	3.2
1	B	426	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	14	ARG	3.2
1	D	173	VAL	3.2
1	D	170	ILE	3.2
1	B	49	LYS	3.1
1	C	151	ALA	3.1
1	D	388	LEU	3.1
1	B	423	SER	3.1
1	A	297	PRO	3.1
1	C	11	GLN	3.1
1	B	180	ILE	3.1
1	A	155	GLY	3.0
1	C	354	ARG	3.0
1	B	544	GLN	3.0
1	C	424	GLN	3.0
1	B	422	VAL	3.0
1	A	346	ASN	3.0
1	C	40	SER	3.0
1	D	354	ARG	3.0
1	D	279	LEU	2.9
1	A	11	GLN	2.9
1	C	455	ARG	2.9
1	B	156	LEU	2.9
1	D	346	ASN	2.9
1	B	201	GLY	2.9
1	C	300	SER	2.9
1	D	280	THR	2.8
1	A	331	GLY	2.8
1	A	271	SER	2.8
1	A	531	THR	2.7
1	B	135	VAL	2.7
1	D	174	LEU	2.7
1	D	141	GLY	2.6
1	A	525	GLU	2.6
1	C	530	ARG	2.6
1	C	54	ASP	2.5
1	B	445	TYR	2.5
1	A	22	PRO	2.5
1	D	50	PRO	2.5
1	B	282	GLY	2.5
1	C	10	TRP	2.4
1	D	517	ARG	2.4
1	D	475	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	324	SER	2.4
1	D	518	ALA	2.4
1	B	43	PHE	2.3
1	B	14	ARG	2.3
1	A	40	SER	2.3
1	C	340	GLY	2.3
1	C	120	SER	2.3
1	D	169	ILE	2.3
1	C	555	ILE	2.3
1	A	13	PHE	2.2
1	A	353	GLY	2.2
1	D	455	ARG	2.2
1	C	476	GLU	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](#)

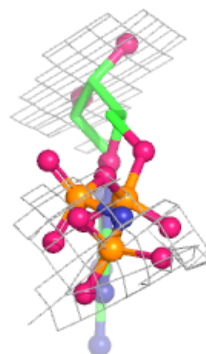
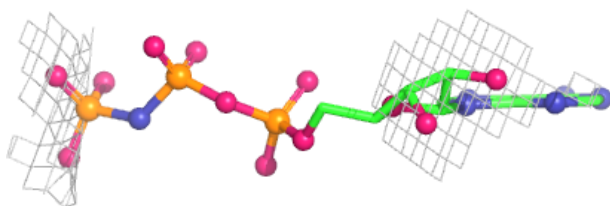
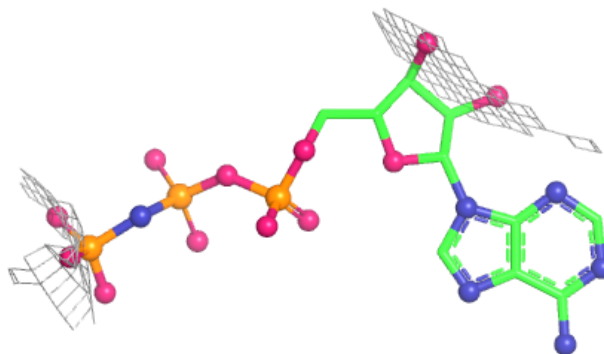
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ANP	A	5002	31/31	0.36	0.91	219,219,219,219	0
2	ANP	B	5001	31/31	0.71	0.83	219,219,219,219	0
2	ANP	D	5003	31/31	0.78	0.72	219,219,219,219	0
2	ANP	C	5004	31/31	0.88	0.69	219,219,219,219	0

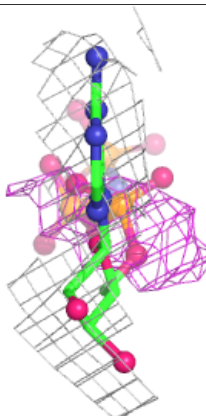
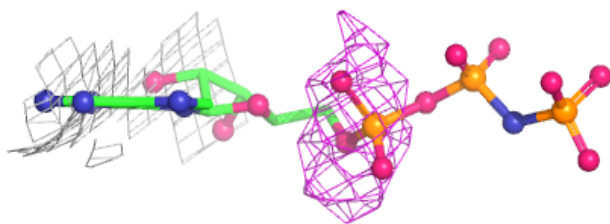
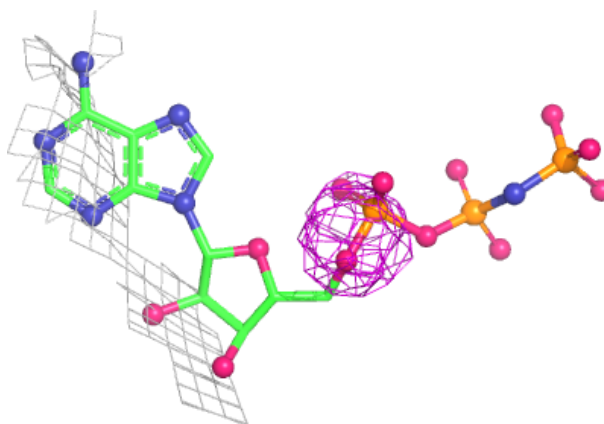
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 5002:

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

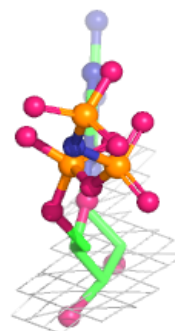
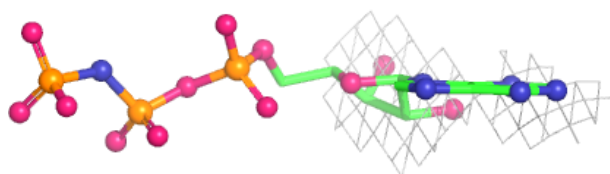
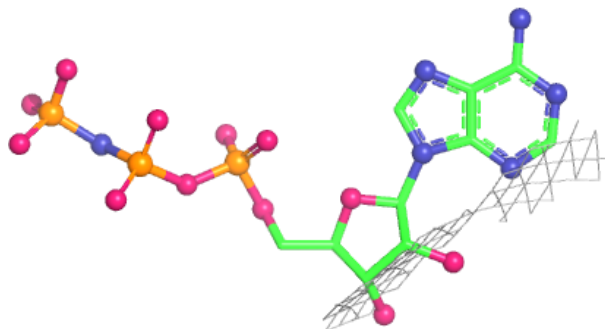
**Electron density around ANP B 5001:**

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

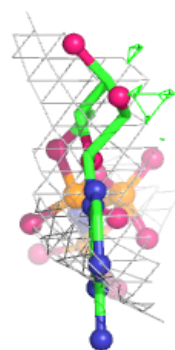
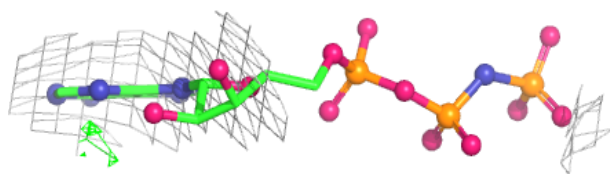
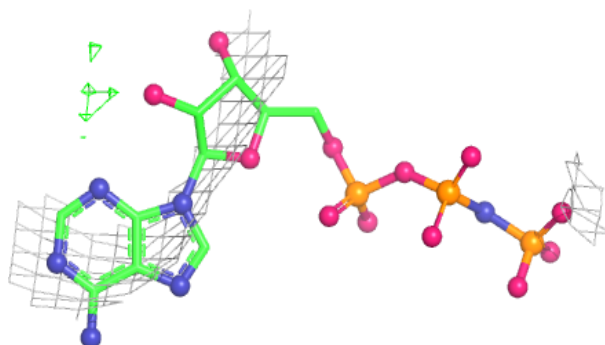


Electron density around ANP D 5003:

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

**Electron density around ANP C 5004:**

$2mF_o-DF_c$ (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.