



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 09:31 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 wwPDB validation summary 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/ValidationPDFNotes.html>

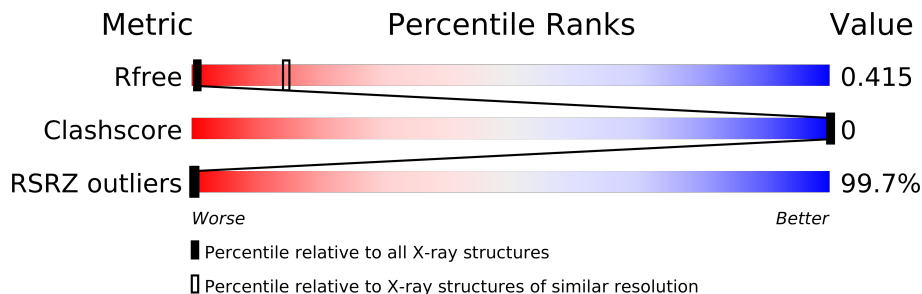
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1029 (5.50-3.50)
Clashscore	79885	1300 (5.50-3.50)
RSRZ outliers	66119	1028 (5.50-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	582	
1	B	582	
1	C	582	
1	D	582	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	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 i

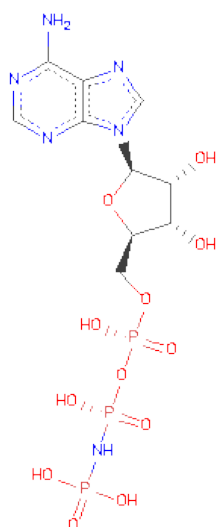
There are 2 unique types of molecules in this entry. The entry contains 2412 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

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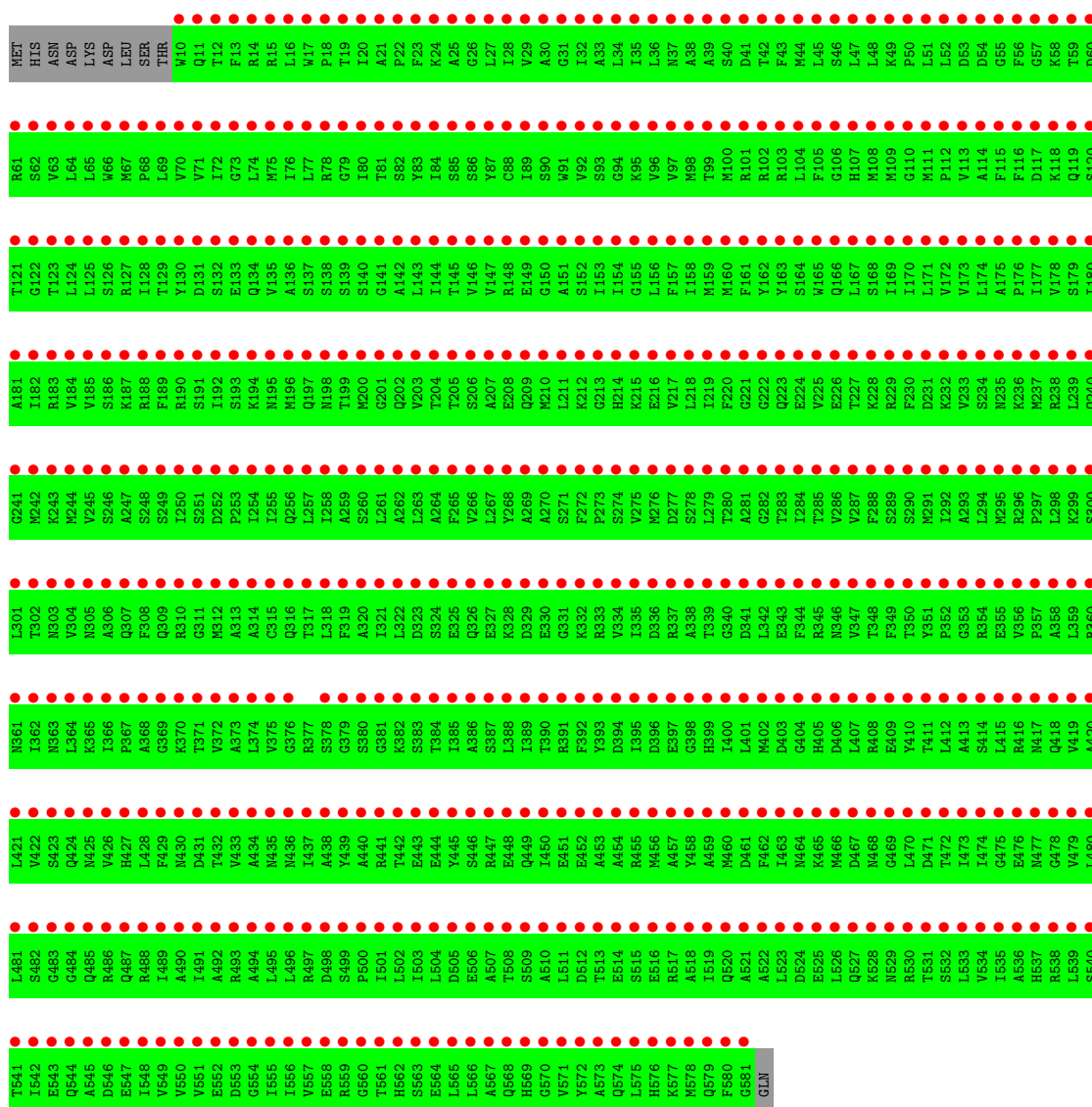
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

Chain A: 



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

Chain B: 



G241	L301	N361	L421	L481	T541
M242	T302	I362	V422	S482	I542
K243	N303	N363	V423	G483	E543
M244	N304	L364	Q424	G484	Q544
N245	N305	K365	N425	Q485	A545
S246	N306	I366	N426	R486	D546
S247	N307	P367	H427	Q487	E547
S248	N308	A368	L428	R488	I548
S249	N309	G369	F429	V549	V549
I250	N310	K370	N430	A490	V550
S251	G311	T371	D431	V551	V551
D252	N312	V372	T432	A492	D552
P253	A313	A373	V433	R493	D553
I254	A314	L374	A434	A494	G554
I255	C315	V375	N435	L495	I555
Q256	Q316	G376	N436	L496	I556
Q257	L317	R377	I437	R497	V557
L258	L318	S378	A438	D498	E558
A259	F319	G379	Y439	S499	R559
S260	A320	S380	A440	P500	G560
A261	L321	R441	A441	L501	T561
L262	L322	K382	T442	L502	H562
L263	D323	S383	E443	I503	S563
A264	S324	T384	E444	L504	E564
F265	E325	I385	Y445	D505	L565
V266	Q326	A386	S446	E506	L566
L267	E327	S387	R447	A507	A567
Y268	K328	L388	E448	T508	Q568
A269	D329	I389	Q449	S509	H569
A270	E330	T390	A450	A510	Q570
S271	G331	R391	E451	L511	V571
F272	K332	F392	E452	D512	Y572
P273	R333	T393	A453	T513	A573
S274	V334	D394	A454	E514	Q574
V275	I335	I395	R455	S515	L575
M276	D336	D396	M456	E516	H576
D277	R337	E397	A457	R517	K577
S278	A338	G398	Y458	A518	M578
L279	T339	H399	A459	I519	Q579
T280	G340	I400	M460	Q520	F580
A281	D341	L401	F461	A521	G581
G282	L342	M402	D462	A522	GLN
T283	E343	D403	I463	L523	
I284	F344	G404	N464	D524	
T285	R345	H405	K465	E525	
V286	N346	D406	M466	L526	
V287	V347	L407	D467	Q527	
F288	T348	R408	N468	K528	
S289	F349	E409	G469	N529	
S290	T350	Y410	L470	R530	
M291	Y351	T411	D471	T531	
L292	P352	L412	T472	S532	
A293	G353	A413	I473	L533	
L294	R354	S414	I474	V534	
M295	E355	L415	G475	T535	
R296	V356	R416	E476	A536	
P297	P357	N417	N477	H537	
L298	A358	Q418	G478	R538	
K299	L359	V419	V479	L539	
S300	R360	A420	L480	S540	

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

Chain D:

MET	ASN	ASP	LYS	ASP	LEU	SER	THR	W10	T12	F13	R14	R15	L16	W17	P18	T19	I20	L21	T56	H56	S56	E56	L56	L56	A56	H56	Q56	V56	Y56	A56	E56	L56	H56	K56	M56	Q56		
R61	S62	V63	L64	N65	W66	M67	P68	R69	V70	T71	G73	L74	M75	I76	L77	R78	G79	I80	T81	S82	Y83	I84	S85	S86	Y87	C88	I89	S90	Y91	V92	S93	G94	K95	V96	V97	M98	T99	M100
T121	G122	T123	L124	N125	S126	R127	I128	T129	Y130	D131	E132	Q133	V135	I136	L137	S138	S139	G140	G141	L142	S143	T144	T145	V146	Y147	R148	E149	G150	A151	S152	T153	I154	G155	L156	F157	I158	M159	M160
A181	I182	V183	W184	N185	S186	K187	F188	R189	R190	S191	S192	K193	M195	M196	Q197	N198	T199	M200	G201	Q202	V203	T204	T205	S206	A207	Q209	A210	M211	K212	G213	H214	K215	E216	V217	L218	I219	F220	
G241	M242	K243	M244	V245	S246	A247	S248	S249	I250	S251	P252	P253	I255	Q256	L257	I258	A259	S260	L261	A262	L263	A264	F265	V266	L267	Y268	A269	A270	S271	F272	P273	S274	V275	M276	D277	S278	L279	T280
L301	T302	N303	V304	N305	A306	Q307	F308	Q309	R310	G311	M312	A313	A314	C315	V316	L317	F319	S320	L321	K322	S323	E324	S325	Q326	E327	K328	D329	E330	G331	K332	T333	D334	I335	D336	R337	A338	T339	G340
N361	I362	N363	L364	K365	I366	P367	A368	G369	T370	T371	V372	A373	L374	G375	G376	R377	S378	G379	S380	R441	K382	S383	T384	I385	A386	S387	I389	T390	I391	F392	T393	D394	I395	D396	E397	G398	I400	L401
L421	V422	S423	Q424	N425	N426	H427	L428	F429	N430	D431	T432	V433	A434	N435	V436	R437	Y439	A440	R441	T442	E443	E444	Y445	S446	R447	Q448	Q449	I450	A451	E452	A453	A454	M455	M456	A457	Y458	M459	M460
L481	S482	G483	Q484	Q485	R486	Q487	R488	L489	A490	L491	A492	R493	A494	L495	L496	R497	S499	P500	L501	L502	S503	E504	D505	E506	A507	T508	S509	A510	L511	D512	A513	E514	S515	E516	R517	A518	I519	Q520
T541	I542	E543	Q544	A545	D546	E547	I548	V549	V550	V551	D552	D553	G554	I555	I556	V557	R559	G560	T561	H562	S563	E564	L565	L566	A567	H569	Q570	V571	Y572	A573	Q574	L575	H576	K577	M578	Q579	G581	
R61	S62	V63	L64	N65	W66	M67	P68	R69	V70	T71	G73	L74	M75	I76	L77	R78	G79	I80	T81	S82	Y83	I84	S85	S86	Y87	C88	I89	S90										

L481	S482	G483	G484	Q485	R486	Q487	R488	I489	A490	I491	A492	R493	A494	L495	L496	R497	D498	S499	P500	I501	L502	I503	L504	D505	E506	A507	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																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
T541	I542	E543	Q544	A545	D546	E547	I548	V549	V550	V551	E552	D553	G554	I555	I556	V557	E558	R559	G560	T561	H562	S563	E564	I565	L566	A567	Q568	H569	G570	V571	V572	A573	Q574	L575	H576	K577	K578	Q579	F580	G581	Gln																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									</

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 0.402 , 0.415	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)	0.86 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25959 reflections	Xtriage
F_o, F_c correlation	0.84	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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	33,33,33	1.55	5 (15%)	51,52,52	2.08	9 (17%)
2	ANP	B	5001	-	33,33,33	2.79	12 (36%)	51,52,52	2.64	12 (23%)
2	ANP	C	5004	-	33,33,33	1.59	5 (15%)	51,52,52	2.08	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	D	5003	-	33,33,33	1.58	5 (15%)	51,52,52	2.08	10 (19%)

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	-	-	0/18/38/38	0/1/3/3
2	ANP	B	5001	-	-	0/18/38/38	0/1/3/3
2	ANP	C	5004	-	-	0/18/38/38	0/1/3/3
2	ANP	D	5003	-	-	0/18/38/38	0/1/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	PB-O1B	-6.20	1.38	1.46
2	B	5001	ANP	PB-N3B	6.07	1.69	1.64
2	B	5001	ANP	C4-N9	5.61	1.45	1.37
2	B	5001	ANP	PG-N3B	5.00	1.68	1.64
2	B	5001	ANP	C8-N9	4.48	1.43	1.36

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	ANP	C4'-O4'-C1'	-9.43	99.50	109.75
2	B	5001	ANP	C8-N9-C4	-8.27	100.58	106.90
2	B	5001	ANP	O4'-C1'-C2'	-6.70	96.50	106.77
2	C	5004	ANP	O4'-C1'-C2'	-6.26	97.18	106.77
2	A	5002	ANP	O4'-C1'-C2'	-6.22	97.24	106.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	28.06	571 (99%) 0 0	142, 225, 277, 312	0
1	B	572/582 (98%)	28.73	570 (99%) 0 0	112, 212, 274, 321	0
1	C	572/582 (98%)	28.92	571 (99%) 0 0	130, 218, 271, 309	0
1	D	572/582 (98%)	31.66	570 (99%) 0 0	132, 220, 271, 314	0
All	All	2288/2328 (98%)	29.34	2282 (99%) 0 0	112, 219, 274, 321	0

The worst 5 of 2282 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	530	ARG	148.7
1	C	49	LYS	145.2
1	B	562	HIS	141.2
1	D	320	ALA	139.2
1	C	345	ARG	135.8

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ANP	D	5003	31/31	1.10	-0.46	219,219,219,219	0
2	ANP	C	5004	31/31	1.11	-0.68	219,219,219,219	0
2	ANP	B	5001	31/31	1.21	-0.69	219,219,219,219	0
2	ANP	A	5002	31/31	1.14	-0.75	219,219,219,219	0

6.5 Other polymers ⓘ

There are no such residues in this entry.