



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:31 AM GMT

PDB ID : 3B5Y
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

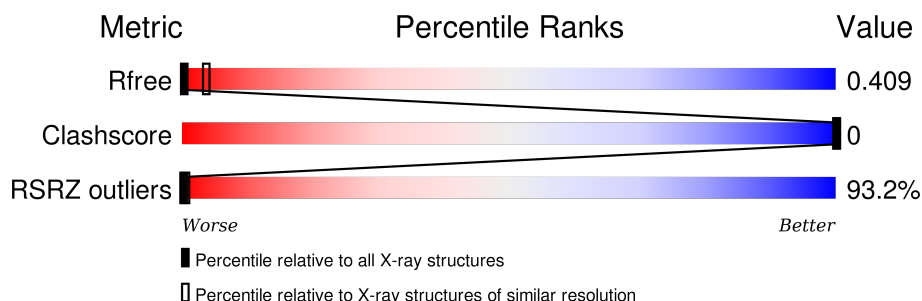
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

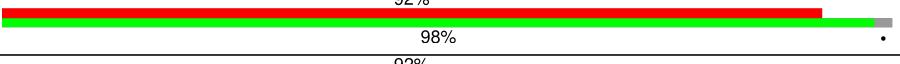
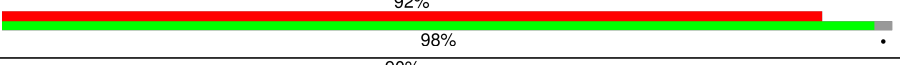
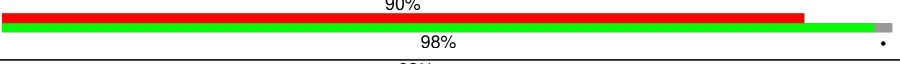
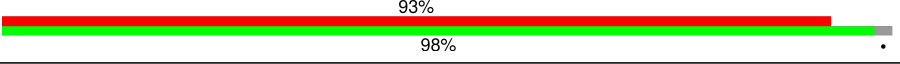
The reported resolution of this entry is 4.50 Å.

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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
RSRZ outliers	91569	1075 (5.40-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 <p>92% (upper red bar), 98% (lower bar)</p>
1	B	582	 <p>92% (upper red bar), 98% (lower bar)</p>
1	C	582	 <p>90% (upper red bar), 98% (lower bar)</p>
1	D	582	 <p>93% (upper red bar), 98% (lower bar)</p>

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	C	5004	-	-	-	X
2	ANP	D	5003	-	-	-	X

2 Entry composition ⓘ

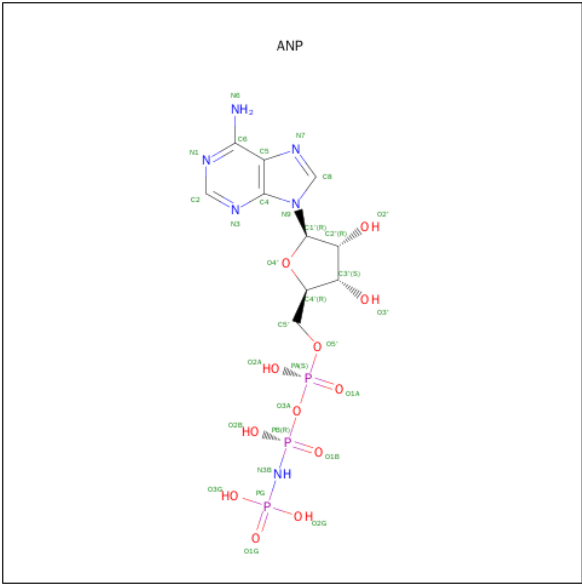
There are 2 unique types of molecules in this entry. The entry contains 2412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

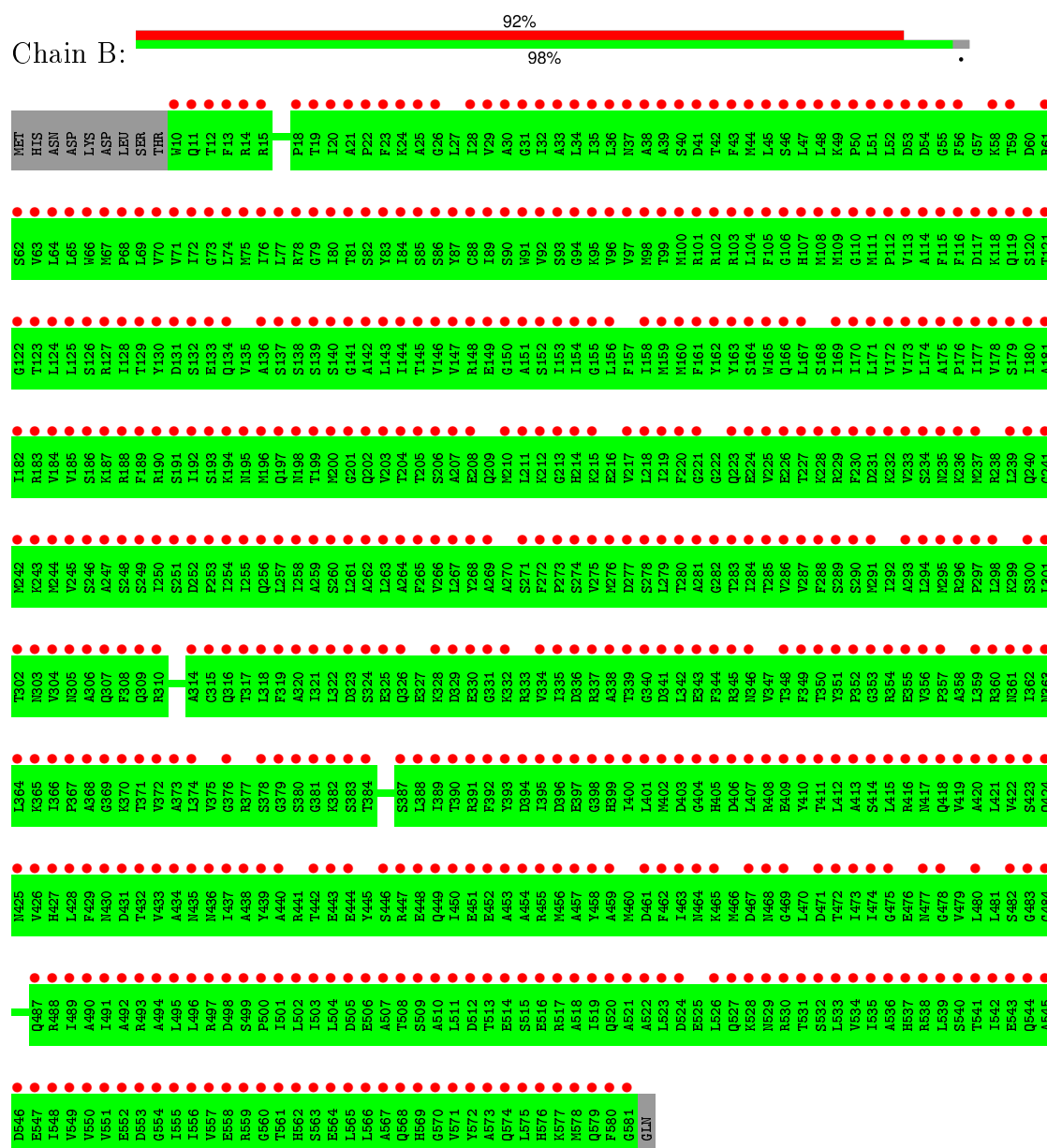
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

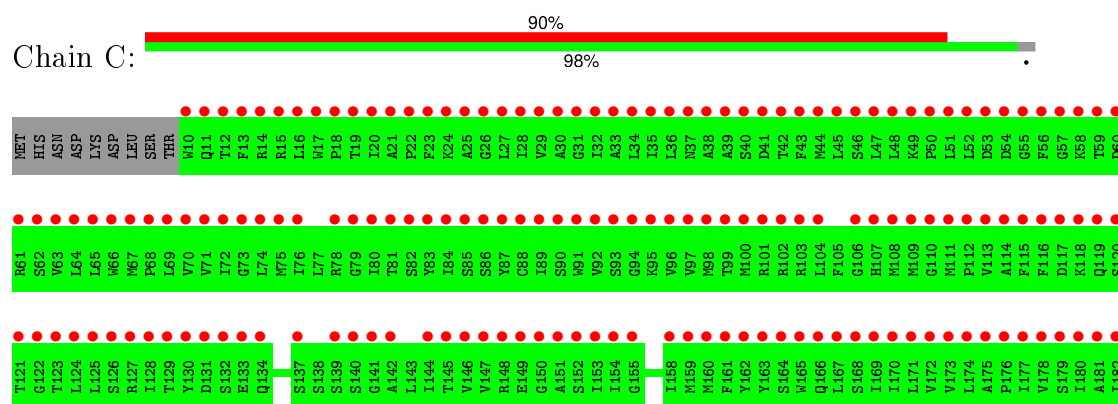
- Molecule 1: Lipid A export ATP-binding/permease protein msbA

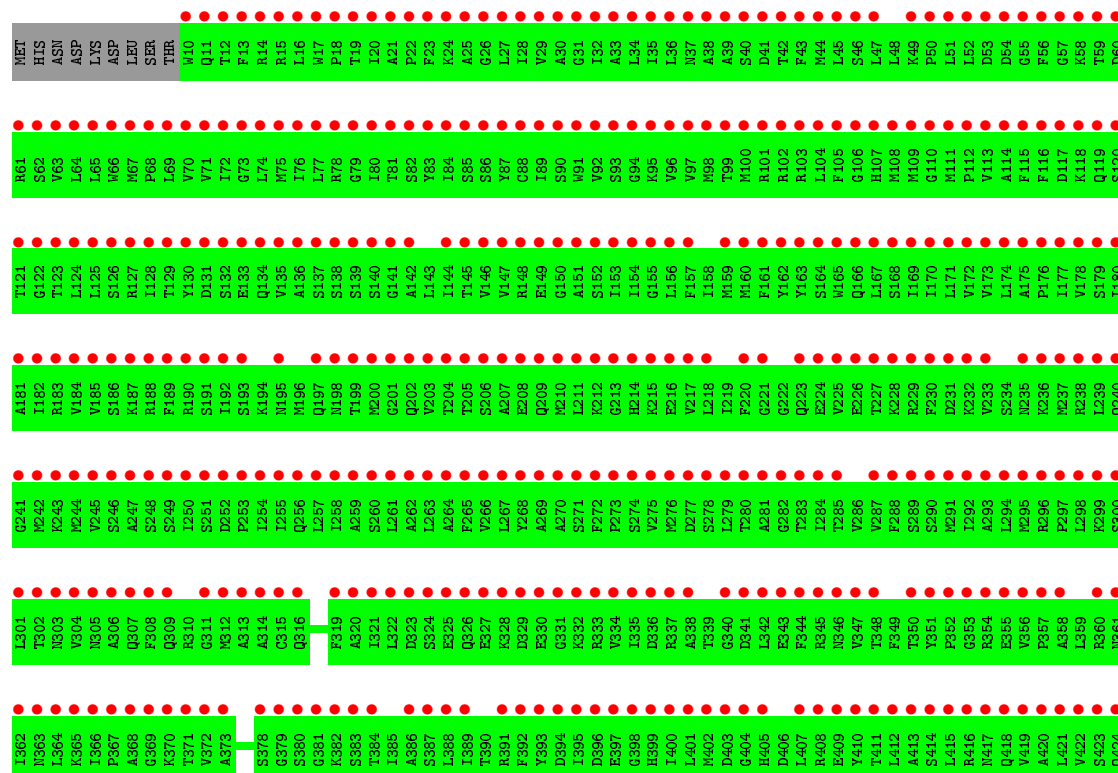


- Molecule 1: Lipid A export ATP-binding/permease protein msbA



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







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) 95.0 (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 0.378 , 0.409	Depositor DCC
R_{free} test set	2602 reflections (10.04%)	DCC
Wilson B-factor (Å ²)	184.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.65 , -9.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25959 reflections	Xtriage
F_o, F_c correlation	0.82	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, 0.375 respectively for untwinned datasets, and 0.333, 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 carbohydrates 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	A	5002	-	27,33,33	1.47	2 (7%)	30,52,52	2.39	8 (26%)
2	ANP	B	5001	-	27,33,33	2.33	9 (33%)	30,52,52	2.81	8 (26%)
2	ANP	C	5004	-	27,33,33	1.51	2 (7%)	30,52,52	2.38	8 (26%)
2	ANP	D	5003	-	27,33,33	1.48	2 (7%)	30,52,52	2.40	7 (23%)

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	A	5002	-	-	0/12/38/38	0/3/3/3
2	ANP	B	5001	-	-	0/12/38/38	0/3/3/3
2	ANP	C	5004	-	-	0/12/38/38	0/3/3/3
2	ANP	D	5003	-	-	0/12/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	PB-O1B	-6.58	1.38	1.46
2	B	5001	ANP	PA-O1A	-4.35	1.35	1.51
2	B	5001	ANP	PB-O2B	-4.25	1.44	1.56
2	C	5004	ANP	PB-O2B	-3.81	1.46	1.56
2	A	5002	ANP	PB-O2B	-3.75	1.46	1.56
2	D	5003	ANP	PB-O2B	-3.73	1.46	1.56
2	B	5001	ANP	O4'-C1'	-3.52	1.36	1.41
2	C	5004	ANP	PG-O2G	-3.46	1.47	1.56
2	D	5003	ANP	PG-O2G	-3.43	1.47	1.56
2	A	5002	ANP	PG-O2G	-3.42	1.47	1.56
2	B	5001	ANP	C3'-C4'	-3.30	1.44	1.53
2	B	5001	ANP	PG-O2G	-2.59	1.49	1.56
2	B	5001	ANP	PG-N3B	2.01	1.68	1.63
2	B	5001	ANP	PB-N3B	2.37	1.69	1.63
2	B	5001	ANP	O3'-C3'	3.04	1.50	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	ANP	C4'-O4'-C1'	-9.30	99.50	109.72
2	D	5003	ANP	C4'-O4'-C1'	-6.12	102.99	109.72
2	A	5002	ANP	C4'-O4'-C1'	-6.08	103.04	109.72
2	C	5004	ANP	C4'-O4'-C1'	-6.05	103.07	109.72
2	C	5004	ANP	O1B-PB-N3B	-4.58	104.87	111.90
2	A	5002	ANP	O1B-PB-N3B	-4.55	104.92	111.90
2	D	5003	ANP	O1B-PB-N3B	-4.54	104.94	111.90
2	C	5004	ANP	O1G-PG-N3B	-4.27	105.34	111.90
2	A	5002	ANP	O1G-PG-N3B	-4.26	105.37	111.90
2	D	5003	ANP	O1G-PG-N3B	-4.25	105.38	111.90
2	B	5001	ANP	O1B-PB-N3B	-3.94	105.85	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	ANP	O3G-PG-O1G	-2.78	106.10	113.49
2	B	5001	ANP	O3A-PA-O5'	-2.06	97.46	102.94
2	A	5002	ANP	C1'-N9-C4	2.02	129.98	126.94
2	C	5004	ANP	C1'-N9-C4	2.02	129.99	126.94
2	A	5002	ANP	O3G-PG-O2G	2.30	114.41	107.58
2	C	5004	ANP	O3G-PG-O2G	2.32	114.46	107.58
2	D	5003	ANP	O3G-PG-O2G	2.32	114.47	107.58
2	A	5002	ANP	C4-C5-N7	2.62	111.89	109.48
2	C	5004	ANP	C4-C5-N7	2.71	111.97	109.48
2	D	5003	ANP	C4-C5-N7	2.86	112.11	109.48
2	B	5001	ANP	C1'-N9-C4	3.57	132.33	126.94
2	A	5002	ANP	O2B-PB-O1B	3.68	117.67	110.00
2	D	5003	ANP	O2B-PB-O1B	3.71	117.74	110.00
2	C	5004	ANP	O2B-PB-O1B	3.71	117.74	110.00
2	B	5001	ANP	O2B-PB-O1B	4.90	120.24	110.00
2	B	5001	ANP	C4-C5-N7	5.02	114.10	109.48
2	B	5001	ANP	C2'-C1'-N9	6.35	123.99	114.29
2	C	5004	ANP	C2'-C1'-N9	6.68	124.49	114.29
2	D	5003	ANP	C2'-C1'-N9	6.79	124.67	114.29
2	A	5002	ANP	C2'-C1'-N9	6.81	124.70	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	6.56	533 (93%) 0 0	142, 225, 277, 312	0
1	B	572/582 (98%)	6.49	535 (93%) 0 0	112, 212, 274, 321	0
1	C	572/582 (98%)	6.68	525 (91%) 0 1	130, 218, 271, 309	0
1	D	572/582 (98%)	6.72	539 (94%) 0 0	132, 220, 271, 314	0
All	All	2288/2328 (98%)	6.61	2132 (93%) 0 0	112, 219, 274, 321	0

All (2132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	THR	28.5
1	B	428	LEU	27.0
1	B	427	HIS	26.7
1	A	300	SER	23.5
1	D	68	PRO	22.5
1	B	177	ILE	21.3
1	C	361	ASN	21.2
1	A	477	ASN	20.9
1	B	325	GLU	20.8
1	C	150	GLY	20.6
1	A	202	GLN	20.3
1	C	400	ILE	19.8
1	B	307	GLN	19.8
1	C	338	ALA	19.7
1	C	80	ILE	19.5
1	D	444	GLU	19.4
1	A	177	ILE	19.4
1	D	236	LYS	19.3
1	C	29	VAL	19.3
1	C	399	HIS	19.3
1	A	423	SER	19.2

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Mol	Chain	Res	Type	RSRZ
1	D	320	ALA	18.9
1	B	231	ASP	18.9
1	D	229	ARG	18.9
1	A	149	GLU	18.8
1	A	414	SER	18.6
1	D	277	ASP	18.3
1	B	360	ARG	18.0
1	C	231	ASP	17.9
1	B	258	ILE	17.6
1	A	365	LYS	17.2
1	C	151	ALA	17.1
1	C	431	ASP	17.1
1	A	303	ASN	17.1
1	C	25	ALA	17.0
1	B	304	VAL	17.0
1	D	473	ILE	17.0
1	D	417	ASN	16.8
1	B	151	ALA	16.5
1	D	567	ALA	16.5
1	D	131	ASP	16.2
1	A	37	ASN	16.1
1	C	213	GLY	16.1
1	D	119	GLN	16.0
1	D	73	GLY	15.9
1	B	115	PHE	15.9
1	C	276	MET	15.9
1	C	159	MET	15.8
1	B	399	HIS	15.8
1	A	394	ASP	15.8
1	C	78	ARG	15.8
1	B	158	ILE	15.8
1	C	247	ALA	15.7
1	A	43	PHE	15.7
1	D	564	GLU	15.6
1	A	546	ASP	15.6
1	D	560	GLY	15.5
1	C	308	PHE	15.4
1	C	196	MET	15.4
1	A	205	THR	15.3
1	C	21	ALA	15.2
1	B	134	GLN	15.2
1	D	576	HIS	15.2

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Mol	Chain	Res	Type	RSRZ
1	C	397	GLU	15.2
1	A	369	GLY	15.1
1	A	117	ASP	15.1
1	A	141	GLY	15.0
1	A	557	VAL	14.9
1	C	473	ILE	14.9
1	C	326	GLN	14.9
1	D	149	GLU	14.8
1	C	50	PRO	14.8
1	D	130	TYR	14.8
1	C	336	ASP	14.7
1	D	39	ALA	14.7
1	C	341	ASP	14.7
1	A	123	THR	14.7
1	D	397	GLU	14.7
1	D	57	GLY	14.6
1	C	309	GLN	14.5
1	A	464	ASN	14.5
1	D	448	GLU	14.5
1	D	178	VAL	14.5
1	A	454	ALA	14.5
1	D	361	ASN	14.4
1	A	403	ASP	14.4
1	D	396	ASP	14.4
1	C	328	LYS	14.4
1	B	328	LYS	14.4
1	C	206	SER	14.4
1	B	92	VAL	14.4
1	D	436	ASN	14.4
1	D	332	LYS	14.3
1	B	330	GLU	14.3
1	B	395	ILE	14.3
1	C	353	GLY	14.3
1	C	329	ASP	14.2
1	A	135	VAL	14.2
1	B	517	ARG	14.1
1	C	246	SER	14.1
1	B	162	TYR	14.1
1	D	162	TYR	14.0
1	A	224	GLU	14.0
1	A	197	GLN	14.0
1	A	201	GLY	14.0

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Mol	Chain	Res	Type	RSRZ
1	A	567	ALA	13.9
1	B	339	THR	13.9
1	C	581	GLY	13.8
1	D	10	TRP	13.8
1	B	453	ALA	13.8
1	B	348	THR	13.8
1	D	333	ARG	13.7
1	B	117	ASP	13.7
1	C	428	LEU	13.7
1	A	114	ALA	13.7
1	C	290	SER	13.7
1	D	371	THR	13.6
1	A	399	HIS	13.6
1	B	53	ASP	13.5
1	D	472	THR	13.5
1	A	417	ASN	13.5
1	D	467	ASP	13.5
1	A	209	GLN	13.5
1	A	137	SER	13.4
1	C	131	ASP	13.4
1	C	427	HIS	13.4
1	C	280	THR	13.4
1	D	402	MET	13.4
1	D	464	ASN	13.3
1	C	181	ALA	13.3
1	B	120	SER	13.3
1	D	326	GLN	13.3
1	B	541	THR	13.3
1	A	145	THR	13.2
1	D	51	LEU	13.2
1	C	71	VAL	13.2
1	A	520	GLN	13.2
1	C	546	ASP	13.2
1	B	18	PRO	13.2
1	A	150	GLY	13.2
1	D	36	LEU	13.1
1	B	236	LYS	13.1
1	C	506	GLU	13.1
1	D	232	LYS	13.1
1	D	123	THR	13.1
1	D	152	SER	13.1
1	B	429	PHE	13.1

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Mol	Chain	Res	Type	RSRZ
1	A	455	ARG	13.1
1	C	203	VAL	13.0
1	D	477	ASN	13.0
1	A	184	VAL	13.0
1	D	231	ASP	13.0
1	D	213	GLY	13.0
1	C	253	PRO	13.0
1	B	285	THR	12.9
1	B	198	ASN	12.9
1	B	568	GLN	12.9
1	B	213	GLY	12.8
1	A	336	ASP	12.7
1	C	368	ALA	12.7
1	C	430	ASN	12.7
1	D	428	LEU	12.7
1	C	39	ALA	12.7
1	B	89	ILE	12.7
1	D	383	SER	12.7
1	B	329	ASP	12.7
1	C	163	TYR	12.6
1	B	367	PRO	12.6
1	C	278	SER	12.6
1	D	199	THR	12.6
1	B	309	GLN	12.6
1	B	283	THR	12.6
1	C	134	GLN	12.5
1	B	314	ALA	12.5
1	B	107	HIS	12.5
1	B	80	ILE	12.5
1	A	84	ILE	12.4
1	C	208	GLU	12.4
1	C	426	VAL	12.4
1	B	544	GLN	12.4
1	D	543	GLU	12.4
1	D	202	GLN	12.4
1	A	502	LEU	12.4
1	D	113	VAL	12.4
1	C	469	GLY	12.4
1	B	114	ALA	12.4
1	C	155	GLY	12.4
1	C	237	MET	12.3
1	B	280	THR	12.3

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Mol	Chain	Res	Type	RSRZ
1	D	468	ASN	12.3
1	A	271	SER	12.3
1	C	209	GLN	12.3
1	C	425	ASN	12.3
1	A	397	GLU	12.2
1	D	187	LYS	12.2
1	D	170	ILE	12.2
1	C	10	TRP	12.2
1	D	148	ARG	12.2
1	B	371	THR	12.2
1	A	578	MET	12.2
1	D	233	VAL	12.1
1	D	93	SER	12.1
1	B	455	ARG	12.1
1	C	391	ARG	12.1
1	B	13	PHE	12.1
1	C	451	GLU	12.1
1	A	400	ILE	12.1
1	C	500	PRO	12.0
1	A	329	ASP	12.0
1	A	506	GLU	12.0
1	B	296	ARG	11.9
1	C	86	SER	11.9
1	C	13	PHE	11.9
1	D	177	ILE	11.9
1	B	449	GLN	11.8
1	C	394	ASP	11.8
1	B	94	GLY	11.8
1	D	21	ALA	11.8
1	B	579	GLN	11.8
1	D	544	GLN	11.7
1	A	319	PHE	11.7
1	D	353	GLY	11.7
1	D	497	ARG	11.7
1	B	214	HIS	11.7
1	C	117	ASP	11.6
1	C	12	THR	11.6
1	A	172	VAL	11.6
1	C	258	ILE	11.6
1	B	149	GLU	11.6
1	A	262	ALA	11.6
1	A	452	GLU	11.5

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Mol	Chain	Res	Type	RSRZ
1	A	235	ASN	11.4
1	D	354	ARG	11.4
1	C	114	ALA	11.4
1	C	210	MET	11.4
1	B	531	THR	11.4
1	C	447	ARG	11.4
1	B	234	SER	11.4
1	C	33	ALA	11.4
1	B	425	ASN	11.4
1	A	79	GLY	11.3
1	C	330	GLU	11.3
1	C	498	ASP	11.3
1	A	428	LEU	11.3
1	A	572	TYR	11.3
1	C	34	LEU	11.2
1	C	505	ASP	11.2
1	A	152	SER	11.2
1	C	467	ASP	11.2
1	A	388	LEU	11.2
1	D	427	HIS	11.2
1	B	81	THR	11.2
1	C	518	ALA	11.1
1	D	71	VAL	11.1
1	D	392	PHE	11.1
1	C	87	TYR	11.1
1	D	235	ASN	11.1
1	C	214	HIS	11.1
1	D	367	PRO	11.1
1	B	444	GLU	11.1
1	C	449	GLN	11.1
1	D	546	ASP	11.1
1	A	239	LEU	11.0
1	D	239	LEU	11.0
1	C	238	ARG	11.0
1	D	40	SER	11.0
1	A	280	THR	11.0
1	A	328	LYS	11.0
1	A	430	ASN	11.0
1	B	223	GLN	11.0
1	B	426	VAL	11.0
1	C	507	ALA	11.0
1	D	25	ALA	11.0

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Mol	Chain	Res	Type	RSRZ
1	C	437	ILE	11.0
1	A	120	SER	11.0
1	D	72	ILE	11.0
1	A	571	VAL	10.9
1	B	172	VAL	10.9
1	D	33	ALA	10.9
1	D	370	LYS	10.9
1	A	429	PHE	10.9
1	C	307	GLN	10.9
1	C	40	SER	10.9
1	C	468	ASN	10.9
1	D	422	VAL	10.9
1	B	423	SER	10.9
1	B	468	ASN	10.9
1	A	181	ALA	10.9
1	D	515	SER	10.8
1	C	220	PHE	10.8
1	A	76	ILE	10.8
1	C	354	ARG	10.8
1	C	95	LYS	10.8
1	A	457	ALA	10.8
1	B	119	GLN	10.8
1	D	118	LYS	10.8
1	B	26	GLY	10.8
1	B	72	ILE	10.8
1	D	471	ASP	10.7
1	A	200	MET	10.7
1	D	20	ILE	10.7
1	D	120	SER	10.7
1	B	121	THR	10.7
1	B	394	ASP	10.7
1	C	576	HIS	10.7
1	B	51	LEU	10.7
1	A	467	ASP	10.7
1	A	416	ARG	10.7
1	D	578	MET	10.7
1	A	198	ASN	10.7
1	B	404	GLY	10.7
1	A	232	LYS	10.6
1	D	172	VAL	10.6
1	B	578	MET	10.6
1	B	225	VAL	10.6

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Mol	Chain	Res	Type	RSRZ
1	D	150	GLY	10.6
1	D	17	TRP	10.6
1	B	145	THR	10.6
1	D	110	GLY	10.6
1	D	84	ILE	10.6
1	B	436	ASN	10.6
1	B	409	GLU	10.6
1	D	443	GLU	10.6
1	A	307	GLN	10.6
1	B	575	LEU	10.5
1	D	372	VAL	10.5
1	D	83	TYR	10.5
1	C	82	SER	10.5
1	C	107	HIS	10.5
1	A	182	ILE	10.5
1	B	281	ALA	10.5
1	A	514	GLU	10.5
1	A	442	THR	10.5
1	D	313	ALA	10.5
1	A	256	GLN	10.4
1	D	522	ALA	10.4
1	D	442	THR	10.4
1	A	193	SER	10.3
1	B	131	ASP	10.3
1	B	137	SER	10.3
1	D	249	SER	10.3
1	A	401	LEU	10.3
1	A	176	PRO	10.3
1	C	174	LEU	10.3
1	C	477	ASN	10.3
1	A	348	THR	10.3
1	A	453	ALA	10.3
1	D	278	SER	10.3
1	C	461	ASP	10.3
1	D	400	ILE	10.3
1	A	61	ARG	10.3
1	D	115	PHE	10.3
1	C	453	ALA	10.3
1	A	311	GLY	10.3
1	A	178	VAL	10.3
1	A	90	SER	10.3
1	C	15	ARG	10.3

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Mol	Chain	Res	Type	RSRZ
1	A	524	ASP	10.3
1	B	235	ASN	10.2
1	C	68	PRO	10.2
1	A	383	SER	10.2
1	B	42	THR	10.2
1	C	202	GLN	10.2
1	D	240	GLN	10.2
1	C	293	ALA	10.2
1	A	560	GLY	10.2
1	A	11	GLN	10.2
1	D	394	ASP	10.1
1	A	361	ASN	10.1
1	B	508	THR	10.1
1	A	191	SER	10.1
1	C	525	GLU	10.1
1	D	192	ILE	10.1
1	C	547	GLU	10.1
1	C	521	ALA	10.1
1	C	262	ALA	10.1
1	D	329	ASP	10.1
1	B	433	VAL	10.0
1	C	99	THR	10.0
1	A	529	ASN	10.0
1	B	253	PRO	10.0
1	A	242	MET	10.0
1	D	399	HIS	10.0
1	C	277	ASP	10.0
1	B	111	MET	10.0
1	D	334	VAL	10.0
1	D	159	MET	10.0
1	C	411	THR	10.0
1	C	239	LEU	10.0
1	C	294	LEU	10.0
1	A	380	SER	10.0
1	C	19	THR	10.0
1	A	344	PHE	10.0
1	B	43	PHE	10.0
1	A	153	ILE	9.9
1	D	482	SER	9.9
1	C	289	SER	9.9
1	A	258	ILE	9.9
1	D	430	ASN	9.9

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Mol	Chain	Res	Type	RSRZ
1	B	23	PHE	9.9
1	C	324	SER	9.9
1	A	39	ALA	9.9
1	D	101	ARG	9.9
1	D	355	GLU	9.9
1	D	378	SER	9.9
1	B	501	ILE	9.9
1	C	53	ASP	9.9
1	D	268	TYR	9.9
1	C	37	ASN	9.8
1	C	314	ALA	9.8
1	C	570	GLY	9.8
1	A	183	ARG	9.8
1	D	490	ALA	9.8
1	C	283	THR	9.8
1	C	448	GLU	9.8
1	D	156	LEU	9.8
1	C	417	ASN	9.8
1	A	305	ASN	9.8
1	A	315	CYS	9.8
1	D	210	MET	9.8
1	D	338	ALA	9.8
1	D	114	ALA	9.8
1	C	362	ILE	9.8
1	A	133	GLU	9.8
1	C	186	SER	9.8
1	C	527	GLN	9.8
1	A	249	SER	9.8
1	A	409	GLU	9.8
1	D	303	ASN	9.8
1	C	228	LYS	9.7
1	C	85	SER	9.7
1	B	98	MET	9.7
1	C	464	ASN	9.7
1	D	369	GLY	9.7
1	B	430	ASN	9.7
1	A	323	ASP	9.7
1	B	336	ASP	9.7
1	A	225	VAL	9.7
1	B	156	LEU	9.7
1	A	113	VAL	9.7
1	A	367	PRO	9.7

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Mol	Chain	Res	Type	RSRZ
1	B	398	GLY	9.7
1	C	35	ILE	9.7
1	B	146	VAL	9.7
1	D	330	GLU	9.7
1	B	521	ALA	9.6
1	B	184	VAL	9.6
1	A	320	ALA	9.6
1	C	54	ASP	9.6
1	D	180	ILE	9.6
1	A	247	ALA	9.6
1	B	353	GLY	9.6
1	A	325	GLU	9.6
1	B	276	MET	9.6
1	D	238	ARG	9.6
1	C	470	LEU	9.5
1	A	491	ILE	9.5
1	C	120	SER	9.5
1	D	226	GLU	9.5
1	B	237	MET	9.5
1	A	427	HIS	9.5
1	C	515	SER	9.5
1	A	121	THR	9.5
1	A	214	HIS	9.5
1	D	13	PHE	9.5
1	B	21	ALA	9.5
1	B	361	ASN	9.5
1	B	472	THR	9.5
1	C	23	PHE	9.5
1	B	224	GLU	9.4
1	B	496	LEU	9.4
1	C	303	ASN	9.4
1	C	531	THR	9.4
1	A	180	ILE	9.4
1	C	81	THR	9.4
1	D	337	ARG	9.4
1	B	303	ASN	9.4
1	B	446	SER	9.4
1	D	514	GLU	9.4
1	D	438	ALA	9.4
1	D	495	LEU	9.4
1	A	507	ALA	9.3
1	B	252	ASP	9.3

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Mol	Chain	Res	Type	RSRZ
1	D	191	SER	9.3
1	B	174	LEU	9.3
1	A	272	PHE	9.3
1	D	179	SER	9.3
1	D	391	ARG	9.3
1	B	343	GLU	9.3
1	C	248	SER	9.3
1	A	33	ALA	9.3
1	B	558	GLU	9.3
1	C	383	SER	9.3
1	D	447	ARG	9.3
1	C	580	PHE	9.3
1	A	322	LEU	9.3
1	D	255	ILE	9.2
1	D	570	GLY	9.2
1	C	191	SER	9.2
1	A	304	VAL	9.2
1	C	103	ARG	9.2
1	C	422	VAL	9.2
1	B	142	ALA	9.2
1	B	543	GLU	9.2
1	D	144	ILE	9.2
1	A	324	SER	9.2
1	D	253	PRO	9.2
1	D	431	ASP	9.2
1	A	188	ARG	9.2
1	B	520	GLN	9.1
1	C	70	VAL	9.1
1	A	164	SER	9.1
1	C	146	VAL	9.1
1	B	102	ARG	9.1
1	D	161	PHE	9.1
1	D	304	VAL	9.1
1	A	440	ALA	9.1
1	C	332	LYS	9.1
1	D	437	ILE	9.1
1	D	193	SER	9.1
1	D	421	LEU	9.0
1	D	163	TYR	9.0
1	B	87	TYR	9.0
1	D	281	ALA	9.0
1	B	396	ASP	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	83	TYR	9.0
1	B	332	LYS	9.0
1	D	530	ARG	9.0
1	D	366	ILE	9.0
1	A	52	LEU	9.0
1	D	32	ILE	9.0
1	C	369	GLY	9.0
1	A	579	GLN	9.0
1	D	135	VAL	9.0
1	A	187	LYS	9.0
1	D	445	TYR	9.0
1	D	569	HIS	9.0
1	C	69	LEU	8.9
1	A	154	ILE	8.9
1	B	540	SER	8.9
1	D	568	GLN	8.9
1	A	558	GLU	8.9
1	D	425	ASN	8.9
1	A	243	LYS	8.9
1	B	556	ILE	8.9
1	A	468	ASN	8.9
1	C	337	ARG	8.9
1	B	277	ASP	8.9
1	D	324	SER	8.9
1	D	491	ILE	8.9
1	D	270	ALA	8.9
1	A	151	ALA	8.9
1	A	525	GLU	8.9
1	A	251	SER	8.8
1	B	271	SER	8.8
1	C	348	THR	8.8
1	C	115	PHE	8.8
1	B	180	ILE	8.8
1	B	33	ALA	8.8
1	A	581	GLY	8.8
1	A	156	LEU	8.8
1	B	232	LYS	8.8
1	D	41	ASP	8.8
1	C	494	ALA	8.8
1	A	252	ASP	8.8
1	D	269	ALA	8.8
1	A	66	TRP	8.8

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Mol	Chain	Res	Type	RSRZ
1	B	442	THR	8.8
1	D	559	ARG	8.8
1	C	296	ARG	8.7
1	D	212	LYS	8.7
1	A	415	LEU	8.7
1	B	403	ASP	8.7
1	B	451	GLU	8.7
1	B	514	GLU	8.7
1	B	530	ARG	8.7
1	B	341	ASP	8.7
1	D	300	SER	8.7
1	C	125	LEU	8.7
1	A	313	ALA	8.7
1	B	29	VAL	8.7
1	A	53	ASP	8.7
1	A	299	LYS	8.7
1	C	569	HIS	8.7
1	A	163	TYR	8.7
1	B	421	LEU	8.7
1	C	279	LEU	8.7
1	A	118	LYS	8.6
1	A	212	LYS	8.6
1	A	236	LYS	8.6
1	C	304	VAL	8.6
1	B	513	THR	8.6
1	B	538	ARG	8.6
1	A	425	ASN	8.6
1	A	98	MET	8.6
1	A	20	ILE	8.6
1	C	302	THR	8.6
1	A	221	GLY	8.6
1	C	184	VAL	8.6
1	C	160	MET	8.6
1	D	22	PRO	8.6
1	D	516	GLU	8.5
1	C	26	GLY	8.5
1	C	256	GLN	8.5
1	D	558	GLU	8.5
1	B	505	ASP	8.5
1	D	441	ARG	8.5
1	D	295	MET	8.5
1	A	72	ILE	8.5

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Mol	Chain	Res	Type	RSRZ
1	B	439	TYR	8.5
1	B	528	LYS	8.5
1	B	28	ILE	8.5
1	B	478	GLY	8.5
1	B	576	HIS	8.5
1	C	197	GLN	8.5
1	A	451	GLU	8.4
1	B	390	THR	8.4
1	C	84	ILE	8.4
1	C	395	ILE	8.4
1	D	141	GLY	8.4
1	C	463	ILE	8.4
1	D	24	LYS	8.4
1	B	24	LYS	8.4
1	B	290	SER	8.4
1	B	73	GLY	8.4
1	B	99	THR	8.4
1	A	107	HIS	8.4
1	C	365	LYS	8.4
1	A	273	PRO	8.4
1	C	36	LEU	8.4
1	C	64	LEU	8.4
1	A	501	ILE	8.4
1	B	308	PHE	8.4
1	D	271	SER	8.4
1	B	383	SER	8.4
1	B	192	ILE	8.4
1	B	500	PRO	8.4
1	D	423	SER	8.4
1	A	296	ARG	8.4
1	C	565	LEU	8.3
1	D	461	ASP	8.3
1	A	396	ASP	8.3
1	C	195	ASN	8.3
1	A	458	TYR	8.3
1	C	152	SER	8.3
1	A	281	ALA	8.3
1	D	43	PHE	8.3
1	D	14	ARG	8.3
1	A	21	ALA	8.3
1	B	411	THR	8.3
1	A	54	ASP	8.3

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Mol	Chain	Res	Type	RSRZ
1	B	141	GLY	8.3
1	A	248	SER	8.3
1	B	14	ARG	8.3
1	D	209	GLN	8.3
1	B	163	TYR	8.3
1	B	297	PRO	8.3
1	D	26	GLY	8.3
1	A	62	SER	8.3
1	A	115	PHE	8.3
1	B	185	VAL	8.2
1	D	525	GLU	8.2
1	A	575	LEU	8.2
1	B	56	PHE	8.2
1	A	449	GLN	8.2
1	B	52	LEU	8.2
1	C	424	GLN	8.2
1	D	498	ASP	8.2
1	D	266	VAL	8.2
1	B	250	ILE	8.2
1	B	32	ILE	8.2
1	D	435	ASN	8.2
1	A	499	SER	8.2
1	D	106	GLY	8.2
1	D	225	VAL	8.1
1	B	113	VAL	8.1
1	C	56	PHE	8.1
1	A	492	ALA	8.1
1	A	161	PHE	8.1
1	B	50	PRO	8.1
1	A	106	GLY	8.1
1	A	290	SER	8.1
1	D	228	LYS	8.1
1	D	335	ILE	8.1
1	D	75	MET	8.1
1	C	300	SER	8.1
1	C	198	ASN	8.1
1	A	338	ALA	8.1
1	B	438	ALA	8.1
1	C	398	GLY	8.1
1	B	84	ILE	8.1
1	D	272	PHE	8.1
1	C	121	THR	8.1

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Mol	Chain	Res	Type	RSRZ
1	C	24	LYS	8.0
1	B	70	VAL	8.0
1	A	144	ILE	8.0
1	D	261	LEU	8.0
1	B	535	ILE	8.0
1	B	123	THR	8.0
1	D	506	GLU	8.0
1	C	366	ILE	8.0
1	A	390	THR	8.0
1	D	322	LEU	8.0
1	D	61	ARG	8.0
1	A	206	SER	8.0
1	B	178	VAL	7.9
1	B	257	LEU	7.9
1	C	579	GLN	7.9
1	B	150	GLY	7.9
1	D	201	GLY	7.9
1	A	353	GLY	7.9
1	A	432	THR	7.9
1	D	496	LEU	7.9
1	B	12	THR	7.9
1	C	432	THR	7.9
1	C	573	ALA	7.9
1	B	118	LYS	7.9
1	B	106	GLY	7.9
1	A	73	GLY	7.9
1	A	259	ALA	7.9
1	B	67	MET	7.9
1	B	241	GLY	7.9
1	D	342	LEU	7.9
1	C	550	VAL	7.9
1	C	429	PHE	7.8
1	A	340	GLY	7.8
1	B	15	ARG	7.8
1	C	164	SER	7.8
1	D	507	ALA	7.8
1	A	116	PHE	7.8
1	A	435	ASN	7.8
1	B	365	LYS	7.8
1	C	343	GLU	7.8
1	D	50	PRO	7.8
1	C	72	ILE	7.8

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Mol	Chain	Res	Type	RSRZ
1	C	291	MET	7.8
1	B	534	VAL	7.8
1	A	94	GLY	7.8
1	D	198	ASN	7.8
1	C	325	GLU	7.8
1	B	454	ALA	7.8
1	A	186	SER	7.8
1	D	171	LEU	7.8
1	A	376	GLY	7.8
1	D	336	ASP	7.8
1	A	270	ALA	7.8
1	C	250	ILE	7.8
1	A	253	PRO	7.8
1	B	310	ARG	7.7
1	A	203	VAL	7.7
1	A	450	ILE	7.7
1	D	296	ARG	7.7
1	A	295	MET	7.7
1	D	297	PRO	7.7
1	D	432	THR	7.7
1	D	547	GLU	7.7
1	A	25	ALA	7.7
1	D	208	GLU	7.7
1	A	227	THR	7.7
1	A	32	ILE	7.7
1	B	370	LYS	7.7
1	B	491	ILE	7.7
1	C	316	GLN	7.7
1	D	325	GLU	7.7
1	C	499	SER	7.6
1	A	517	ARG	7.6
1	D	67	MET	7.6
1	D	518	ALA	7.6
1	A	230	PHE	7.6
1	B	90	SER	7.6
1	B	324	SER	7.6
1	A	439	TYR	7.6
1	A	544	GLN	7.6
1	B	105	PHE	7.6
1	A	528	LYS	7.6
1	B	154	ILE	7.5
1	B	109	MET	7.5

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Mol	Chain	Res	Type	RSRZ
1	B	294	LEU	7.5
1	A	516	GLU	7.5
1	C	564	GLU	7.5
1	D	37	ASN	7.5
1	B	40	SER	7.5
1	B	456	MET	7.5
1	D	214	HIS	7.5
1	C	257	LEU	7.5
1	D	94	GLY	7.5
1	B	259	ALA	7.5
1	A	192	ILE	7.5
1	A	341	ASP	7.5
1	A	531	THR	7.5
1	D	134	GLN	7.5
1	B	155	GLY	7.5
1	B	186	SER	7.5
1	B	434	ALA	7.5
1	C	243	LYS	7.5
1	B	570	GLY	7.4
1	C	66	TRP	7.4
1	B	473	ILE	7.4
1	B	509	SER	7.4
1	D	533	LEU	7.4
1	B	199	THR	7.4
1	C	28	ILE	7.4
1	B	547	GLU	7.4
1	D	382	LYS	7.4
1	C	523	LEU	7.4
1	D	341	ASP	7.4
1	D	363	ASN	7.4
1	C	240	GLN	7.4
1	D	529	ASN	7.4
1	A	343	GLU	7.4
1	C	543	GLU	7.4
1	B	477	ASN	7.4
1	A	298	LEU	7.3
1	B	101	ARG	7.3
1	C	530	ARG	7.3
1	D	283	THR	7.3
1	B	516	GLU	7.3
1	D	223	GLN	7.3
1	A	139	SER	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	265	PHE	7.3
1	D	200	MET	7.3
1	A	223	GLN	7.3
1	B	402	MET	7.3
1	A	112	PRO	7.3
1	B	522	ALA	7.3
1	A	421	LEU	7.3
1	D	19	THR	7.3
1	B	557	VAL	7.3
1	B	492	ALA	7.3
1	D	52	LEU	7.3
1	B	337	ARG	7.3
1	A	88	CYS	7.3
1	D	59	THR	7.3
1	D	81	THR	7.3
1	B	321	ILE	7.3
1	D	501	ILE	7.3
1	D	364	LEU	7.2
1	B	46	SER	7.2
1	A	294	LEU	7.2
1	A	498	ASP	7.2
1	A	208	GLU	7.2
1	B	68	PRO	7.2
1	C	281	ALA	7.2
1	B	62	SER	7.2
1	D	31	GLY	7.2
1	A	237	MET	7.2
1	D	307	GLN	7.2
1	C	409	GLU	7.2
1	B	464	ASN	7.2
1	B	110	GLY	7.2
1	C	558	GLU	7.2
1	A	146	VAL	7.2
1	B	563	SER	7.2
1	B	95	LYS	7.2
1	B	240	GLN	7.2
1	D	452	GLU	7.2
1	D	112	PRO	7.1
1	B	191	SER	7.1
1	C	189	PHE	7.1
1	D	175	ALA	7.1
1	C	401	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
1	D	290	SER	7.1
1	C	284	ILE	7.1
1	D	321	ILE	7.1
1	A	436	ASN	7.1
1	B	201	GLY	7.1
1	B	243	LYS	7.1
1	D	502	LEU	7.1
1	B	139	SER	7.1
1	D	42	THR	7.1
1	C	31	GLY	7.1
1	C	43	PHE	7.1
1	B	82	SER	7.1
1	B	83	TYR	7.1
1	C	390	THR	7.1
1	B	524	ASP	7.1
1	A	462	PHE	7.1
1	D	45	LEU	7.1
1	D	302	THR	7.1
1	A	318	LEU	7.1
1	B	251	SER	7.1
1	D	453	ALA	7.1
1	B	459	ALA	7.0
1	B	227	THR	7.0
1	A	126	SER	7.0
1	A	128	ILE	7.0
1	A	562	HIS	7.0
1	C	320	ALA	7.0
1	A	246	SER	7.0
1	C	116	PHE	7.0
1	B	469	GLY	7.0
1	D	387	SER	7.0
1	A	210	MET	7.0
1	C	491	ILE	7.0
1	A	413	ALA	7.0
1	A	533	LEU	7.0
1	B	418	GLN	7.0
1	D	247	ALA	7.0
1	A	261	LEU	7.0
1	D	230	PHE	7.0
1	D	314	ALA	7.0
1	D	580	PHE	7.0
1	B	116	PHE	6.9

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Mol	Chain	Res	Type	RSRZ
1	C	313	ALA	6.9
1	D	237	MET	6.9
1	B	93	SER	6.9
1	A	556	ILE	6.9
1	C	372	VAL	6.9
1	B	206	SER	6.9
1	D	29	VAL	6.9
1	A	85	SER	6.9
1	C	141	GLY	6.9
1	A	505	ASP	6.9
1	B	523	LEU	6.9
1	D	127	ARG	6.9
1	B	397	GLU	6.9
1	D	505	ASP	6.9
1	D	256	GLN	6.9
1	D	517	ARG	6.9
1	C	418	GLN	6.9
1	A	564	GLU	6.9
1	D	572	TYR	6.9
1	C	367	PRO	6.9
1	D	262	ALA	6.9
1	A	378	SER	6.9
1	B	497	ARG	6.9
1	D	15	ARG	6.9
1	C	169	ILE	6.9
1	A	346	ASN	6.8
1	B	424	GLN	6.8
1	A	278	SER	6.8
1	C	58	LYS	6.8
1	C	108	MET	6.8
1	B	498	ASP	6.8
1	C	119	GLN	6.8
1	D	455	ARG	6.8
1	B	233	VAL	6.8
1	D	426	VAL	6.8
1	B	400	ILE	6.8
1	C	118	LYS	6.8
1	C	245	VAL	6.8
1	B	208	GLU	6.8
1	A	26	GLY	6.8
1	B	566	LEU	6.8
1	C	538	ARG	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	424	GLN	6.8
1	A	93	SER	6.8
1	C	263	LEU	6.8
1	A	122	GLY	6.7
1	B	322	LEU	6.7
1	A	67	MET	6.7
1	C	516	GLU	6.7
1	D	418	GLN	6.7
1	C	471	ASP	6.7
1	C	482	SER	6.7
1	B	54	ASP	6.7
1	B	63	VAL	6.7
1	B	529	ASN	6.7
1	A	508	THR	6.7
1	C	355	GLU	6.7
1	B	181	ALA	6.7
1	A	362	ILE	6.7
1	A	548	ILE	6.7
1	D	30	ALA	6.7
1	A	240	GLN	6.6
1	C	271	SER	6.6
1	C	100	MET	6.6
1	D	227	THR	6.6
1	D	552	GLU	6.6
1	D	555	ILE	6.6
1	A	580	PHE	6.6
1	D	76	ILE	6.6
1	B	75	MET	6.6
1	C	412	LEU	6.6
1	C	172	VAL	6.6
1	D	207	ALA	6.6
1	C	528	LYS	6.6
1	D	499	SER	6.6
1	B	555	ILE	6.6
1	C	145	THR	6.6
1	C	553	ASP	6.6
1	B	247	ALA	6.6
1	A	532	SER	6.6
1	A	102	ARG	6.6
1	C	20	ILE	6.6
1	D	87	TYR	6.6
1	B	58	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	123	THR	6.6
1	C	154	ILE	6.6
1	C	242	MET	6.6
1	B	422	VAL	6.5
1	B	503	ILE	6.5
1	A	13	PHE	6.5
1	A	366	ILE	6.5
1	C	264	ALA	6.5
1	C	555	ILE	6.5
1	D	54	ASP	6.5
1	C	572	TYR	6.5
1	B	125	LEU	6.5
1	C	476	GLU	6.5
1	A	47	LEU	6.5
1	A	422	VAL	6.5
1	B	169	ILE	6.5
1	B	203	VAL	6.5
1	A	46	SER	6.5
1	A	283	THR	6.5
1	D	107	HIS	6.5
1	A	494	ALA	6.5
1	C	339	THR	6.5
1	C	229	ARG	6.5
1	B	413	ALA	6.5
1	C	223	GLN	6.5
1	A	199	THR	6.5
1	C	32	ILE	6.5
1	A	268	TYR	6.5
1	C	334	VAL	6.4
1	B	573	ALA	6.4
1	B	22	PRO	6.4
1	A	395	ILE	6.4
1	C	110	GLY	6.4
1	C	562	HIS	6.4
1	C	94	GLY	6.4
1	A	36	LEU	6.4
1	C	455	ARG	6.4
1	D	474	ILE	6.4
1	D	205	THR	6.4
1	C	566	LEU	6.4
1	D	340	GLY	6.4
1	C	315	CYS	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	533	LEU	6.4
1	B	338	ALA	6.4
1	B	246	SER	6.4
1	C	295	MET	6.4
1	C	509	SER	6.4
1	C	333	ARG	6.4
1	C	305	ASN	6.4
1	B	489	ILE	6.4
1	B	261	LEU	6.3
1	C	456	MET	6.3
1	C	544	GLN	6.3
1	A	87	TYR	6.3
1	A	332	LYS	6.3
1	C	227	THR	6.3
1	C	535	ILE	6.3
1	C	90	SER	6.3
1	A	130	TYR	6.3
1	C	557	VAL	6.3
1	D	243	LYS	6.3
1	B	518	ALA	6.3
1	B	326	GLN	6.3
1	A	132	SER	6.3
1	B	432	THR	6.3
1	D	137	SER	6.3
1	D	315	CYS	6.3
1	D	181	ALA	6.3
1	B	226	GLU	6.3
1	C	438	ALA	6.3
1	D	220	PHE	6.3
1	B	507	ALA	6.3
1	D	98	MET	6.3
1	C	457	ALA	6.2
1	C	48	LEU	6.2
1	D	566	LEU	6.2
1	B	195	ASN	6.2
1	B	300	SER	6.2
1	C	148	ARG	6.2
1	C	571	VAL	6.2
1	A	371	THR	6.2
1	C	444	GLU	6.2
1	A	504	LEU	6.2
1	C	421	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	D	145	THR	6.2
1	B	574	GLN	6.2
1	D	541	THR	6.2
1	A	74	LEU	6.2
1	A	233	VAL	6.2
1	A	446	SER	6.2
1	C	446	SER	6.2
1	A	99	THR	6.2
1	C	98	MET	6.2
1	A	509	SER	6.2
1	D	446	SER	6.2
1	D	500	PRO	6.2
1	A	97	VAL	6.2
1	B	193	SER	6.2
1	D	11	GLN	6.2
1	A	194	LYS	6.2
1	B	461	ASP	6.2
1	D	154	ILE	6.2
1	D	203	VAL	6.1
1	D	299	LYS	6.1
1	C	102	ARG	6.1
1	B	490	ALA	6.1
1	D	562	HIS	6.1
1	D	508	THR	6.1
1	A	418	GLN	6.1
1	D	365	LYS	6.1
1	B	356	VAL	6.1
1	D	116	PHE	6.1
1	D	257	LEU	6.1
1	D	95	LYS	6.1
1	C	346	ASN	6.1
1	B	254	ILE	6.1
1	B	66	TRP	6.1
1	A	330	GLU	6.1
1	C	188	ARG	6.1
1	A	316	GLN	6.1
1	C	436	ASN	6.1
1	A	155	GLY	6.1
1	B	205	THR	6.1
1	D	254	ILE	6.1
1	A	42	THR	6.1
1	A	173	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	195	ASN	6.1
1	B	97	VAL	6.1
1	A	471	ASP	6.0
1	B	228	LYS	6.0
1	C	212	LYS	6.0
1	C	577	LYS	6.0
1	C	46	SER	6.0
1	B	282	GLY	6.0
1	C	524	ASP	6.0
1	D	122	GLY	6.0
1	B	315	CYS	6.0
1	A	95	LYS	6.0
1	D	169	ILE	6.0
1	C	162	TYR	6.0
1	B	44	MET	6.0
1	C	178	VAL	6.0
1	C	433	VAL	6.0
1	D	56	PHE	6.0
1	B	239	LEU	6.0
1	B	458	TYR	6.0
1	D	509	SER	6.0
1	D	454	ALA	6.0
1	A	31	GLY	6.0
1	C	207	ALA	6.0
1	A	142	ALA	6.0
1	C	370	LYS	6.0
1	C	396	ASP	6.0
1	D	245	VAL	6.0
1	C	201	GLY	6.0
1	D	275	VAL	6.0
1	A	68	PRO	6.0
1	A	342	LEU	6.0
1	C	378	SER	6.0
1	D	513	THR	5.9
1	A	354	ARG	5.9
1	D	92	VAL	5.9
1	D	28	ILE	5.9
1	D	563	SER	5.9
1	D	96	VAL	5.9
1	B	38	ALA	5.9
1	C	147	VAL	5.9
1	C	381	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	269	ALA	5.9
1	B	218	LEU	5.9
1	D	183	ARG	5.9
1	C	113	VAL	5.9
1	A	404	GLY	5.9
1	D	456	MET	5.9
1	B	69	LEU	5.9
1	B	316	GLN	5.9
1	C	578	MET	5.9
1	D	312	MET	5.9
1	B	88	CYS	5.9
1	C	441	ARG	5.9
1	D	85	SER	5.9
1	A	103	ARG	5.9
1	D	80	ILE	5.9
1	D	429	PHE	5.8
1	A	75	MET	5.8
1	C	563	SER	5.8
1	A	92	VAL	5.8
1	B	147	VAL	5.8
1	D	185	VAL	5.8
1	A	352	PRO	5.8
1	B	346	ASN	5.8
1	B	487	GLN	5.8
1	A	108	MET	5.8
1	B	567	ALA	5.8
1	B	45	LEU	5.8
1	B	467	ASP	5.8
1	B	366	ILE	5.8
1	D	344	PHE	5.8
1	C	442	THR	5.8
1	A	545	ALA	5.8
1	C	170	ILE	5.8
1	D	484	GLY	5.8
1	C	232	LYS	5.8
1	C	233	VAL	5.8
1	C	380	SER	5.8
1	C	200	MET	5.8
1	C	317	THR	5.8
1	A	419	VAL	5.8
1	C	177	ILE	5.8
1	C	548	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	168	SER	5.8
1	D	510	ALA	5.8
1	D	35	ILE	5.8
1	C	363	ASN	5.8
1	D	64	LEU	5.8
1	A	254	ILE	5.8
1	C	254	ILE	5.7
1	B	417	ASN	5.7
1	A	241	GLY	5.7
1	B	136	ALA	5.7
1	B	372	VAL	5.7
1	C	111	MET	5.7
1	C	185	VAL	5.7
1	C	91	TRP	5.7
1	D	293	ALA	5.7
1	D	189	PHE	5.7
1	A	444	GLU	5.7
1	B	167	LEU	5.7
1	C	236	LYS	5.7
1	D	415	LEU	5.7
1	C	93	SER	5.7
1	A	553	ASP	5.7
1	A	57	GLY	5.7
1	A	521	ALA	5.7
1	A	80	ILE	5.7
1	B	183	ARG	5.7
1	C	41	ASP	5.7
1	D	102	ARG	5.7
1	D	108	MET	5.7
1	D	221	GLY	5.7
1	A	387	SER	5.7
1	A	40	SER	5.7
1	A	461	ASP	5.7
1	B	71	VAL	5.7
1	C	44	MET	5.7
1	A	41	ASP	5.7
1	C	180	ILE	5.7
1	D	282	GLY	5.7
1	B	526	LEU	5.7
1	A	554	GLY	5.6
1	D	160	MET	5.6
1	B	36	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	260	SER	5.6
1	C	331	GLY	5.6
1	A	131	ASP	5.6
1	A	476	GLU	5.6
1	C	497	ARG	5.6
1	D	82	SER	5.6
1	B	182	ILE	5.6
1	B	160	MET	5.6
1	A	335	ILE	5.6
1	B	166	GLN	5.6
1	A	105	PHE	5.6
1	A	228	LYS	5.6
1	C	22	PRO	5.6
1	A	350	THR	5.6
1	D	526	LEU	5.6
1	A	574	GLN	5.6
1	A	10	TRP	5.6
1	B	200	MET	5.6
1	D	206	SER	5.6
1	B	91	TRP	5.6
1	A	136	ALA	5.6
1	B	345	ARG	5.6
1	B	484	GLY	5.6
1	D	301	LEU	5.6
1	B	291	MET	5.6
1	A	555	ILE	5.6
1	A	69	LEU	5.6
1	B	108	MET	5.6
1	C	322	LEU	5.6
1	A	364	LEU	5.5
1	D	343	GLU	5.5
1	A	231	ASP	5.5
1	B	331	GLY	5.5
1	D	457	ALA	5.5
1	D	69	LEU	5.5
1	C	192	ILE	5.5
1	C	226	GLU	5.5
1	C	459	ALA	5.5
1	D	184	VAL	5.5
1	A	89	ILE	5.5
1	B	362	ILE	5.5
1	C	508	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	235	ASN	5.5
1	B	244	MET	5.5
1	D	409	GLU	5.5
1	B	30	ALA	5.5
1	D	465	LYS	5.5
1	B	124	LEU	5.5
1	A	349	PHE	5.5
1	B	364	LEU	5.5
1	C	272	PHE	5.5
1	A	166	GLN	5.5
1	A	420	ALA	5.5
1	D	531	THR	5.5
1	B	352	PRO	5.5
1	A	195	ASN	5.5
1	A	512	ASP	5.5
1	D	128	ILE	5.5
1	A	541	THR	5.5
1	A	171	LEU	5.4
1	C	488	ARG	5.4
1	A	179	SER	5.4
1	A	308	PHE	5.4
1	B	138	SER	5.4
1	D	99	THR	5.4
1	D	449	GLN	5.4
1	A	59	THR	5.4
1	C	514	GLU	5.4
1	D	323	ASP	5.4
1	B	373	ALA	5.4
1	B	405	HIS	5.4
1	A	91	TRP	5.4
1	C	406	ASP	5.4
1	A	257	LEU	5.4
1	C	127	ARG	5.4
1	C	101	ARG	5.4
1	D	125	LEU	5.4
1	C	534	VAL	5.4
1	A	481	LEU	5.4
1	B	539	LEU	5.4
1	C	144	ILE	5.4
1	A	540	SER	5.4
1	D	265	PHE	5.4
1	A	393	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	426	VAL	5.4
1	C	268	TYR	5.3
1	A	469	GLY	5.3
1	A	569	HIS	5.3
1	B	515	SER	5.3
1	C	16	LEU	5.3
1	B	369	GLY	5.3
1	C	60	ASP	5.3
1	A	22	PRO	5.3
1	B	221	GLY	5.3
1	D	182	ILE	5.3
1	D	242	MET	5.3
1	D	373	ALA	5.3
1	C	128	ILE	5.3
1	C	142	ALA	5.3
1	C	230	PHE	5.3
1	C	503	ILE	5.3
1	D	571	VAL	5.3
1	A	222	GLY	5.3
1	C	560	GLY	5.3
1	C	139	SER	5.3
1	C	261	LEU	5.3
1	B	334	VAL	5.3
1	D	250	ILE	5.3
1	C	434	ALA	5.3
1	A	547	GLU	5.3
1	C	183	ARG	5.2
1	C	42	THR	5.2
1	A	386	ALA	5.2
1	C	402	MET	5.2
1	D	346	ASN	5.2
1	B	242	MET	5.2
1	D	524	ASP	5.2
1	D	246	SER	5.2
1	B	196	MET	5.2
1	A	213	GLY	5.2
1	A	337	ARG	5.2
1	A	219	ILE	5.2
1	B	79	GLY	5.2
1	D	204	THR	5.2
1	B	443	GLU	5.2
1	D	478	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	463	ILE	5.2
1	B	248	SER	5.2
1	D	407	LEU	5.2
1	B	143	LEU	5.2
1	A	402	MET	5.2
1	D	12	THR	5.2
1	B	220	PHE	5.2
1	D	521	ALA	5.2
1	D	557	VAL	5.1
1	A	285	THR	5.1
1	D	493	ARG	5.1
1	C	137	SER	5.1
1	A	448	GLU	5.1
1	B	273	PRO	5.1
1	D	486	ARG	5.1
1	D	124	LEU	5.1
1	A	138	SER	5.1
1	B	197	GLN	5.1
1	B	161	PHE	5.1
1	A	327	GLU	5.1
1	D	581	GLY	5.1
1	A	301	LEU	5.1
1	C	574	GLN	5.1
1	D	166	GLN	5.1
1	A	275	VAL	5.1
1	C	356	VAL	5.1
1	D	224	GLU	5.1
1	D	100	MET	5.1
1	B	553	ASP	5.1
1	A	276	MET	5.1
1	C	483	GLY	5.1
1	D	462	PHE	5.1
1	A	71	VAL	5.1
1	A	389	ILE	5.1
1	D	480	LEU	5.1
1	B	126	SER	5.1
1	D	276	MET	5.1
1	C	83	TYR	5.1
1	C	38	ALA	5.0
1	B	393	TYR	5.0
1	D	217	VAL	5.0
1	B	581	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	573	ALA	5.0
1	C	373	ALA	5.0
1	C	76	ILE	5.0
1	D	97	VAL	5.0
1	A	244	MET	5.0
1	B	207	ALA	5.0
1	C	435	ASN	5.0
1	C	490	ALA	5.0
1	C	301	LEU	5.0
1	A	470	LEU	5.0
1	B	536	ALA	5.0
1	C	517	ARG	5.0
1	D	520	GLN	5.0
1	D	398	GLY	5.0
1	A	207	ALA	5.0
1	A	96	VAL	5.0
1	D	554	GLY	5.0
1	B	382	LYS	5.0
1	A	559	ARG	5.0
1	D	556	ILE	5.0
1	B	564	GLU	5.0
1	D	142	ALA	5.0
1	D	434	ALA	5.0
1	B	554	GLY	4.9
1	A	431	ASP	4.9
1	B	552	GLU	4.9
1	D	538	ARG	4.9
1	A	513	THR	4.9
1	C	504	LEU	4.9
1	D	241	GLY	4.9
1	C	556	ILE	4.9
1	A	447	ARG	4.9
1	C	89	ILE	4.9
1	C	559	ARG	4.9
1	B	49	LYS	4.9
1	A	500	PRO	4.9
1	A	82	SER	4.9
1	C	275	VAL	4.9
1	C	260	SER	4.9
1	B	260	SER	4.9
1	B	301	LEU	4.9
1	D	412	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	405	HIS	4.9
1	A	306	ALA	4.8
1	C	218	LEU	4.8
1	C	168	SER	4.8
1	B	502	LEU	4.8
1	B	562	HIS	4.8
1	B	100	MET	4.8
1	A	445	TYR	4.8
1	B	437	ILE	4.8
1	B	189	PHE	4.8
1	C	297	PRO	4.8
1	A	15	ARG	4.8
1	D	117	ASP	4.8
1	A	265	PHE	4.8
1	A	217	VAL	4.8
1	B	74	LEU	4.8
1	D	77	LEU	4.8
1	B	128	ILE	4.8
1	C	403	ASP	4.8
1	B	465	LYS	4.8
1	B	499	SER	4.8
1	D	309	GLN	4.8
1	D	188	ARG	4.8
1	C	166	GLN	4.8
1	C	67	MET	4.8
1	A	488	ARG	4.8
1	C	384	THR	4.8
1	C	49	LYS	4.7
1	A	12	THR	4.7
1	C	74	LEU	4.7
1	D	362	ILE	4.7
1	A	86	SER	4.7
1	C	193	SER	4.7
1	D	419	VAL	4.7
1	B	471	ASP	4.7
1	C	335	ILE	4.7
1	D	403	ASP	4.7
1	B	10	TRP	4.7
1	C	388	LEU	4.7
1	C	311	GLY	4.7
1	B	286	VAL	4.7
1	A	522	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	112	PRO	4.7
1	A	363	ASN	4.7
1	C	537	HIS	4.7
1	B	85	SER	4.7
1	A	215	LYS	4.6
1	A	326	GLN	4.6
1	A	226	GLU	4.6
1	C	472	THR	4.6
1	A	65	LEU	4.6
1	A	539	LEU	4.6
1	B	293	ALA	4.6
1	B	202	GLN	4.6
1	D	18	PRO	4.6
1	B	342	LEU	4.6
1	C	541	THR	4.6
1	D	103	ARG	4.6
1	A	189	PHE	4.6
1	C	350	THR	4.6
1	C	219	ILE	4.6
1	D	360	ARG	4.6
1	C	502	LEU	4.6
1	A	487	GLN	4.6
1	C	407	LEU	4.6
1	D	109	MET	4.6
1	D	287	VAL	4.6
1	B	560	GLY	4.6
1	D	306	ALA	4.6
1	C	414	SER	4.6
1	A	443	GLU	4.6
1	D	46	SER	4.6
1	A	530	ARG	4.6
1	A	478	GLY	4.6
1	C	149	GLU	4.6
1	D	579	GLN	4.6
1	D	49	LYS	4.5
1	A	314	ALA	4.5
1	B	506	GLU	4.5
1	A	408	ARG	4.5
1	A	119	GLN	4.5
1	C	11	GLN	4.5
1	C	122	GLY	4.5
1	B	104	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	463	ILE	4.5
1	D	527	GLN	4.5
1	B	37	ASN	4.5
1	A	565	LEU	4.5
1	B	388	LEU	4.5
1	B	175	ALA	4.5
1	D	153	ILE	4.5
1	A	16	LEU	4.5
1	C	249	SER	4.5
1	B	410	TYR	4.5
1	B	302	THR	4.5
1	A	190	ARG	4.5
1	B	20	ILE	4.5
1	B	153	ILE	4.5
1	C	124	LEU	4.5
1	D	62	SER	4.5
1	A	333	ARG	4.5
1	B	268	TYR	4.5
1	D	408	ARG	4.5
1	B	452	GLU	4.5
1	B	495	LEU	4.5
1	D	258	ILE	4.4
1	A	104	LEU	4.4
1	B	580	PHE	4.4
1	A	158	ILE	4.4
1	B	414	SER	4.4
1	C	466	MET	4.4
1	A	438	ALA	4.4
1	C	182	ILE	4.4
1	A	373	ALA	4.4
1	B	264	ALA	4.4
1	B	488	ARG	4.4
1	D	176	PRO	4.4
1	A	552	GLU	4.4
1	B	275	VAL	4.4
1	D	512	ASP	4.4
1	A	534	VAL	4.4
1	C	495	LEU	4.4
1	C	199	THR	4.4
1	B	188	ARG	4.4
1	C	554	GLY	4.4
1	B	483	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	14	ARG	4.4
1	C	371	THR	4.4
1	C	360	ARG	4.4
1	A	561	THR	4.3
1	B	284	ILE	4.3
1	A	480	LEU	4.3
1	C	321	ILE	4.3
1	C	52	LEU	4.3
1	D	151	ALA	4.3
1	D	132	SER	4.3
1	C	97	VAL	4.3
1	C	340	GLY	4.3
1	A	167	LEU	4.3
1	D	90	SER	4.3
1	D	78	ARG	4.3
1	C	568	GLN	4.3
1	B	212	LYS	4.3
1	A	255	ILE	4.3
1	A	482	SER	4.3
1	A	267	LEU	4.3
1	C	513	THR	4.3
1	D	327	GLU	4.3
1	A	473	ILE	4.3
1	D	416	ARG	4.3
1	C	561	THR	4.3
1	A	291	MET	4.3
1	A	543	GLU	4.3
1	C	224	GLU	4.3
1	C	478	GLY	4.3
1	B	39	ALA	4.3
1	D	470	LEU	4.3
1	A	27	LEU	4.3
1	B	164	SER	4.2
1	B	374	LEU	4.2
1	A	357	PRO	4.2
1	B	510	ALA	4.2
1	C	176	PRO	4.2
1	D	466	MET	4.2
1	D	487	GLN	4.2
1	D	458	TYR	4.2
1	A	64	LEU	4.2
1	B	561	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	419	VAL	4.2
1	C	532	SER	4.2
1	D	129	THR	4.2
1	A	407	LEU	4.2
1	C	153	ILE	4.2
1	D	133	GLU	4.2
1	B	532	SER	4.2
1	B	391	ARG	4.2
1	B	435	ASN	4.2
1	D	532	SER	4.2
1	C	342	LEU	4.2
1	A	391	ARG	4.2
1	A	334	VAL	4.2
1	A	143	LEU	4.2
1	D	451	GLU	4.1
1	C	299	LYS	4.1
1	D	450	ILE	4.1
1	C	510	ALA	4.1
1	D	86	SER	4.1
1	B	384	THR	4.1
1	C	18	PRO	4.1
1	A	44	MET	4.1
1	A	260	SER	4.1
1	C	552	GLU	4.1
1	A	360	ARG	4.1
1	D	252	ASP	4.1
1	D	350	THR	4.1
1	B	11	GLN	4.1
1	A	50	PRO	4.1
1	B	306	ALA	4.1
1	A	563	SER	4.1
1	D	139	SER	4.1
1	A	384	THR	4.1
1	D	389	ILE	4.1
1	C	364	LEU	4.1
1	D	553	ASP	4.1
1	A	30	ALA	4.1
1	C	450	ILE	4.1
1	C	30	ALA	4.1
1	B	527	GLN	4.0
1	D	264	ALA	4.0
1	A	19	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	298	LEU	4.0
1	A	147	VAL	4.0
1	C	88	CYS	4.0
1	D	211	LEU	4.0
1	A	465	LYS	4.0
1	C	132	SER	4.0
1	B	440	ALA	4.0
1	A	159	MET	4.0
1	B	420	ALA	4.0
1	D	138	SER	4.0
1	D	440	ALA	4.0
1	A	196	MET	4.0
1	C	167	LEU	4.0
1	A	58	LYS	4.0
1	A	109	MET	4.0
1	B	380	SER	4.0
1	D	460	MET	4.0
1	B	350	THR	4.0
1	D	476	GLU	4.0
1	B	159	MET	4.0
1	A	287	VAL	4.0
1	D	368	ALA	4.0
1	A	100	MET	4.0
1	B	378	SER	4.0
1	B	47	LEU	4.0
1	D	16	LEU	4.0
1	B	318	LEU	4.0
1	D	55	GLY	3.9
1	C	292	ILE	3.9
1	C	79	GLY	3.9
1	C	318	LEU	3.9
1	C	439	TYR	3.9
1	A	519	ILE	3.9
1	D	401	LEU	3.9
1	D	311	GLY	3.9
1	B	550	VAL	3.9
1	C	165	TRP	3.9
1	A	351	TYR	3.9
1	B	78	ARG	3.9
1	A	309	GLN	3.9
1	B	267	LEU	3.9
1	A	124	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	415	LEU	3.9
1	D	53	ASP	3.9
1	A	38	ALA	3.9
1	A	496	LEU	3.9
1	C	312	MET	3.9
1	D	292	ILE	3.9
1	D	167	LEU	3.9
1	C	454	ALA	3.8
1	A	101	ARG	3.8
1	D	395	ILE	3.8
1	C	387	SER	3.8
1	C	65	LEU	3.8
1	C	27	LEU	3.8
1	C	241	GLY	3.8
1	D	294	LEU	3.8
1	A	538	ARG	3.8
1	B	354	ARG	3.8
1	C	104	LEU	3.8
1	D	248	SER	3.8
1	B	457	ALA	3.8
1	A	264	ALA	3.8
1	A	486	ARG	3.8
1	A	289	SER	3.8
1	C	484	GLY	3.8
1	D	136	ALA	3.8
1	A	28	ILE	3.8
1	C	410	TYR	3.8
1	B	279	LEU	3.8
1	B	533	LEU	3.8
1	B	548	ILE	3.8
1	C	92	VAL	3.8
1	D	146	VAL	3.8
1	D	285	THR	3.8
1	A	162	TYR	3.8
1	B	130	TYR	3.8
1	B	542	ILE	3.8
1	C	306	ALA	3.8
1	C	109	MET	3.8
1	A	535	ILE	3.8
1	D	404	GLY	3.8
1	B	387	SER	3.8
1	D	173	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	515	SER	3.8
1	B	569	HIS	3.8
1	C	542	ILE	3.8
1	C	75	MET	3.7
1	C	140	SER	3.7
1	D	47	LEU	3.7
1	D	251	SER	3.7
1	A	286	VAL	3.7
1	B	77	LEU	3.7
1	D	23	PHE	3.7
1	D	511	LEU	3.7
1	D	34	LEU	3.7
1	D	298	LEU	3.7
1	B	34	LEU	3.7
1	A	134	GLN	3.7
1	B	447	ARG	3.7
1	B	86	SER	3.7
1	A	370	LYS	3.7
1	D	463	ILE	3.7
1	A	459	ALA	3.7
1	D	259	ALA	3.7
1	D	165	TRP	3.7
1	B	165	TRP	3.7
1	C	251	SER	3.7
1	A	460	MET	3.6
1	B	571	VAL	3.6
1	A	250	ILE	3.6
1	A	497	ARG	3.6
1	A	570	GLY	3.6
1	C	129	THR	3.6
1	B	129	THR	3.6
1	C	285	THR	3.6
1	B	269	ALA	3.6
1	C	496	LEU	3.6
1	A	484	GLY	3.6
1	D	523	LEU	3.6
1	C	45	LEU	3.6
1	C	190	ARG	3.6
1	C	175	ALA	3.6
1	B	401	LEU	3.6
1	D	174	LEU	3.6
1	B	61	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	392	PHE	3.6
1	B	19	THR	3.6
1	D	244	MET	3.6
1	B	171	LEU	3.6
1	A	170	ILE	3.6
1	B	173	VAL	3.5
1	B	298	LEU	3.5
1	D	534	VAL	3.5
1	B	140	SER	3.5
1	D	483	GLY	3.5
1	C	287	VAL	3.5
1	C	458	TYR	3.5
1	D	157	PHE	3.5
1	D	384	THR	3.5
1	C	493	ARG	3.5
1	B	96	VAL	3.5
1	D	63	VAL	3.5
1	A	292	ILE	3.5
1	B	190	ARG	3.5
1	A	229	ARG	3.5
1	C	126	SER	3.5
1	B	215	LYS	3.5
1	D	575	LEU	3.5
1	B	25	ALA	3.5
1	B	512	ASP	3.5
1	D	216	GLU	3.5
1	D	379	GLY	3.5
1	B	493	ARG	3.5
1	A	284	ILE	3.4
1	B	256	GLN	3.4
1	D	316	GLN	3.4
1	B	187	LYS	3.4
1	B	194	LYS	3.4
1	B	450	ILE	3.4
1	D	38	ALA	3.4
1	C	61	ARG	3.4
1	D	352	PRO	3.4
1	B	295	MET	3.4
1	C	161	PHE	3.4
1	A	441	ARG	3.4
1	A	127	ARG	3.4
1	D	357	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	545	ALA	3.4
1	A	49	LYS	3.4
1	D	60	ASP	3.4
1	D	147	VAL	3.4
1	A	356	VAL	3.4
1	D	414	SER	3.4
1	B	262	ALA	3.4
1	D	104	LEU	3.4
1	D	413	ALA	3.4
1	A	412	LEU	3.4
1	C	327	GLU	3.4
1	C	55	GLY	3.4
1	A	411	THR	3.4
1	C	520	GLN	3.3
1	A	568	GLN	3.3
1	C	382	LYS	3.3
1	B	65	LEU	3.3
1	D	411	THR	3.3
1	D	70	VAL	3.3
1	A	125	LEU	3.3
1	C	51	LEU	3.3
1	A	18	PRO	3.3
1	A	518	ALA	3.3
1	B	266	VAL	3.3
1	B	572	TYR	3.3
1	C	130	TYR	3.3
1	A	51	LEU	3.3
1	A	358	ALA	3.3
1	B	392	PHE	3.3
1	C	344	PHE	3.3
1	A	238	ARG	3.2
1	A	266	VAL	3.2
1	C	273	PRO	3.2
1	D	215	LYS	3.2
1	B	475	GLY	3.2
1	A	204	THR	3.2
1	C	460	MET	3.2
1	D	503	ILE	3.2
1	D	439	TYR	3.2
1	A	434	ALA	3.2
1	B	305	ASN	3.2
1	D	381	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	148	ARG	3.2
1	C	474	ILE	3.2
1	D	577	LYS	3.2
1	B	229	ARG	3.2
1	B	577	LYS	3.2
1	C	286	VAL	3.2
1	A	245	VAL	3.2
1	C	265	PHE	3.2
1	A	129	THR	3.2
1	B	132	SER	3.2
1	A	110	GLY	3.2
1	C	106	GLY	3.2
1	D	288	PHE	3.2
1	B	363	ASN	3.2
1	C	211	LEU	3.2
1	B	349	PHE	3.2
1	C	47	LEU	3.2
1	D	388	LEU	3.2
1	A	140	SER	3.1
1	C	352	PRO	3.1
1	D	536	ALA	3.1
1	C	419	VAL	3.1
1	A	437	ILE	3.1
1	B	148	ARG	3.1
1	B	511	LEU	3.1
1	B	122	GLY	3.1
1	B	287	VAL	3.1
1	A	17	TRP	3.1
1	B	357	PRO	3.1
1	C	62	SER	3.1
1	A	175	ALA	3.1
1	C	511	LEU	3.1
1	C	539	LEU	3.1
1	D	540	SER	3.1
1	B	211	LEU	3.1
1	D	539	LEU	3.1
1	C	489	ILE	3.1
1	D	351	TYR	3.1
1	A	185	VAL	3.1
1	D	319	PHE	3.1
1	B	323	ASP	3.1
1	C	194	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	127	ARG	3.1
1	A	493	ARG	3.0
1	D	347	VAL	3.0
1	B	412	LEU	3.0
1	C	487	GLN	3.0
1	A	527	GLN	3.0
1	B	407	LEU	3.0
1	C	96	VAL	3.0
1	A	23	PHE	3.0
1	B	355	GLU	3.0
1	C	345	ARG	3.0
1	A	551	VAL	3.0
1	B	482	SER	3.0
1	B	376	GLY	3.0
1	B	179	SER	3.0
1	A	234	SER	3.0
1	B	59	THR	3.0
1	B	133	GLU	3.0
1	C	269	ALA	3.0
1	B	344	PHE	2.9
1	B	245	VAL	2.9
1	D	126	SER	2.9
1	C	57	GLY	2.9
1	B	389	ILE	2.9
1	D	305	ASN	2.9
1	A	288	PHE	2.9
1	D	91	TRP	2.9
1	D	356	VAL	2.9
1	A	29	VAL	2.9
1	A	70	VAL	2.9
1	B	64	LEU	2.9
1	C	522	ALA	2.9
1	D	273	PRO	2.9
1	D	197	GLN	2.9
1	B	31	GLY	2.9
1	C	575	LEU	2.9
1	A	345	ARG	2.9
1	A	472	THR	2.9
1	B	549	VAL	2.9
1	C	133	GLU	2.9
1	B	103	ARG	2.9
1	B	272	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	59	THR	2.9
1	B	537	HIS	2.8
1	B	249	SER	2.8
1	C	545	ALA	2.8
1	D	358	ALA	2.8
1	A	78	ARG	2.8
1	B	381	GLY	2.8
1	A	211	LEU	2.8
1	C	244	MET	2.8
1	C	536	ALA	2.8
1	C	357	PRO	2.8
1	D	489	ILE	2.8
1	B	504	LEU	2.8
1	D	267	LEU	2.8
1	D	140	SER	2.8
1	B	546	ASP	2.8
1	D	44	MET	2.8
1	B	76	ILE	2.8
1	C	452	GLU	2.8
1	A	368	ALA	2.8
1	B	335	ILE	2.8
1	D	410	TYR	2.8
1	C	551	VAL	2.8
1	B	565	LEU	2.8
1	B	494	ALA	2.8
1	B	274	SER	2.8
1	D	380	SER	2.8
1	C	465	LYS	2.8
1	D	535	ILE	2.8
1	A	81	THR	2.8
1	C	179	SER	2.8
1	A	577	LYS	2.8
1	C	526	LEU	2.8
1	D	348	THR	2.8
1	A	479	VAL	2.7
1	C	323	ASP	2.7
1	A	433	VAL	2.7
1	B	204	THR	2.7
1	B	545	ALA	2.7
1	B	480	LEU	2.7
1	D	121	THR	2.7
1	D	561	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	111	MET	2.7
1	A	566	LEU	2.7
1	D	345	ARG	2.7
1	B	288	PHE	2.7
1	B	176	PRO	2.7
1	D	420	ALA	2.7
1	D	405	HIS	2.7
1	B	230	PHE	2.7
1	C	389	ILE	2.7
1	D	551	VAL	2.7
1	B	170	ILE	2.6
1	D	308	PHE	2.6
1	D	89	ILE	2.6
1	A	495	LEU	2.6
1	D	492	ALA	2.6
1	C	374	LEU	2.6
1	C	234	SER	2.6
1	C	63	VAL	2.6
1	D	393	TYR	2.6
1	A	542	ILE	2.6
1	C	404	GLY	2.6
1	B	474	ILE	2.6
1	B	35	ILE	2.6
1	B	319	PHE	2.6
1	A	220	PHE	2.6
1	A	14	ARG	2.6
1	C	171	LEU	2.6
1	C	112	PRO	2.6
1	B	551	VAL	2.5
1	C	512	ASP	2.6
1	B	368	ALA	2.5
1	D	433	VAL	2.5
1	C	445	TYR	2.5
1	B	210	MET	2.5
1	C	282	GLY	2.5
1	D	537	HIS	2.5
1	D	550	VAL	2.5
1	A	355	GLU	2.5
1	A	379	GLY	2.5
1	B	289	SER	2.5
1	C	423	SER	2.5
1	D	574	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	219	ILE	2.5
1	B	408	ARG	2.5
1	B	340	GLY	2.5
1	B	144	ILE	2.4
1	D	263	LEU	2.4
1	A	485	GLN	2.4
1	C	158	ILE	2.4
1	C	73	GLY	2.4
1	C	393	TYR	2.4
1	A	489	ILE	2.4
1	B	278	SER	2.4
1	D	190	ARG	2.4
1	C	255	ILE	2.4
1	C	420	ALA	2.4
1	D	218	LEU	2.4
1	B	317	THR	2.4
1	C	173	VAL	2.4
1	D	274	SER	2.4
1	B	48	LEU	2.4
1	D	289	SER	2.4
1	A	302	THR	2.4
1	D	66	TRP	2.4
1	C	252	ASP	2.4
1	D	279	LEU	2.4
1	D	475	GLY	2.4
1	C	479	VAL	2.4
1	B	41	ASP	2.3
1	D	155	GLY	2.3
1	B	416	ARG	2.3
1	D	291	MET	2.3
1	A	279	LEU	2.3
1	C	187	LYS	2.3
1	A	372	VAL	2.3
1	B	379	GLY	2.3
1	C	17	TRP	2.3
1	A	359	LEU	2.3
1	B	359	LEU	2.3
1	D	164	SER	2.3
1	D	386	ALA	2.3
1	D	27	LEU	2.3
1	A	576	HIS	2.3
1	B	152	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	105	PHE	2.3
1	C	415	LEU	2.3
1	B	462	PHE	2.3
1	A	168	SER	2.3
1	C	204	THR	2.3
1	B	351	TYR	2.3
1	B	255	ILE	2.3
1	A	277	ASP	2.2
1	D	488	ARG	2.2
1	A	321	ILE	2.2
1	A	511	LEU	2.2
1	D	74	LEU	2.2
1	A	483	GLY	2.2
1	A	424	GLN	2.2
1	B	217	VAL	2.2
1	A	474	ILE	2.2
1	D	186	SER	2.2
1	B	431	ASP	2.2
1	B	320	ALA	2.2
1	D	65	LEU	2.2
1	A	34	LEU	2.2
1	A	536	ALA	2.2
1	B	448	GLU	2.2
1	D	481	LEU	2.2
1	A	466	MET	2.2
1	D	459	ALA	2.2
1	D	58	LYS	2.2
1	B	406	ASP	2.1
1	B	559	ARG	2.1
1	A	456	MET	2.1
1	B	55	GLY	2.1
1	D	284	ILE	2.1
1	C	529	ASN	2.1
1	B	263	LEU	2.1
1	C	270	ALA	2.1
1	C	347	VAL	2.1
1	D	494	ALA	2.1
1	A	48	LEU	2.1
1	A	523	LEU	2.1
1	A	24	LYS	2.1
1	A	382	LYS	2.1
1	A	274	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	519	ILE	2.1
1	C	413	ALA	2.1
1	D	328	LYS	2.1
1	A	375	VAL	2.0
1	A	218	LEU	2.0
1	C	319	PHE	2.0
1	A	77	LEU	2.0
1	D	88	CYS	2.0
1	D	331	GLY	2.0
1	D	79	GLY	2.0
1	C	440	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ANP	A	5002	31/31	-0.03	1.01	-0.16	219,219,219,219	0
2	ANP	B	5001	31/31	-0.02	0.99	-0.22	219,219,219,219	0
2	ANP	D	5003	31/31	0.20	1.04	-0.34	219,219,219,219	0
2	ANP	C	5004	31/31	-0.01	1.00	-0.44	219,219,219,219	0

6.5 Other polymers [i](#)

There are no such residues in this entry.