



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:31 AM GMT

PDB ID : 3B5Z
Title : Crystal Structure of MsbA from Salmonella typhimurium with ADP Vanadate
Authors : Ward, A.; Reyes, C.L.; Yu, J.; Roth, C.B.; Chang, G.
Deposited on : 2007-10-26
Resolution : 4.20 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

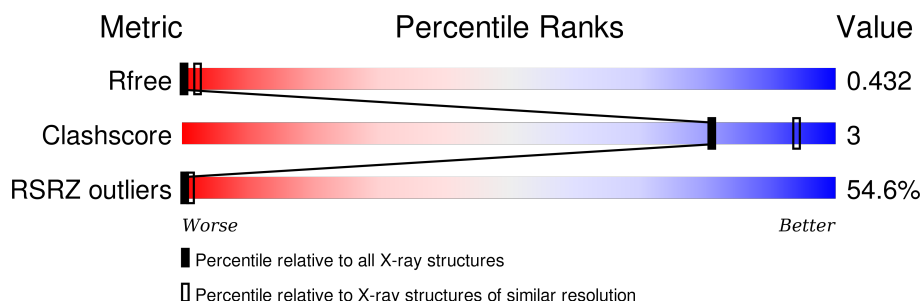
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	<div> <div>48%</div> <div>98%</div> </div>
1	B	582	<div> <div>53%</div> <div>98%</div> </div>
1	C	582	<div> <div>54%</div> <div>98%</div> </div>
1	D	582	<div> <div>59%</div> <div>98%</div> </div>

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	ADP	A	5001	-	-	-	X
2	ADP	B	601	-	-	-	X
2	ADP	C	601	-	-	-	X
2	ADP	D	601	-	-	-	X

2 Entry composition [i](#)

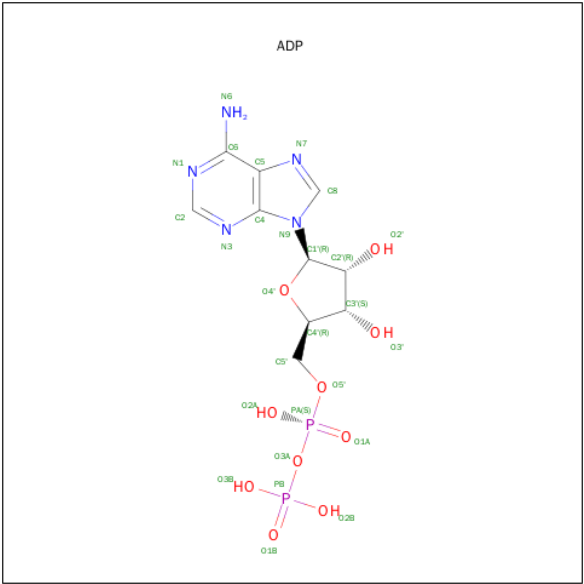
There are 3 unique types of molecules in this entry. The entry contains 2400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

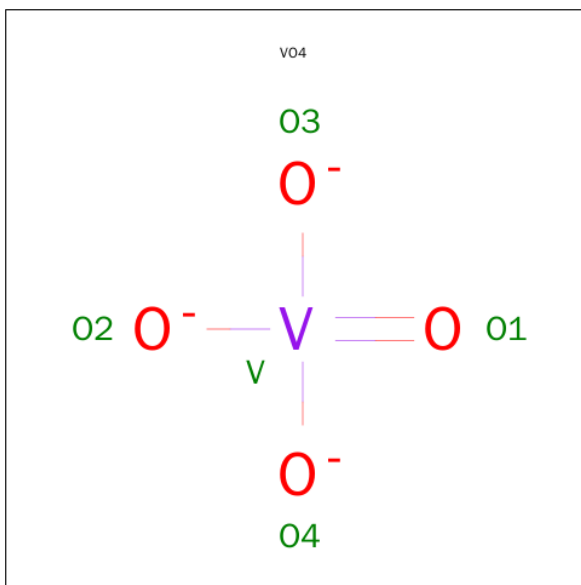
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
2	D	1	Total	C	N	O	P	0	0
			26	10	5	9	2		

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O₄V).

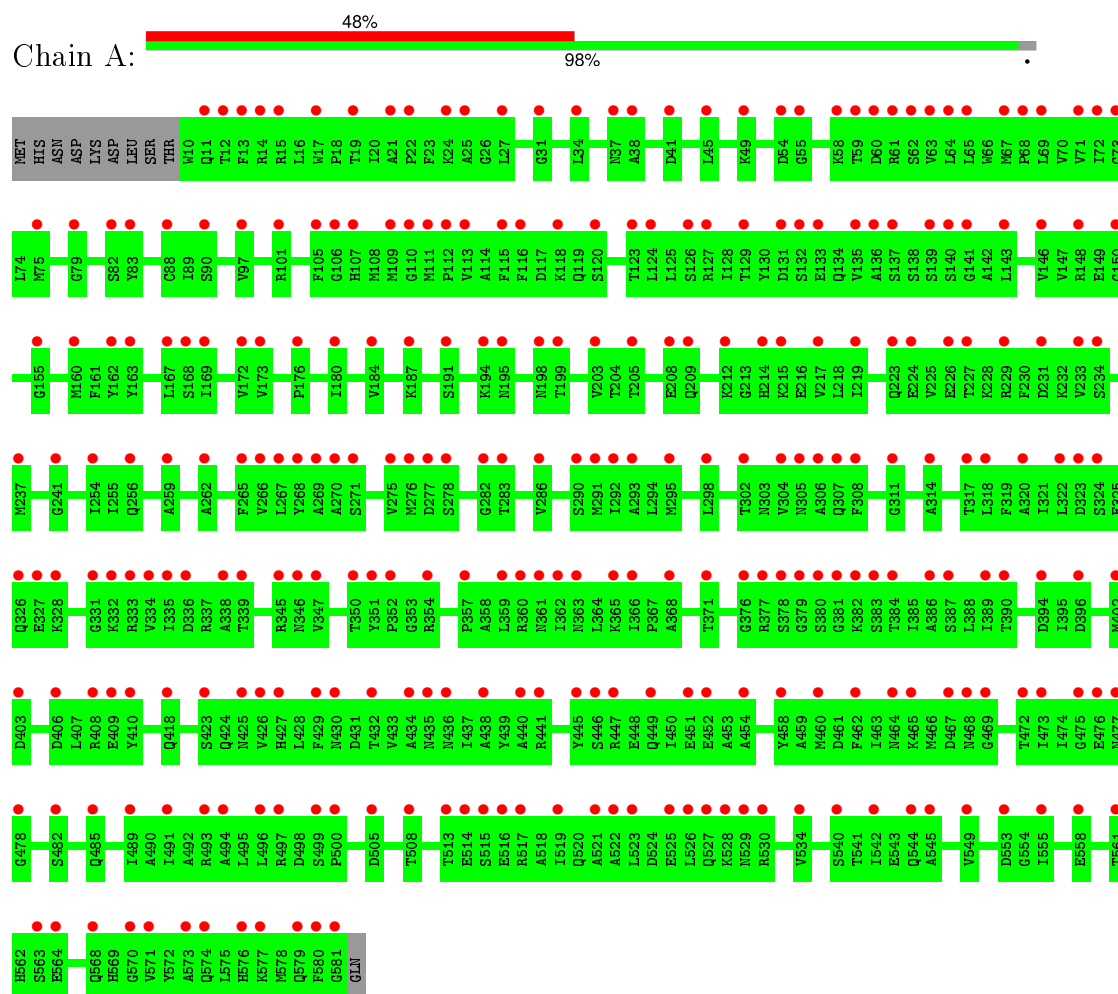


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			2	1	1		
3	B	1	Total	O	V	0	0
			2	1	1		
3	C	1	Total	O	V	0	0
			2	1	1		
3	D	1	Total	O	V	0	0
			2	1	1		

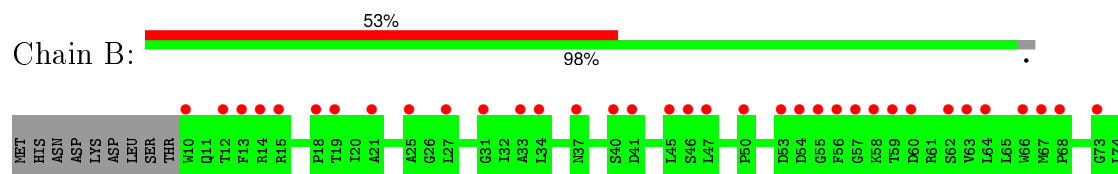
3 Residue-property plots

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.

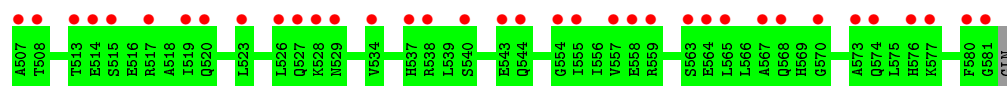
- Molecule 1: Lipid A export ATP-binding/permease protein msbA



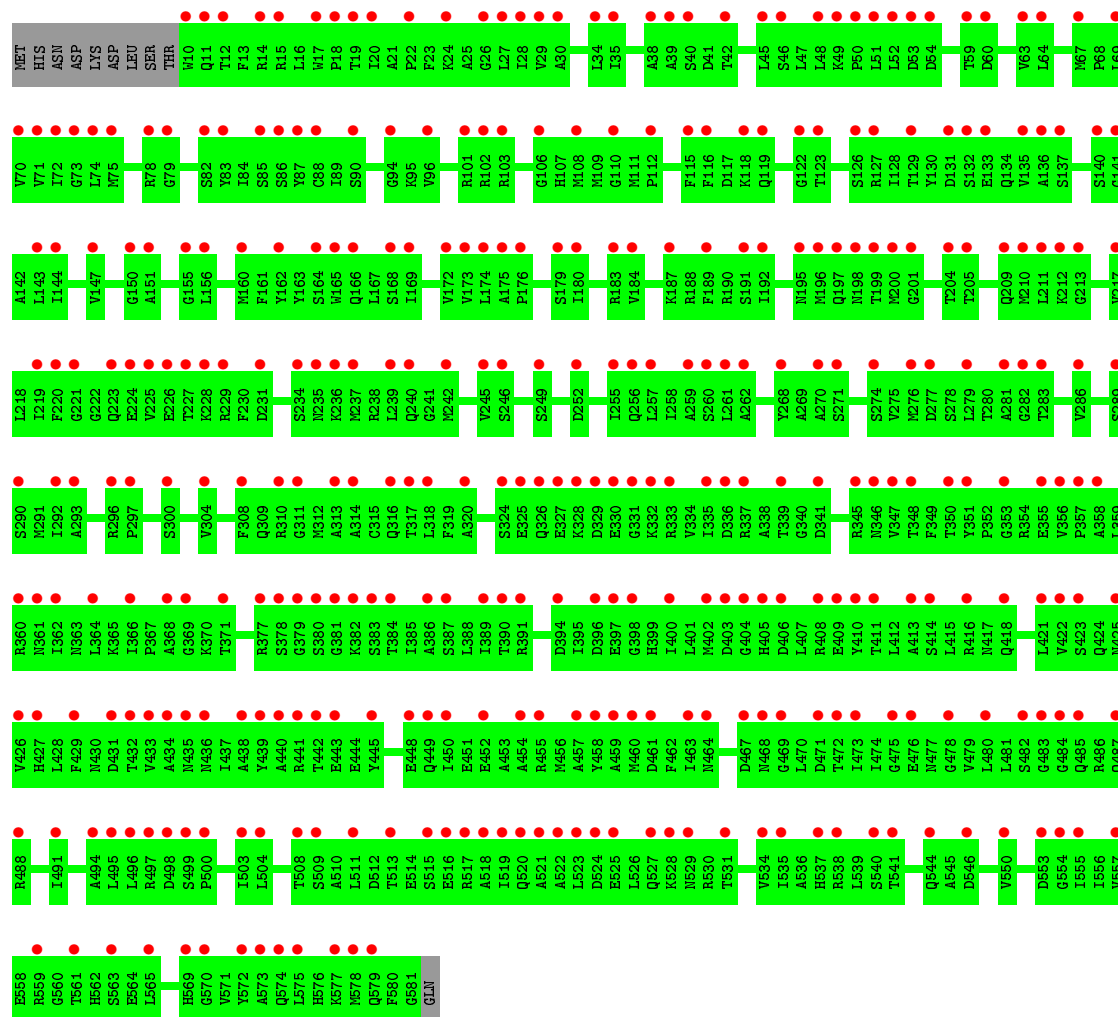
- Molecule 1: Lipid A export ATP-binding/permease protein msbA







- 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	267.17Å 121.10Å 176.74Å 90.00° 121.57° 90.00°	Depositor
Resolution (Å)	20.00 – 4.20 20.00 – 4.20	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-4.20) 86.3 (20.00-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 4.21Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.336 , 0.362 0.413 , 0.432	Depositor DCC
R_{free} test set	2121 reflections (7.04%)	DCC
Wilson B-factor (Å ²)	173.0	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.72 , 314.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30164 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2400	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: VO4, ADP

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	26	0	12	2	0
2	B	26	0	12	2	0
2	C	26	0	12	2	0
2	D	26	0	12	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	2400	0	48	8	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 3.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:ADP:O2A	2:C:601:ADP:O1B	2.27	0.52
2:B:601:ADP:O2B	2:B:601:ADP:O1A	2.28	0.50
2:A:5001:ADP:O1A	2:A:5001:ADP:O2B	2.30	0.50
2:B:601:ADP:O1B	2:B:601:ADP:O2A	2.30	0.49
2:C:601:ADP:O2B	2:C:601:ADP:O1A	2.31	0.47
2:D:601:ADP:O1B	2:D:601:ADP:O2A	2.33	0.45
2:D:601:ADP:O1A	2:D:601:ADP:O2B	2.35	0.45
2:A:5001:ADP:O1B	2:A:5001:ADP:O2A	2.35	0.44

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

8 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	ADP	A	5001	3	19,28,29	1.33	2 (10%)	21,42,45	2.60	2 (9%)
3	VO4	A	5002	2	0,1,4	0.00	-	0,0,6	0.00	-
2	ADP	B	601	3	19,28,29	1.15	2 (10%)	21,42,45	2.36	3 (14%)
3	VO4	B	602	2	0,1,4	0.00	-	0,0,6	0.00	-
2	ADP	C	601	3	19,28,29	1.44	2 (10%)	21,42,45	2.45	2 (9%)
3	VO4	C	602	2	0,1,4	0.00	-	0,0,6	0.00	-
2	ADP	D	601	3	19,28,29	1.44	2 (10%)	21,42,45	2.47	3 (14%)
3	VO4	D	602	2	0,1,4	0.00	-	0,0,6	0.00	-

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	ADP	A	5001	3	-	0/9/31/32	0/3/3/3
3	VO4	A	5002	2	-	0/0/0/0	0/0/0/0
2	ADP	B	601	3	-	0/9/31/32	0/3/3/3
3	VO4	B	602	2	-	0/0/0/0	0/0/0/0
2	ADP	C	601	3	-	0/9/31/32	0/3/3/3
3	VO4	C	602	2	-	0/0/0/0	0/0/0/0
2	ADP	D	601	3	-	0/9/31/32	0/3/3/3
3	VO4	D	602	2	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ADP	C8-N7	-2.80	1.29	1.34
2	D	601	ADP	C8-N7	-2.65	1.29	1.34
2	A	5001	ADP	C8-N7	-2.53	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C8-N7	-2.01	1.30	1.34
2	B	601	ADP	O4'-C1'	3.59	1.45	1.41
2	A	5001	ADP	O4'-C1'	4.23	1.46	1.41
2	C	601	ADP	O4'-C1'	4.56	1.47	1.41
2	D	601	ADP	O4'-C1'	4.71	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	ADP	N3-C2-N1	-10.20	121.09	128.89
2	D	601	ADP	N3-C2-N1	-9.88	121.33	128.89
2	C	601	ADP	N3-C2-N1	-9.72	121.45	128.89
2	B	601	ADP	N3-C2-N1	-9.47	121.64	128.89
2	D	601	ADP	C4-C5-N7	-2.23	107.43	109.48
2	B	601	ADP	C4-C5-N7	-2.12	107.53	109.48
2	B	601	ADP	O3A-PA-O5'	2.99	110.88	102.94
2	C	601	ADP	O3A-PA-O5'	3.26	111.58	102.94
2	D	601	ADP	O3A-PA-O5'	3.49	112.19	102.94
2	A	5001	ADP	O3A-PA-O5'	4.10	113.80	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	ADP	2	0
2	B	601	ADP	2	0
2	C	601	ADP	2	0
2	D	601	ADP	2	0

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%)	2.57	281 (49%) 0 1	116, 152, 169, 183	0
1	B	572/582 (98%)	2.79	307 (53%) 0 1	125, 155, 170, 184	0
1	C	572/582 (98%)	2.87	316 (55%) 0 1	114, 153, 171, 184	0
1	D	572/582 (98%)	3.05	346 (60%) 0 1	124, 156, 171, 188	0
All	All	2288/2328 (98%)	2.82	1250 (54%) 0 1	114, 154, 170, 188	0

All (1250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	60	ASP	16.1
1	B	325	GLU	15.0
1	D	529	ASN	14.4
1	B	18	PRO	14.2
1	B	115	PHE	13.8
1	C	336	ASP	13.7
1	A	75	MET	13.2
1	C	432	THR	12.9
1	B	60	ASP	12.8
1	A	129	THR	12.7
1	A	71	VAL	12.6
1	A	49	LYS	12.6
1	C	573	ALA	12.4
1	D	524	ASP	12.1
1	B	129	THR	11.9
1	D	10	TRP	11.5
1	A	45	LEU	11.3
1	D	151	ALA	11.2
1	B	45	LEU	11.2
1	B	119	GLN	11.0
1	D	442	THR	11.0

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Mol	Chain	Res	Type	RSRZ
1	C	468	ASN	11.0
1	A	11	GLN	10.7
1	D	402	MET	10.7
1	B	527	GLN	10.7
1	D	327	GLU	10.6
1	C	320	ALA	10.5
1	B	320	ALA	10.4
1	B	50	PRO	10.4
1	A	234	SER	10.3
1	D	570	GLY	10.3
1	C	122	GLY	10.3
1	C	19	THR	10.3
1	A	462	PHE	10.3
1	D	136	ALA	10.3
1	B	94	GLY	10.3
1	C	67	MET	10.2
1	B	522	ALA	10.1
1	B	259	ALA	10.1
1	D	409	GLU	10.0
1	C	439	TYR	10.0
1	D	60	ASP	9.9
1	C	271	SER	9.9
1	C	278	SER	9.9
1	B	140	SER	9.8
1	D	129	THR	9.8
1	B	59	THR	9.7
1	B	274	SER	9.7
1	C	470	LEU	9.7
1	C	126	SER	9.6
1	C	217	VAL	9.6
1	B	465	LYS	9.5
1	A	563	SER	9.5
1	C	451	GLU	9.4
1	B	445	TYR	9.3
1	D	324	SER	9.3
1	A	564	GLU	9.2
1	B	151	ALA	9.2
1	A	458	TYR	9.2
1	C	427	HIS	9.1
1	B	197	GLN	9.0
1	C	167	LEU	9.0
1	C	298	LEU	9.0

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Mol	Chain	Res	Type	RSRZ
1	C	237	MET	9.0
1	D	310	ARG	8.9
1	D	119	GLN	8.9
1	D	522	ALA	8.9
1	C	305	ASN	8.8
1	D	348	THR	8.8
1	A	136	ALA	8.7
1	A	576	HIS	8.7
1	D	516	GLU	8.7
1	C	332	LYS	8.7
1	D	292	ILE	8.7
1	D	14	ARG	8.6
1	D	452	GLU	8.6
1	D	544	GLN	8.6
1	B	425	ASN	8.6
1	B	278	SER	8.6
1	B	567	ALA	8.6
1	D	423	SER	8.5
1	C	324	SER	8.5
1	D	246	SER	8.5
1	D	34	LEU	8.4
1	A	574	GLN	8.4
1	A	68	PRO	8.4
1	C	361	ASN	8.4
1	B	55	GLY	8.3
1	A	112	PRO	8.3
1	D	555	ILE	8.3
1	B	494	ALA	8.3
1	D	406	ASP	8.2
1	D	227	THR	8.2
1	B	516	GLU	8.1
1	A	302	THR	8.1
1	A	137	SER	8.1
1	D	289	SER	8.1
1	C	442	THR	8.1
1	B	155	GLY	8.1
1	D	463	ILE	8.1
1	D	553	ASP	8.1
1	C	227	THR	8.1
1	D	11	GLN	8.1
1	A	406	ASP	8.0
1	B	520	GLN	8.0

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Mol	Chain	Res	Type	RSRZ
1	B	555	ILE	8.0
1	C	27	LEU	8.0
1	C	387	SER	7.9
1	B	63	VAL	7.9
1	D	488	ARG	7.9
1	C	328	LYS	7.9
1	D	49	LYS	7.9
1	D	537	HIS	7.8
1	D	410	TYR	7.8
1	C	213	GLY	7.8
1	A	497	ARG	7.8
1	D	398	GLY	7.8
1	B	282	GLY	7.7
1	B	402	MET	7.7
1	C	268	TYR	7.7
1	C	534	VAL	7.7
1	B	498	ASP	7.6
1	B	184	VAL	7.6
1	B	41	ASP	7.6
1	A	237	MET	7.6
1	C	173	VAL	7.5
1	D	413	ALA	7.5
1	A	266	VAL	7.5
1	D	515	SER	7.5
1	D	172	VAL	7.5
1	D	476	GLU	7.5
1	C	82	SER	7.5
1	A	436	ASN	7.4
1	D	242	MET	7.4
1	B	327	GLU	7.4
1	A	477	ASN	7.4
1	A	333	ARG	7.4
1	C	436	ASN	7.4
1	D	332	LYS	7.4
1	C	257	LEU	7.3
1	C	458	TYR	7.3
1	A	545	ALA	7.3
1	D	473	ILE	7.3
1	B	214	HIS	7.3
1	B	414	SER	7.2
1	B	452	GLU	7.2
1	C	337	ARG	7.2

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Mol	Chain	Res	Type	RSRZ
1	D	436	ASN	7.2
1	D	259	ALA	7.2
1	D	449	GLN	7.2
1	A	270	ALA	7.2
1	A	460	MET	7.1
1	A	115	PHE	7.1
1	B	143	LEU	7.1
1	C	199	THR	7.1
1	A	570	GLY	7.0
1	D	540	SER	7.0
1	A	525	GLU	7.0
1	B	353	GLY	7.0
1	D	318	LEU	7.0
1	D	180	ILE	7.0
1	A	259	ALA	7.0
1	C	45	LEU	7.0
1	B	410	TYR	7.0
1	C	115	PHE	6.9
1	A	150	GLY	6.9
1	C	172	VAL	6.9
1	C	537	HIS	6.9
1	C	14	ARG	6.9
1	B	442	THR	6.9
1	D	461	ASP	6.9
1	A	326	GLN	6.9
1	B	443	GLU	6.8
1	D	274	SER	6.8
1	D	140	SER	6.8
1	D	346	ASN	6.8
1	D	337	ARG	6.8
1	D	404	GLY	6.8
1	C	577	LYS	6.8
1	A	101	ARG	6.8
1	D	565	LEU	6.7
1	C	292	ILE	6.7
1	D	432	THR	6.6
1	C	121	THR	6.6
1	B	201	GLY	6.6
1	D	380	SER	6.6
1	A	368	ALA	6.6
1	B	75	MET	6.5
1	C	307	GLN	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	162	TYR	6.5
1	A	162	TYR	6.5
1	A	320	ALA	6.5
1	C	270	ALA	6.5
1	C	34	LEU	6.5
1	D	19	THR	6.4
1	A	25	ALA	6.4
1	B	262	ALA	6.4
1	B	462	PHE	6.4
1	B	332	LYS	6.4
1	B	564	GLU	6.4
1	D	460	MET	6.3
1	A	362	ILE	6.3
1	B	497	ARG	6.3
1	B	169	ILE	6.3
1	B	57	GLY	6.3
1	C	316	GLN	6.3
1	C	195	ASN	6.3
1	C	357	PRO	6.2
1	C	224	GLU	6.2
1	D	213	GLY	6.2
1	A	13	PHE	6.2
1	A	345	ARG	6.2
1	D	239	LEU	6.2
1	B	261	LEU	6.2
1	C	529	ASN	6.2
1	D	67	MET	6.2
1	B	476	GLU	6.2
1	B	240	GLN	6.2
1	B	346	ASN	6.1
1	C	389	ILE	6.1
1	D	454	ALA	6.1
1	B	339	THR	6.1
1	D	425	ASN	6.1
1	C	11	GLN	6.1
1	A	491	ILE	6.1
1	C	59	THR	6.1
1	B	336	ASP	6.1
1	C	574	GLN	6.1
1	A	580	PHE	6.0
1	B	106	GLY	6.0
1	B	221	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	459	ALA	6.0
1	D	519	ILE	6.0
1	D	15	ARG	6.0
1	A	447	ARG	6.0
1	D	64	LEU	6.0
1	C	86	SER	6.0
1	D	183	ARG	6.0
1	A	452	GLU	6.0
1	A	60	ASP	6.0
1	A	275	VAL	5.9
1	C	570	GLY	5.9
1	C	117	ASP	5.9
1	B	451	GLU	5.9
1	B	573	ALA	5.9
1	B	534	VAL	5.9
1	A	227	THR	5.9
1	C	101	ARG	5.9
1	A	494	ALA	5.9
1	B	213	GLY	5.9
1	C	108	MET	5.9
1	D	24	LYS	5.9
1	B	101	ARG	5.9
1	C	38	ALA	5.8
1	C	41	ASP	5.8
1	C	88	CYS	5.8
1	C	13	PHE	5.8
1	C	55	GLY	5.8
1	C	406	ASP	5.8
1	B	302	THR	5.8
1	A	476	GLU	5.8
1	D	59	THR	5.7
1	A	64	LEU	5.7
1	C	75	MET	5.7
1	B	86	SER	5.7
1	C	558	GLU	5.7
1	A	581	GLY	5.7
1	A	54	ASP	5.7
1	C	520	GLN	5.7
1	A	493	ARG	5.7
1	A	167	LEU	5.7
1	D	187	LYS	5.7
1	D	27	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	445	TYR	5.7
1	A	408	ARG	5.7
1	B	448	GLU	5.7
1	C	367	PRO	5.6
1	C	275	VAL	5.6
1	C	513	THR	5.6
1	D	237	MET	5.6
1	B	19	THR	5.6
1	A	513	THR	5.6
1	D	160	MET	5.6
1	D	379	GLY	5.6
1	C	214	HIS	5.6
1	A	327	GLU	5.6
1	D	271	SER	5.6
1	A	311	GLY	5.5
1	C	280	THR	5.5
1	D	249	SER	5.5
1	B	408	ARG	5.5
1	B	574	GLN	5.5
1	B	553	ASP	5.5
1	D	508	THR	5.5
1	D	528	LYS	5.5
1	C	410	TYR	5.4
1	A	106	GLY	5.4
1	B	440	ALA	5.4
1	D	520	GLN	5.4
1	B	25	ALA	5.4
1	C	112	PRO	5.4
1	C	249	SER	5.4
1	B	324	SER	5.4
1	A	410	TYR	5.4
1	D	112	PRO	5.4
1	B	391	ARG	5.4
1	B	304	VAL	5.4
1	D	482	SER	5.4
1	C	25	ALA	5.3
1	B	54	ASP	5.3
1	D	431	ASP	5.3
1	A	146	VAL	5.3
1	D	199	THR	5.3
1	D	394	ASP	5.3
1	B	134	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	526	LEU	5.3
1	C	18	PRO	5.3
1	A	521	ALA	5.3
1	B	517	ARG	5.3
1	D	351	TYR	5.3
1	B	136	ALA	5.3
1	C	308	PHE	5.3
1	A	339	THR	5.2
1	D	317	THR	5.2
1	A	555	ILE	5.2
1	C	198	ASN	5.2
1	D	471	ASP	5.2
1	A	131	ASP	5.2
1	C	76	ILE	5.2
1	A	561	THR	5.2
1	B	397	GLU	5.2
1	D	200	MET	5.2
1	B	138	SER	5.2
1	D	290	SER	5.1
1	A	187	LYS	5.1
1	B	345	ARG	5.1
1	B	447	ARG	5.1
1	B	357	PRO	5.1
1	D	116	PHE	5.1
1	C	405	HIS	5.1
1	C	223	GLN	5.1
1	C	360	ARG	5.1
1	C	73	GLY	5.1
1	A	127	ARG	5.1
1	C	254	ILE	5.1
1	C	477	ASN	5.1
1	A	59	THR	5.1
1	B	409	GLU	5.1
1	D	223	GLN	5.1
1	A	425	ASN	5.1
1	B	118	LYS	5.1
1	C	430	ASN	5.1
1	A	21	ALA	5.0
1	D	210	MET	5.0
1	D	54	ASP	5.0
1	A	31	GLY	5.0
1	C	260	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	523	LEU	5.0
1	C	200	MET	5.0
1	D	83	TYR	5.0
1	B	170	ILE	5.0
1	A	427	HIS	5.0
1	A	396	ASP	5.0
1	C	204	THR	5.0
1	A	140	SER	5.0
1	B	181	ALA	4.9
1	B	242	MET	4.9
1	D	281	ALA	4.9
1	D	438	ALA	4.9
1	B	557	VAL	4.9
1	C	540	SER	4.9
1	A	434	ALA	4.9
1	A	173	VAL	4.9
1	B	348	THR	4.9
1	D	191	SER	4.9
1	A	331	GLY	4.8
1	D	141	GLY	4.8
1	B	579	GLN	4.8
1	C	454	ALA	4.8
1	C	169	ILE	4.8
1	D	574	GLN	4.8
1	D	369	GLY	4.8
1	D	518	ALA	4.8
1	C	425	ASN	4.8
1	D	405	HIS	4.8
1	A	465	LYS	4.8
1	A	378	SER	4.8
1	C	576	HIS	4.8
1	D	575	LEU	4.8
1	C	402	MET	4.8
1	A	295	MET	4.8
1	C	246	SER	4.8
1	D	484	GLY	4.7
1	A	22	PRO	4.7
1	C	63	VAL	4.7
1	B	210	MET	4.7
1	D	577	LYS	4.7
1	A	472	THR	4.7
1	D	525	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	180	ILE	4.7
1	A	409	GLU	4.7
1	C	434	ALA	4.7
1	C	378	SER	4.7
1	B	306	ALA	4.7
1	B	351	TYR	4.7
1	A	58	LYS	4.6
1	A	293	ALA	4.6
1	B	67	MET	4.6
1	D	381	GLY	4.6
1	C	282	GLY	4.6
1	A	432	THR	4.6
1	A	445	TYR	4.6
1	B	471	ASP	4.6
1	D	96	VAL	4.6
1	D	184	VAL	4.6
1	B	131	ASP	4.6
1	C	129	THR	4.6
1	A	214	HIS	4.6
1	C	232	LYS	4.6
1	D	450	ILE	4.6
1	C	30	ALA	4.5
1	D	234	SER	4.5
1	C	355	GLU	4.5
1	C	289	SER	4.5
1	D	468	ASN	4.5
1	C	131	ASP	4.5
1	D	329	ASP	4.5
1	B	429	PHE	4.5
1	D	28	ILE	4.5
1	B	406	ASP	4.5
1	A	517	ARG	4.5
1	D	42	THR	4.5
1	D	22	PRO	4.5
1	C	154	ILE	4.5
1	A	549	VAL	4.5
1	A	305	ASN	4.5
1	A	322	LEU	4.5
1	B	180	ILE	4.5
1	C	161	PHE	4.5
1	A	123	THR	4.5
1	D	383	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	387	SER	4.4
1	B	493	ARG	4.4
1	A	105	PHE	4.4
1	C	90	SER	4.4
1	A	212	LYS	4.4
1	A	403	ASP	4.4
1	D	204	THR	4.4
1	D	311	GLY	4.4
1	A	357	PRO	4.4
1	B	68	PRO	4.4
1	A	534	VAL	4.4
1	A	38	ALA	4.4
1	D	106	GLY	4.4
1	B	458	TYR	4.4
1	C	118	LYS	4.3
1	D	389	ILE	4.3
1	B	539	LEU	4.3
1	C	443	GLU	4.3
1	A	61	ARG	4.3
1	D	494	ALA	4.3
1	B	15	ARG	4.3
1	A	516	GLU	4.3
1	B	117	ASP	4.3
1	C	351	TYR	4.3
1	A	79	GLY	4.3
1	B	315	CYS	4.3
1	A	380	SER	4.3
1	C	251	SER	4.3
1	D	408	ARG	4.3
1	C	49	LYS	4.3
1	C	221	GLY	4.3
1	D	457	ALA	4.2
1	B	162	TYR	4.2
1	D	427	HIS	4.2
1	C	143	LEU	4.2
1	B	127	ARG	4.2
1	B	37	ASN	4.2
1	D	378	SER	4.2
1	B	251	SER	4.2
1	D	168	SER	4.2
1	B	467	ASP	4.2
1	A	271	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	40	SER	4.2
1	D	434	ALA	4.2
1	D	403	ASP	4.2
1	B	204	THR	4.2
1	D	260	SER	4.2
1	A	209	GLN	4.2
1	C	17	TRP	4.2
1	D	155	GLY	4.2
1	C	567	ALA	4.2
1	C	465	LYS	4.2
1	D	579	GLN	4.2
1	A	376	GLY	4.1
1	A	500	PRO	4.1
1	A	540	SER	4.1
1	C	568	GLN	4.1
1	C	346	ASN	4.1
1	A	544	GLN	4.1
1	B	352	PRO	4.1
1	D	270	ALA	4.1
1	D	51	LEU	4.1
1	D	88	CYS	4.1
1	C	461	ASP	4.1
1	A	268	TYR	4.1
1	C	330	GLU	4.1
1	B	235	ASN	4.1
1	B	12	THR	4.1
1	C	274	SER	4.1
1	B	381	GLY	4.1
1	A	379	GLY	4.1
1	A	41	ASP	4.1
1	A	336	ASP	4.1
1	B	248	SER	4.1
1	A	389	ILE	4.1
1	B	199	THR	4.1
1	C	382	LYS	4.0
1	B	418	GLN	4.0
1	C	302	THR	4.0
1	D	314	ALA	4.0
1	D	72	ILE	4.0
1	D	475	GLY	4.0
1	D	12	THR	4.0
1	B	326	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	361	ASN	4.0
1	D	320	ALA	4.0
1	B	187	LYS	4.0
1	A	335	ILE	4.0
1	A	438	ALA	3.9
1	A	514	GLU	3.9
1	C	370	LYS	3.9
1	D	353	GLY	3.9
1	C	319	PHE	3.9
1	A	120	SER	3.9
1	A	446	SER	3.9
1	C	384	THR	3.9
1	B	460	MET	3.9
1	D	296	ARG	3.9
1	A	199	THR	3.9
1	A	208	GLU	3.9
1	A	354	ARG	3.9
1	A	505	ASP	3.9
1	A	350	THR	3.9
1	B	524	ASP	3.9
1	A	205	THR	3.9
1	B	208	GLU	3.9
1	C	350	THR	3.9
1	B	518	ALA	3.9
1	C	394	ASP	3.9
1	A	217	VAL	3.9
1	B	217	VAL	3.9
1	C	491	ILE	3.9
1	D	487	GLN	3.9
1	B	172	VAL	3.9
1	C	508	THR	3.9
1	D	30	ALA	3.9
1	D	45	LEU	3.9
1	A	530	ARG	3.9
1	D	220	PHE	3.9
1	D	209	GLN	3.8
1	C	150	GLY	3.8
1	A	111	MET	3.8
1	C	449	GLN	3.8
1	A	394	ASP	3.8
1	A	402	MET	3.8
1	C	469	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	427	HIS	3.8
1	A	328	LYS	3.8
1	B	330	GLU	3.8
1	D	164	SER	3.8
1	A	307	GLN	3.7
1	C	440	ALA	3.7
1	C	476	GLU	3.7
1	B	543	GLU	3.7
1	C	517	ARG	3.7
1	B	254	ILE	3.7
1	B	230	PHE	3.7
1	C	381	GLY	3.7
1	A	485	GLN	3.7
1	A	55	GLY	3.7
1	B	97	VAL	3.7
1	B	186	SER	3.7
1	B	236	LYS	3.7
1	C	147	VAL	3.7
1	A	529	ASN	3.7
1	C	398	GLY	3.7
1	D	70	VAL	3.7
1	A	231	ASP	3.7
1	D	38	ALA	3.7
1	B	108	MET	3.7
1	D	20	ILE	3.7
1	C	252	ASP	3.7
1	D	48	LEU	3.7
1	B	382	LYS	3.7
1	B	450	ILE	3.7
1	C	555	ILE	3.7
1	B	227	THR	3.7
1	C	408	ARG	3.7
1	D	118	LYS	3.7
1	B	256	GLN	3.6
1	A	107	HIS	3.6
1	D	286	VAL	3.6
1	B	380	SER	3.6
1	C	580	PHE	3.6
1	C	311	GLY	3.6
1	D	304	VAL	3.6
1	A	317	THR	3.6
1	A	435	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	144	ILE	3.6
1	B	112	PRO	3.6
1	D	101	ARG	3.6
1	C	407	LEU	3.6
1	D	563	SER	3.6
1	D	147	VAL	3.6
1	A	27	LEU	3.6
1	B	540	SER	3.6
1	C	438	ALA	3.6
1	C	333	ARG	3.6
1	D	122	GLY	3.6
1	D	150	GLY	3.6
1	B	255	ILE	3.5
1	A	571	VAL	3.5
1	C	145	THR	3.5
1	C	304	VAL	3.5
1	B	376	GLY	3.5
1	B	464	ASN	3.5
1	A	382	LYS	3.5
1	A	290	SER	3.5
1	A	304	VAL	3.5
1	D	509	SER	3.5
1	D	400	ILE	3.5
1	C	471	ASP	3.5
1	A	469	GLY	3.5
1	D	333	ARG	3.5
1	C	231	ASP	3.5
1	D	132	SER	3.5
1	C	331	GLY	3.5
1	C	527	GLN	3.5
1	C	380	SER	3.5
1	A	203	VAL	3.5
1	A	519	ILE	3.5
1	B	363	ASN	3.5
1	D	535	ILE	3.5
1	D	561	THR	3.5
1	D	356	VAL	3.5
1	D	480	LEU	3.5
1	A	82	SER	3.5
1	A	126	SER	3.5
1	C	482	SER	3.5
1	B	190	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	158	ILE	3.5
1	A	387	SER	3.4
1	B	99	THR	3.4
1	D	366	ILE	3.4
1	B	572	TYR	3.4
1	D	17	TRP	3.4
1	A	124	LEU	3.4
1	C	321	ILE	3.4
1	A	440	ALA	3.4
1	D	336	ASP	3.4
1	A	318	LEU	3.4
1	D	511	LEU	3.4
1	B	369	GLY	3.4
1	A	19	THR	3.4
1	A	283	THR	3.4
1	C	339	THR	3.4
1	D	331	GLY	3.4
1	A	143	LEU	3.4
1	C	396	ASP	3.4
1	A	113	VAL	3.4
1	A	191	SER	3.4
1	A	306	ALA	3.4
1	D	231	ASP	3.4
1	B	531	THR	3.4
1	D	196	MET	3.4
1	C	130	TYR	3.3
1	C	383	SER	3.3
1	D	252	ASP	3.3
1	A	219	ILE	3.3
1	C	29	VAL	3.3
1	A	579	GLN	3.3
1	A	346	ASN	3.3
1	D	377	ARG	3.3
1	D	313	ALA	3.3
1	D	71	VAL	3.3
1	B	514	GLU	3.3
1	C	487	GLN	3.3
1	C	242	MET	3.3
1	C	317	THR	3.3
1	A	464	ASN	3.3
1	B	222	GLY	3.3
1	C	368	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	511	LEU	3.3
1	C	495	LEU	3.3
1	C	348	THR	3.3
1	A	269	ALA	3.3
1	C	250	ILE	3.3
1	C	353	GLY	3.3
1	C	272	PHE	3.3
1	D	426	VAL	3.3
1	B	513	THR	3.3
1	C	31	GLY	3.3
1	A	155	GLY	3.3
1	D	504	LEU	3.3
1	D	176	PRO	3.3
1	C	456	MET	3.3
1	C	16	LEU	3.3
1	B	563	SER	3.3
1	C	386	ALA	3.3
1	A	449	GLN	3.3
1	A	282	GLY	3.3
1	D	94	GLY	3.3
1	C	523	LEU	3.3
1	D	443	GLU	3.3
1	C	215	LYS	3.3
1	C	176	PRO	3.2
1	A	383	SER	3.2
1	B	298	LEU	3.2
1	D	29	VAL	3.2
1	A	256	GLN	3.2
1	A	426	VAL	3.2
1	B	454	ALA	3.2
1	B	478	GLY	3.2
1	D	74	LEU	3.2
1	A	90	SER	3.2
1	D	478	GLY	3.2
1	D	328	LYS	3.2
1	D	557	VAL	3.2
1	A	467	ASP	3.2
1	A	69	LEU	3.2
1	C	197	GLN	3.2
1	D	467	ASP	3.2
1	A	298	LEU	3.2
1	D	360	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	498	ASP	3.2
1	D	433	VAL	3.2
1	B	159	MET	3.2
1	B	361	ASN	3.2
1	D	257	LEU	3.2
1	A	441	ARG	3.2
1	C	152	SER	3.2
1	C	526	LEU	3.2
1	D	358	ALA	3.2
1	C	445	TYR	3.2
1	A	169	ILE	3.2
1	B	383	SER	3.2
1	D	131	ASP	3.2
1	D	221	GLY	3.2
1	B	166	GLN	3.2
1	A	226	GLU	3.2
1	B	347	VAL	3.2
1	B	576	HIS	3.2
1	B	379	GLY	3.2
1	B	205	THR	3.2
1	B	423	SER	3.2
1	D	224	GLU	3.2
1	C	494	ALA	3.1
1	C	208	GLU	3.1
1	A	276	MET	3.1
1	C	411	THR	3.1
1	C	277	ASP	3.1
1	D	240	GLN	3.1
1	D	416	ARG	3.1
1	D	498	ASP	3.1
1	A	241	GLY	3.1
1	B	194	LYS	3.1
1	D	397	GLU	3.1
1	A	163	TYR	3.1
1	B	53	ASP	3.1
1	C	309	GLN	3.1
1	C	554	GLY	3.1
1	B	289	SER	3.1
1	B	331	GLY	3.1
1	D	236	LYS	3.1
1	D	357	PRO	3.1
1	A	386	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	347	VAL	3.1
1	B	168	SER	3.1
1	B	394	ASP	3.1
1	A	141	GLY	3.1
1	C	403	ASP	3.1
1	B	441	ARG	3.1
1	A	286	VAL	3.1
1	C	107	HIS	3.1
1	D	325	GLU	3.1
1	D	578	MET	3.1
1	B	64	LEU	3.1
1	A	133	GLU	3.1
1	C	219	ILE	3.1
1	A	363	ASN	3.1
1	B	232	LYS	3.1
1	B	234	SER	3.1
1	B	444	GLU	3.1
1	C	230	PHE	3.1
1	C	192	ILE	3.1
1	D	256	GLN	3.1
1	C	116	PHE	3.1
1	B	436	ASN	3.0
1	C	42	THR	3.0
1	C	463	ILE	3.0
1	A	351	TYR	3.0
1	D	491	ILE	3.0
1	D	335	ILE	3.0
1	C	104	LEU	3.0
1	B	411	THR	3.0
1	A	468	ASN	3.0
1	D	26	GLY	3.0
1	D	559	ARG	3.0
1	D	569	HIS	3.0
1	B	559	ARG	3.0
1	A	215	LYS	3.0
1	A	430	ASN	3.0
1	C	490	ALA	3.0
1	D	85	SER	3.0
1	C	475	GLY	3.0
1	C	444	GLU	3.0
1	A	229	ARG	3.0
1	B	211	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	273	PRO	3.0
1	B	270	ALA	3.0
1	C	514	GLU	3.0
1	B	358	ALA	3.0
1	D	308	PHE	3.0
1	A	573	ALA	3.0
1	D	513	THR	3.0
1	C	478	GLY	3.0
1	B	160	MET	3.0
1	B	223	GLN	3.0
1	A	265	PHE	3.0
1	A	14	ARG	3.0
1	A	522	ALA	3.0
1	B	328	LYS	3.0
1	C	226	GLU	3.0
1	D	362	ILE	3.0
1	B	224	GLU	2.9
1	B	565	LEU	2.9
1	C	123	THR	2.9
1	C	377	ARG	2.9
1	D	371	THR	2.9
1	C	326	GLN	2.9
1	D	192	ILE	2.9
1	B	56	PHE	2.9
1	C	344	PHE	2.9
1	A	475	GLY	2.9
1	A	515	SER	2.9
1	B	484	GLY	2.9
1	B	468	ASN	2.9
1	D	538	ARG	2.9
1	D	217	VAL	2.9
1	A	223	GLN	2.9
1	D	123	THR	2.9
1	D	79	GLY	2.9
1	D	297	PRO	2.9
1	C	362	ILE	2.9
1	D	102	ARG	2.9
1	D	197	GLN	2.9
1	B	34	LEU	2.9
1	D	390	THR	2.9
1	D	485	GLN	2.9
1	D	355	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	495	LEU	2.9
1	B	121	THR	2.9
1	B	368	ALA	2.9
1	C	492	ALA	2.9
1	B	27	LEU	2.9
1	B	435	ASN	2.9
1	C	61	ARG	2.9
1	B	105	PHE	2.9
1	A	34	LEU	2.9
1	C	139	SER	2.9
1	A	160	MET	2.9
1	A	324	SER	2.9
1	C	244	MET	2.9
1	D	300	SER	2.9
1	C	180	ILE	2.9
1	C	342	LEU	2.9
1	A	63	VAL	2.8
1	D	115	PHE	2.8
1	D	550	VAL	2.8
1	D	497	ARG	2.8
1	C	276	MET	2.8
1	D	472	THR	2.8
1	D	541	THR	2.8
1	B	178	VAL	2.8
1	C	132	SER	2.8
1	C	564	GLU	2.8
1	A	526	LEU	2.8
1	C	480	LEU	2.8
1	D	86	SER	2.8
1	C	379	GLY	2.8
1	C	503	ILE	2.8
1	D	391	ARG	2.8
1	D	455	ARG	2.8
1	D	347	VAL	2.8
1	B	477	ASN	2.8
1	C	58	LYS	2.8
1	D	189	PHE	2.8
1	A	359	LEU	2.8
1	C	431	ASP	2.8
1	D	225	VAL	2.8
1	C	295	MET	2.8
1	C	300	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	366	ILE	2.8
1	B	293	ALA	2.8
1	B	147	VAL	2.8
1	C	71	VAL	2.8
1	C	565	LEU	2.8
1	A	262	ALA	2.8
1	B	219	ILE	2.8
1	A	116	PHE	2.8
1	D	219	ILE	2.8
1	B	104	LEU	2.8
1	B	386	ALA	2.8
1	C	248	SER	2.7
1	D	211	LEU	2.7
1	D	421	LEU	2.7
1	C	373	ALA	2.7
1	C	158	ILE	2.7
1	B	359	LEU	2.7
1	C	376	GLY	2.7
1	D	435	ASN	2.7
1	C	363	ASN	2.7
1	D	235	ASN	2.7
1	C	211	LEU	2.7
1	D	175	ALA	2.7
1	D	396	ASP	2.7
1	B	480	LEU	2.7
1	C	466	MET	2.7
1	B	62	SER	2.7
1	B	73	GLY	2.7
1	B	424	GLN	2.7
1	C	22	PRO	2.7
1	D	326	GLN	2.7
1	A	12	THR	2.7
1	C	216	GLU	2.7
1	D	262	ALA	2.7
1	B	102	ARG	2.7
1	D	441	ARG	2.7
1	C	413	ALA	2.7
1	D	521	ALA	2.7
1	B	333	ARG	2.7
1	B	107	HIS	2.7
1	C	235	ASN	2.7
1	B	488	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	418	GLN	2.7
1	B	295	MET	2.7
1	A	360	ARG	2.7
1	B	150	GLY	2.7
1	A	62	SER	2.7
1	B	377	ARG	2.7
1	A	184	VAL	2.7
1	D	245	VAL	2.7
1	D	127	ARG	2.6
1	C	203	VAL	2.6
1	D	469	GLY	2.6
1	B	482	SER	2.6
1	B	556	ILE	2.6
1	B	473	ILE	2.6
1	C	53	ASP	2.6
1	C	113	VAL	2.6
1	D	53	ASP	2.6
1	D	283	THR	2.6
1	C	111	MET	2.6
1	B	212	LYS	2.6
1	D	279	LEU	2.6
1	C	210	MET	2.6
1	A	24	LYS	2.6
1	B	237	MET	2.6
1	C	68	PRO	2.6
1	D	90	SER	2.6
1	C	187	LYS	2.6
1	A	172	VAL	2.6
1	D	418	GLN	2.6
1	D	169	ILE	2.6
1	A	267	LEU	2.6
1	B	549	VAL	2.6
1	D	496	LEU	2.6
1	A	553	ASP	2.6
1	D	282	GLY	2.6
1	D	229	ARG	2.6
1	D	18	PRO	2.6
1	D	63	VAL	2.6
1	A	523	LEU	2.6
1	D	87	TYR	2.6
1	C	544	GLN	2.6
1	B	269	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	438	ALA	2.6
1	B	10	TRP	2.6
1	A	332	LYS	2.6
1	D	52	LEU	2.6
1	C	507	ALA	2.6
1	D	341	ASP	2.6
1	D	440	ALA	2.6
1	D	546	ASP	2.6
1	B	66	TRP	2.5
1	C	366	ILE	2.5
1	D	212	LYS	2.5
1	A	168	SER	2.5
1	B	525	GLU	2.5
1	A	73	GLY	2.5
1	B	307	GLN	2.5
1	B	272	PHE	2.5
1	C	189	PHE	2.5
1	A	482	SER	2.5
1	B	323	ASP	2.5
1	D	39	ALA	2.5
1	B	79	GLY	2.5
1	B	314	ALA	2.5
1	A	132	SER	2.5
1	B	133	GLU	2.5
1	B	276	MET	2.5
1	B	31	GLY	2.5
1	C	423	SER	2.5
1	B	13	PHE	2.5
1	B	568	GLN	2.5
1	D	195	ASN	2.5
1	A	558	GLU	2.5
1	A	508	THR	2.5
1	B	398	GLY	2.5
1	A	454	ALA	2.5
1	D	411	THR	2.5
1	B	228	LYS	2.5
1	A	195	ASN	2.5
1	D	572	TYR	2.5
1	C	559	ARG	2.5
1	C	40	SER	2.5
1	C	269	ALA	2.5
1	D	339	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	201	GLY	2.5
1	A	384	THR	2.5
1	B	338	ALA	2.5
1	C	286	VAL	2.5
1	A	451	GLU	2.5
1	C	349	PHE	2.5
1	A	88	CYS	2.5
1	A	377	ARG	2.5
1	A	423	SER	2.5
1	D	483	GLY	2.5
1	B	385	ILE	2.4
1	A	381	GLY	2.4
1	D	531	THR	2.4
1	A	278	SER	2.4
1	B	141	GLY	2.4
1	D	110	GLY	2.4
1	D	534	VAL	2.4
1	D	75	MET	2.4
1	D	143	LEU	2.4
1	B	461	ASP	2.4
1	B	537	HIS	2.4
1	C	26	GLY	2.4
1	C	165	TRP	2.4
1	C	262	ALA	2.4
1	B	496	LEU	2.4
1	B	486	ARG	2.4
1	C	484	GLY	2.4
1	D	69	LEU	2.4
1	A	528	LYS	2.4
1	B	156	LEU	2.4
1	B	173	VAL	2.4
1	D	108	MET	2.4
1	B	90	SER	2.4
1	A	194	LYS	2.4
1	C	299	LYS	2.4
1	D	527	GLN	2.4
1	D	82	SER	2.4
1	C	437	ILE	2.4
1	C	110	GLY	2.4
1	D	414	SER	2.4
1	A	83	TYR	2.4
1	D	500	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	543	GLU	2.4
1	B	378	SER	2.4
1	B	515	SER	2.4
1	C	162	TYR	2.4
1	B	175	ALA	2.4
1	A	15	ARG	2.4
1	B	46	SER	2.4
1	A	72	ILE	2.4
1	A	37	ASN	2.4
1	B	83	TYR	2.4
1	B	512	ASP	2.4
1	C	105	PHE	2.4
1	D	345	ARG	2.4
1	A	118	LYS	2.4
1	A	568	GLN	2.4
1	A	314	ALA	2.4
1	B	33	ALA	2.4
1	C	264	ALA	2.4
1	D	174	LEU	2.4
1	A	473	ILE	2.4
1	B	561	THR	2.4
1	C	391	ARG	2.4
1	A	323	ASP	2.4
1	B	334	VAL	2.3
1	D	255	ILE	2.3
1	C	10	TRP	2.3
1	D	205	THR	2.3
1	C	385	ILE	2.3
1	C	64	LEU	2.3
1	B	489	ILE	2.3
1	C	358	ALA	2.3
1	A	135	VAL	2.3
1	C	447	ARG	2.3
1	C	483	GLY	2.3
1	C	581	GLY	2.3
1	D	165	TRP	2.3
1	D	554	GLY	2.3
1	D	386	ALA	2.3
1	A	176	PRO	2.3
1	B	384	THR	2.3
1	D	46	SER	2.3
1	D	78	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	137	SER	2.3
1	D	166	GLN	2.3
1	D	503	ILE	2.3
1	B	179	SER	2.3
1	B	426	VAL	2.3
1	B	87	TYR	2.3
1	D	135	VAL	2.3
1	C	538	ARG	2.3
1	B	207	ALA	2.3
1	A	110	GLY	2.3
1	C	201	GLY	2.3
1	D	226	GLU	2.3
1	A	254	ILE	2.3
1	D	103	ARG	2.3
1	C	418	GLN	2.3
1	B	280	THR	2.3
1	A	429	PHE	2.3
1	B	459	ALA	2.3
1	C	134	GLN	2.3
1	C	563	SER	2.3
1	C	228	LYS	2.3
1	A	365	LYS	2.3
1	D	156	LEU	2.3
1	D	126	SER	2.3
1	B	14	ARG	2.3
1	C	485	GLN	2.2
1	A	489	ILE	2.2
1	C	247	ALA	2.2
1	C	519	ILE	2.2
1	D	277	ASP	2.2
1	B	40	SER	2.2
1	A	224	GLU	2.2
1	B	470	LEU	2.2
1	A	17	TRP	2.2
1	C	79	GLY	2.2
1	B	132	SER	2.2
1	A	308	PHE	2.2
1	B	114	ALA	2.2
1	A	527	GLN	2.2
1	A	67	MET	2.2
1	A	577	LYS	2.2
1	D	316	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	21	ALA	2.2
1	D	133	GLU	2.2
1	B	367	PRO	2.2
1	C	354	ARG	2.2
1	C	528	LYS	2.2
1	B	570	GLY	2.2
1	B	58	LYS	2.2
1	B	245	VAL	2.2
1	D	459	ALA	2.2
1	D	268	TYR	2.2
1	A	148	ARG	2.2
1	A	361	ASN	2.2
1	D	350	THR	2.2
1	B	137	SER	2.2
1	A	334	VAL	2.2
1	C	97	VAL	2.2
1	D	50	PRO	2.2
1	C	397	GLU	2.2
1	A	198	ASN	2.2
1	B	239	LEU	2.2
1	B	492	ALA	2.2
1	A	291	MET	2.2
1	B	362	ILE	2.2
1	C	28	ILE	2.2
1	D	573	ALA	2.2
1	A	496	LEU	2.2
1	A	338	ALA	2.1
1	B	122	GLY	2.1
1	D	330	GLU	2.1
1	D	517	ARG	2.1
1	A	390	THR	2.1
1	D	429	PHE	2.1
1	A	97	VAL	2.1
1	D	228	LYS	2.1
1	C	479	VAL	2.1
1	C	12	THR	2.1
1	C	467	ASP	2.1
1	D	439	TYR	2.1
1	A	292	ILE	2.1
1	B	322	LEU	2.1
1	B	396	ASP	2.1
1	C	557	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	255	ILE	2.1
1	D	458	TYR	2.1
1	C	94	GLY	2.1
1	A	139	SER	2.1
1	B	249	SER	2.1
1	C	191	SER	2.1
1	B	215	LYS	2.1
1	D	368	ALA	2.1
1	D	422	VAL	2.1
1	D	73	GLY	2.1
1	A	109	MET	2.1
1	B	82	SER	2.1
1	B	430	ASN	2.1
1	D	198	ASN	2.1
1	D	382	LYS	2.1
1	D	384	THR	2.1
1	A	277	ASP	2.1
1	C	294	LEU	2.1
1	D	464	ASN	2.1
1	C	388	LEU	2.1
1	B	431	ASP	2.1
1	B	300	SER	2.1
1	A	352	PRO	2.1
1	A	233	VAL	2.1
1	B	195	ASN	2.1
1	A	65	LEU	2.0
1	C	245	VAL	2.0
1	B	88	CYS	2.0
1	D	448	GLU	2.0
1	C	127	ARG	2.0
1	D	179	SER	2.0
1	B	318	LEU	2.0
1	C	497	ARG	2.0
1	C	515	SER	2.0
1	D	35	ILE	2.0
1	B	21	ALA	2.0
1	B	457	ALA	2.0
1	D	293	ALA	2.0
1	A	499	SER	2.0
1	A	371	THR	2.0
1	B	485	GLN	2.0
1	D	364	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	276	MET	2.0
1	B	47	LEU	2.0
1	A	542	ILE	2.0
1	B	390	THR	2.0
1	C	329	ASP	2.0
1	D	261	LEU	2.0
1	D	499	SER	2.0
1	A	478	GLY	2.0
1	D	173	VAL	2.0
1	C	395	ILE	2.0
1	B	80	ILE	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(Å ²)	Q<0.9
2	ADP	B	601	26/27	0.63	0.83	0.38	156,156,156,156	0
2	ADP	A	5001	26/27	0.64	0.82	-0.50	156,156,156,156	0
2	ADP	C	601	26/27	0.74	0.81	-0.68	156,156,156,156	0
2	ADP	D	601	26/27	0.69	0.80	-0.88	156,156,156,156	0
3	VO4	A	5002	2/5	0.84	0.75	-	156,156,156,156	0
3	VO4	D	602	2/5	0.66	0.74	-	156,156,156,156	0
3	VO4	C	602	2/5	0.81	0.72	-	156,156,156,156	0
3	VO4	B	602	2/5	0.74	0.86	-	156,156,156,156	0

6.5 Other polymers

There are no such residues in this entry.