



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:35 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

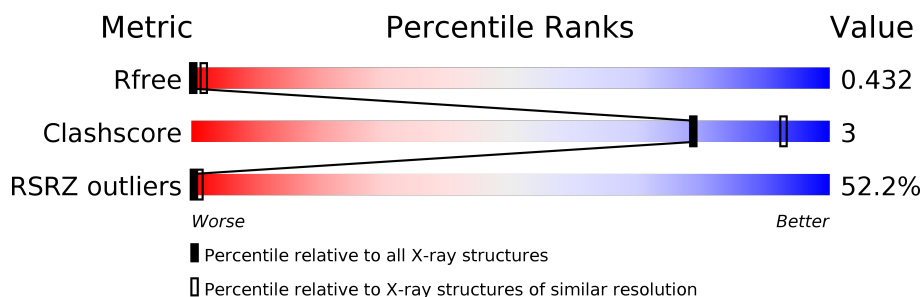
1 Overall quality at a glance

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}	100719	1177 (4.80-3.60)
Clashscore	112137	1025 (4.72-3.66)
RSRZ outliers	101464	1188 (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	
1	B	582	
1	C	582	
1	D	582	

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](#)

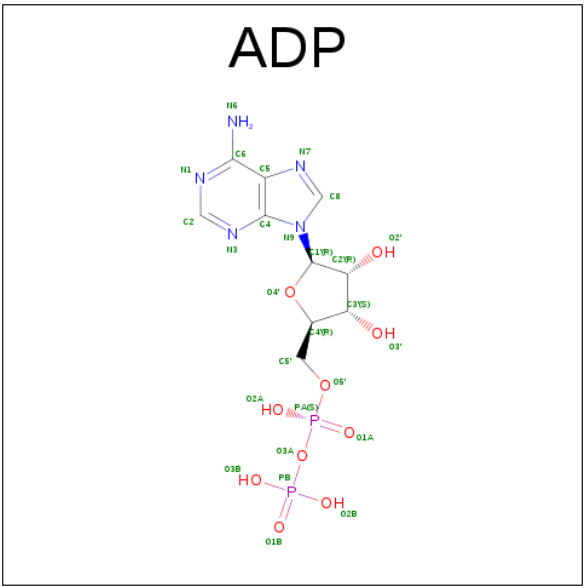
There are 3 unique types of molecules in this entry. The entry contains 2400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₁₀H₁₅N₅O₁₀P₂).



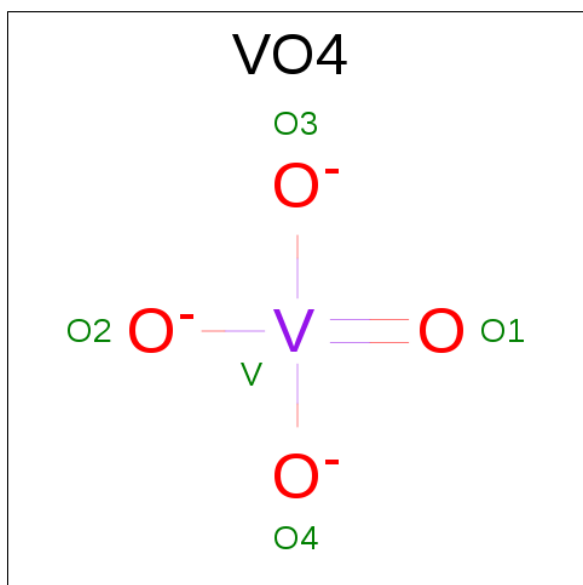
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
2	B	1	Total	C	N	O	P	0	0
			26	10	5	9	2		

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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).

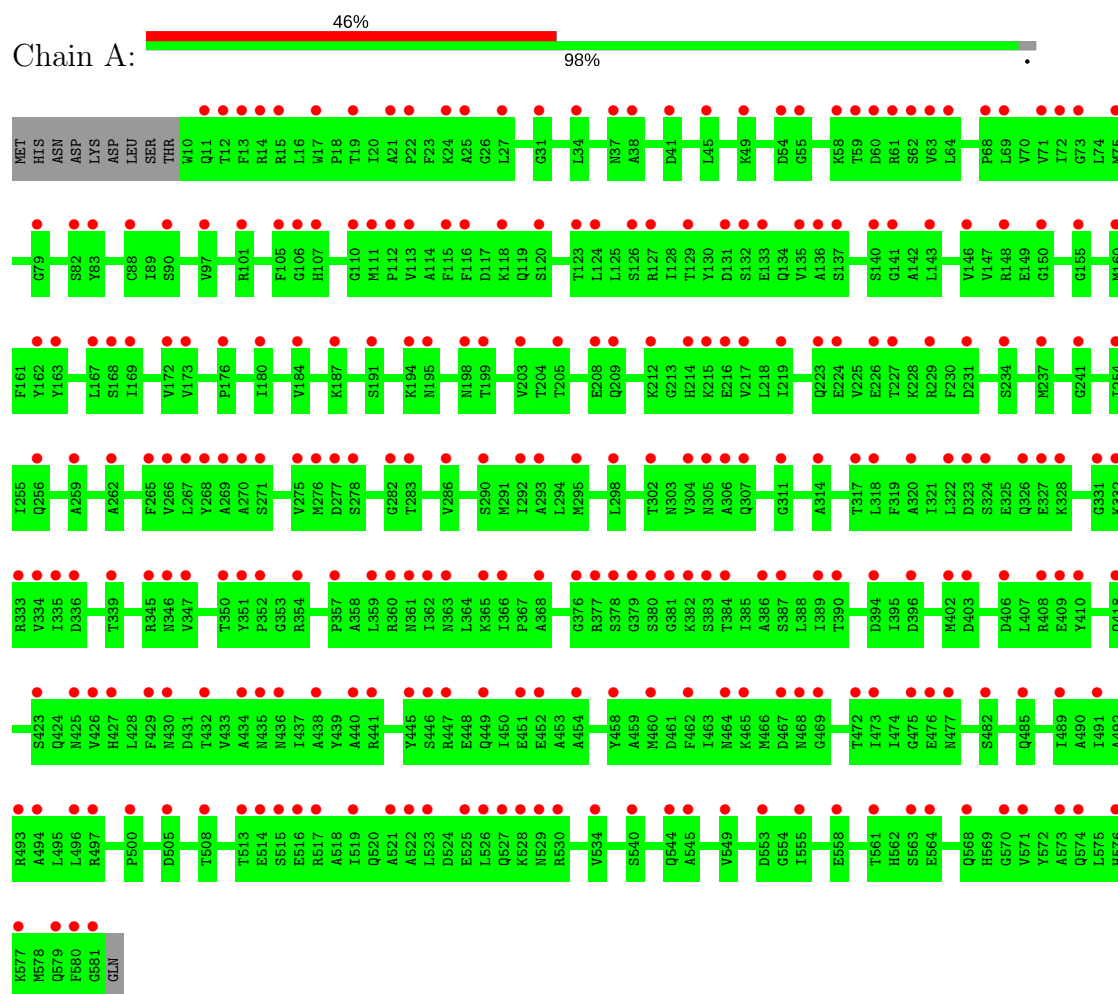


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			2	1	1		
3	B	1	Total	O	V	0	0
			2	1	1		
3	C	1	Total	O	V	0	0
			2	1	1		
3	D	1	Total	O	V	0	0
			2	1	1		

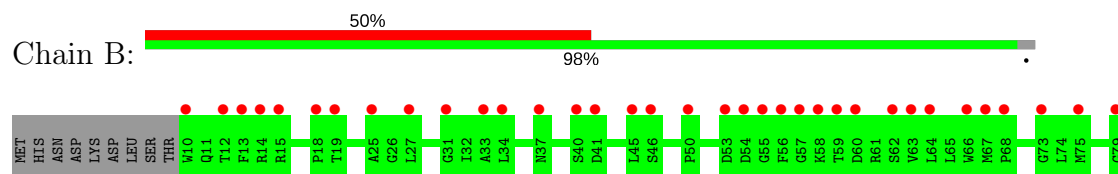
3 Residue-property plots

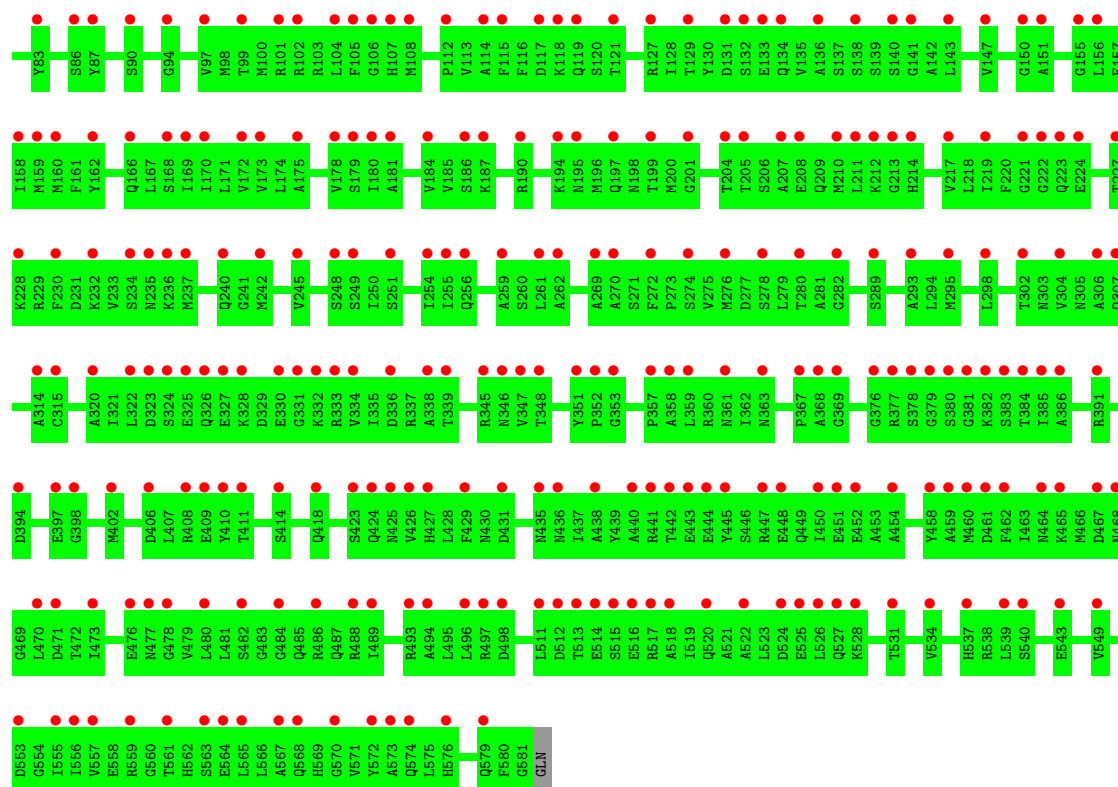
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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

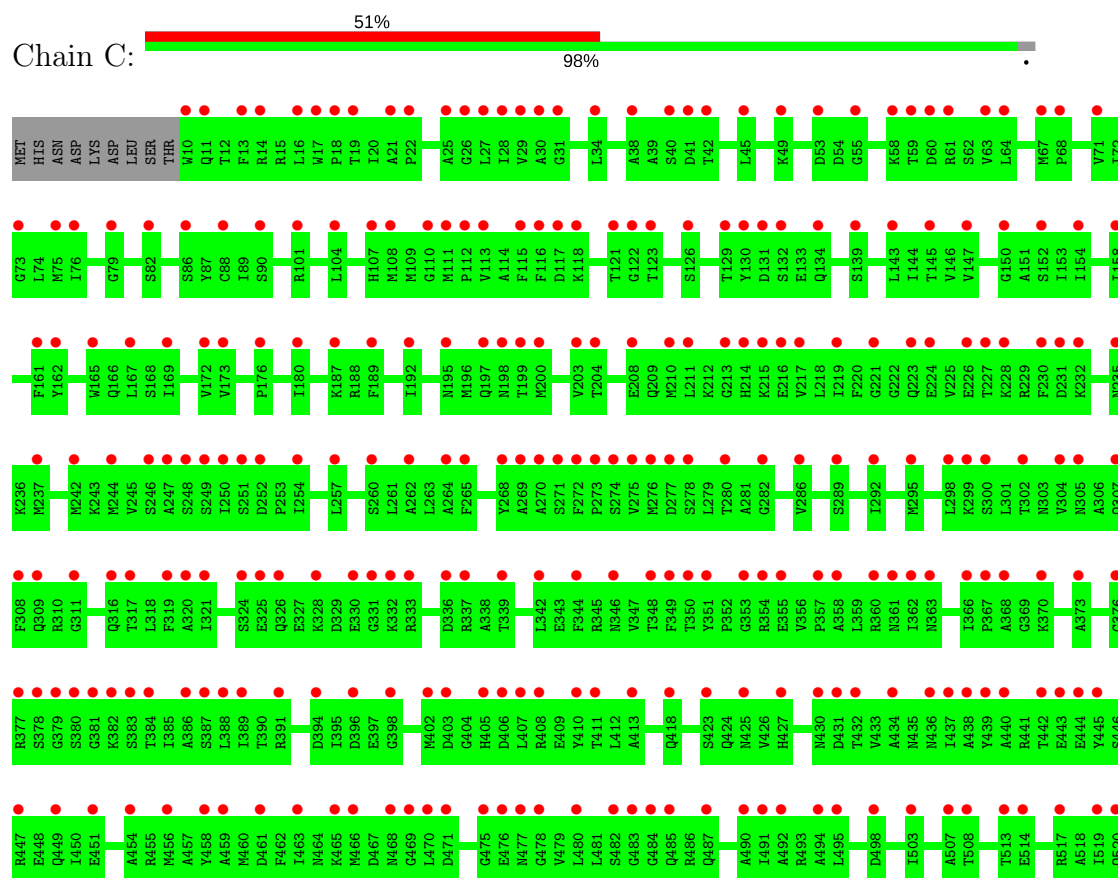


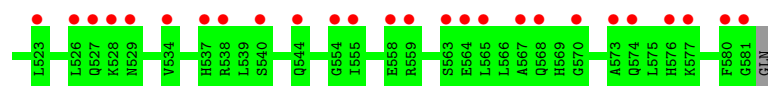
- Molecule 1: Lipid A export ATP-binding/permease protein msbA



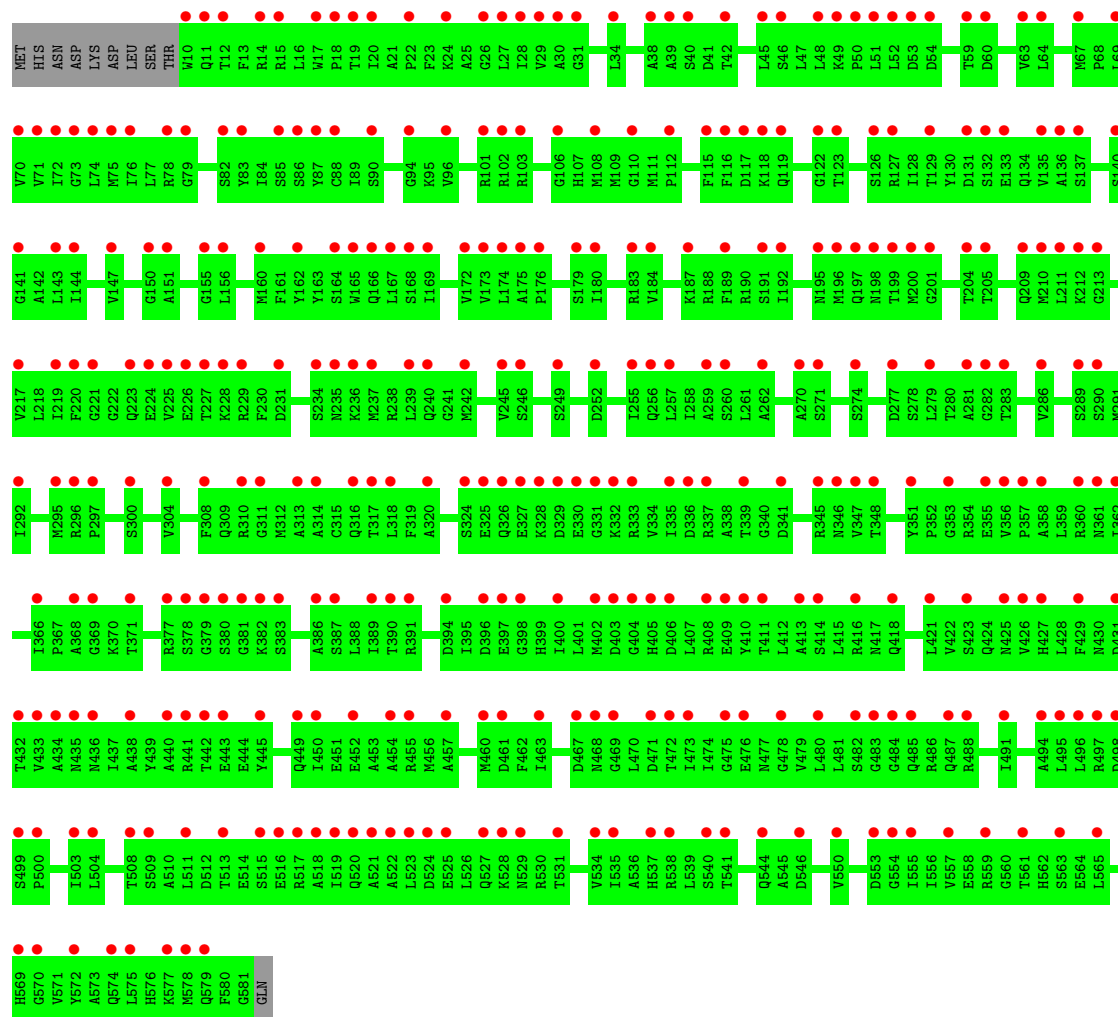


- Molecule 1: Lipid A export ATP-binding/permease protein msbA





- 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)	1.71 , 314.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	22,28,29	1.41	3 (13%)	21,42,45	2.33	2 (9%)
3	VO4	A	5002	2	0,1,4	0.00	-	0,0,6	0.00	-
2	ADP	B	601	3	22,28,29	1.12	2 (9%)	21,42,45	2.09	2 (9%)
3	VO4	B	602	2	0,1,4	0.00	-	0,0,6	0.00	-
2	ADP	C	601	3	22,28,29	1.32	2 (9%)	21,42,45	2.16	2 (9%)
3	VO4	C	602	2	0,1,4	0.00	-	0,0,6	0.00	-
2	ADP	D	601	3	22,28,29	1.42	3 (13%)	21,42,45	2.20	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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ADP	C8-N7	-2.90	1.29	1.34
2	D	601	ADP	C8-N7	-2.75	1.29	1.34
2	A	5001	ADP	C8-N7	-2.62	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C8-N7	-2.09	1.30	1.34
2	D	601	ADP	PA-O3A	2.67	1.64	1.59
2	B	601	ADP	O4'-C1'	3.24	1.45	1.41
2	A	5001	ADP	PA-O3A	3.50	1.66	1.59
2	A	5001	ADP	O4'-C1'	3.82	1.46	1.41
2	C	601	ADP	O4'-C1'	4.12	1.47	1.41
2	D	601	ADP	O4'-C1'	4.27	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	ADP	N3-C2-N1	-8.92	121.09	128.86
2	D	601	ADP	N3-C2-N1	-8.64	121.33	128.86
2	C	601	ADP	N3-C2-N1	-8.50	121.45	128.86
2	B	601	ADP	N3-C2-N1	-8.29	121.64	128.86
2	D	601	ADP	C4-C5-N7	-2.05	107.43	109.41
2	B	601	ADP	O3A-PA-O5'	2.75	110.88	103.07
2	C	601	ADP	O3A-PA-O5'	3.00	111.58	103.07
2	D	601	ADP	O3A-PA-O5'	3.21	112.19	103.07
2	A	5001	ADP	O3A-PA-O5'	3.78	113.80	103.07

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%)	2.44	270 (47%) 0 1	116, 152, 169, 183	0
1	B	572/582 (98%)	2.64	290 (50%) 0 1	125, 155, 170, 184	0
1	C	572/582 (98%)	2.71	298 (52%) 0 1	114, 153, 171, 184	0
1	D	572/582 (98%)	2.91	336 (58%) 0 1	124, 156, 171, 188	0
All	All	2288/2328 (98%)	2.68	1194 (52%) 0 1	114, 154, 170, 188	0

All (1194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	60	ASP	15.4
1	B	18	PRO	14.4
1	B	325	GLU	14.3
1	D	529	ASN	13.9
1	C	336	ASP	13.6
1	A	49	LYS	12.4
1	B	115	PHE	12.4
1	A	75	MET	12.4
1	A	129	THR	12.0
1	D	524	ASP	12.0
1	B	60	ASP	12.0
1	C	432	THR	12.0
1	C	573	ALA	11.7
1	C	468	ASN	11.5
1	A	71	VAL	11.2
1	B	129	THR	11.2
1	D	10	TRP	11.1
1	D	151	ALA	10.9
1	B	50	PRO	10.8
1	C	470	LEU	10.6
1	B	119	GLN	10.5

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Mol	Chain	Res	Type	RSRZ
1	B	45	LEU	10.4
1	B	94	GLY	10.3
1	A	11	GLN	10.2
1	B	140	SER	10.2
1	D	60	ASP	10.2
1	A	45	LEU	10.1
1	C	278	SER	10.1
1	A	234	SER	10.1
1	D	409	GLU	10.0
1	D	570	GLY	10.0
1	B	527	GLN	10.0
1	C	451	GLU	9.8
1	D	442	THR	9.8
1	C	271	SER	9.7
1	D	402	MET	9.7
1	C	67	MET	9.7
1	D	327	GLU	9.7
1	A	462	PHE	9.5
1	B	320	ALA	9.5
1	A	563	SER	9.4
1	B	274	SER	9.3
1	C	237	MET	9.3
1	D	310	ARG	9.3
1	C	19	THR	9.2
1	B	522	ALA	9.2
1	D	136	ALA	9.1
1	D	324	SER	9.0
1	B	59	THR	9.0
1	D	292	ILE	9.0
1	D	129	THR	9.0
1	C	122	GLY	9.0
1	B	465	LYS	9.0
1	C	126	SER	9.0
1	D	14	ARG	9.0
1	C	332	LYS	8.8
1	C	320	ALA	8.8
1	C	217	VAL	8.8
1	B	445	TYR	8.8
1	D	522	ALA	8.8
1	C	324	SER	8.7
1	A	574	GLN	8.7
1	B	151	ALA	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	576	HIS	8.7
1	C	167	LEU	8.6
1	B	259	ALA	8.6
1	C	305	ASN	8.6
1	C	427	HIS	8.6
1	B	55	GLY	8.6
1	C	439	TYR	8.5
1	A	564	GLU	8.4
1	D	119	GLN	8.4
1	D	49	LYS	8.4
1	A	68	PRO	8.3
1	A	137	SER	8.3
1	D	452	GLU	8.2
1	A	458	TYR	8.2
1	D	423	SER	8.2
1	B	282	GLY	8.1
1	D	227	THR	8.1
1	D	406	ASP	8.1
1	D	348	THR	8.1
1	B	197	GLN	8.1
1	D	544	GLN	8.0
1	D	246	SER	8.0
1	B	520	GLN	8.0
1	D	398	GLY	8.0
1	D	553	ASP	8.0
1	B	516	GLU	8.0
1	C	328	LYS	7.9
1	A	436	ASN	7.9
1	C	298	LEU	7.9
1	A	112	PRO	7.9
1	B	425	ASN	7.9
1	D	34	LEU	7.9
1	D	289	SER	7.8
1	C	361	ASN	7.8
1	A	406	ASP	7.8
1	D	463	ILE	7.8
1	D	516	GLU	7.7
1	A	302	THR	7.7
1	B	278	SER	7.7
1	D	332	LYS	7.7
1	A	525	GLU	7.7
1	D	172	VAL	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	136	ALA	7.7
1	D	11	GLN	7.6
1	D	449	GLN	7.6
1	B	555	ILE	7.6
1	D	555	ILE	7.6
1	C	27	LEU	7.5
1	A	237	MET	7.5
1	A	477	ASN	7.5
1	B	494	ALA	7.5
1	B	184	VAL	7.5
1	C	442	THR	7.5
1	C	227	THR	7.5
1	D	515	SER	7.4
1	A	333	ARG	7.4
1	B	327	GLU	7.4
1	B	567	ALA	7.4
1	D	537	HIS	7.4
1	C	534	VAL	7.3
1	C	436	ASN	7.3
1	B	402	MET	7.3
1	D	488	ARG	7.3
1	B	155	GLY	7.2
1	D	476	GLU	7.2
1	C	213	GLY	7.1
1	A	497	ARG	7.1
1	B	41	ASP	7.1
1	A	545	ALA	7.1
1	D	413	ALA	7.1
1	B	498	ASP	7.1
1	D	461	ASP	7.1
1	A	570	GLY	7.0
1	B	443	GLU	7.0
1	C	387	SER	7.0
1	A	115	PHE	7.0
1	D	432	THR	7.0
1	B	63	VAL	7.0
1	C	14	ARG	7.0
1	C	337	ARG	7.0
1	C	82	SER	7.0
1	D	436	ASN	7.0
1	A	460	MET	7.0
1	D	242	MET	7.0

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Mol	Chain	Res	Type	RSRZ
1	C	257	LEU	6.9
1	B	452	GLU	6.9
1	B	414	SER	6.9
1	C	199	THR	6.8
1	A	266	VAL	6.8
1	D	410	TYR	6.8
1	B	143	LEU	6.8
1	B	214	HIS	6.7
1	D	540	SER	6.7
1	D	318	LEU	6.7
1	D	180	ILE	6.7
1	C	268	TYR	6.7
1	C	537	HIS	6.7
1	C	45	LEU	6.7
1	D	64	LEU	6.7
1	B	353	GLY	6.6
1	C	574	GLN	6.6
1	C	307	GLN	6.6
1	C	577	LYS	6.6
1	D	346	ASN	6.6
1	D	274	SER	6.6
1	D	473	ILE	6.6
1	D	259	ALA	6.6
1	C	115	PHE	6.5
1	D	140	SER	6.5
1	C	173	VAL	6.5
1	B	410	TYR	6.5
1	B	442	THR	6.5
1	C	13	PHE	6.5
1	A	101	ARG	6.5
1	C	195	ASN	6.5
1	B	497	ARG	6.4
1	B	57	GLY	6.4
1	D	337	ARG	6.4
1	D	380	SER	6.4
1	A	259	ALA	6.4
1	D	19	THR	6.4
1	A	368	ALA	6.4
1	D	404	GLY	6.4
1	A	25	ALA	6.4
1	C	458	TYR	6.4
1	A	270	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	150	GLY	6.3
1	C	292	ILE	6.3
1	C	357	PRO	6.2
1	C	529	ASN	6.2
1	D	15	ARG	6.2
1	B	106	GLY	6.2
1	B	346	ASN	6.2
1	C	121	THR	6.2
1	A	320	ALA	6.2
1	B	448	GLU	6.2
1	B	240	GLN	6.2
1	B	462	PHE	6.1
1	B	201	GLY	6.1
1	B	564	GLU	6.1
1	A	326	GLN	6.1
1	A	362	ILE	6.1
1	D	24	LYS	6.1
1	B	169	ILE	6.1
1	C	367	PRO	6.0
1	D	213	GLY	6.0
1	C	172	VAL	6.0
1	C	34	LEU	6.0
1	A	345	ARG	6.0
1	C	11	GLN	6.0
1	D	565	LEU	6.0
1	B	332	LYS	6.0
1	C	88	CYS	6.0
1	B	391	ARG	6.0
1	C	108	MET	6.0
1	D	162	TYR	6.0
1	C	224	GLU	5.9
1	B	534	VAL	5.9
1	A	13	PHE	5.9
1	A	162	TYR	5.9
1	C	117	ASP	5.9
1	A	227	THR	5.9
1	D	460	MET	5.9
1	B	573	ALA	5.8
1	A	447	ARG	5.8
1	C	316	GLN	5.8
1	C	389	ILE	5.8
1	D	239	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	339	THR	5.8
1	A	580	PHE	5.8
1	B	324	SER	5.8
1	C	75	MET	5.8
1	C	270	ALA	5.7
1	D	183	ARG	5.7
1	A	408	ARG	5.7
1	A	581	GLY	5.7
1	C	275	VAL	5.7
1	D	454	ALA	5.7
1	D	508	THR	5.7
1	B	101	ARG	5.7
1	B	517	ARG	5.7
1	B	262	ALA	5.7
1	C	520	GLN	5.7
1	D	67	MET	5.7
1	A	327	GLU	5.7
1	B	302	THR	5.7
1	C	86	SER	5.6
1	A	60	ASP	5.6
1	A	275	VAL	5.6
1	B	75	MET	5.6
1	A	54	ASP	5.6
1	B	451	GLU	5.6
1	D	528	LYS	5.6
1	D	249	SER	5.6
1	D	425	ASN	5.6
1	B	476	GLU	5.6
1	C	513	THR	5.5
1	A	491	ILE	5.5
1	C	41	ASP	5.5
1	D	519	ILE	5.5
1	D	187	LYS	5.5
1	B	134	GLN	5.5
1	C	459	ALA	5.5
1	D	59	THR	5.5
1	B	213	GLY	5.5
1	D	271	SER	5.4
1	B	397	GLU	5.4
1	B	574	GLN	5.4
1	B	357	PRO	5.4
1	C	59	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	379	GLY	5.4
1	C	570	GLY	5.4
1	A	106	GLY	5.4
1	B	336	ASP	5.4
1	C	558	GLU	5.4
1	A	64	LEU	5.4
1	B	408	ARG	5.4
1	A	493	ARG	5.4
1	B	86	SER	5.4
1	D	431	ASP	5.3
1	A	131	ASP	5.3
1	B	54	ASP	5.3
1	A	494	ALA	5.3
1	A	127	ARG	5.3
1	A	452	GLU	5.3
1	B	261	LEU	5.3
1	C	55	GLY	5.3
1	A	167	LEU	5.3
1	C	280	THR	5.3
1	B	118	LYS	5.3
1	C	406	ASP	5.3
1	B	553	ASP	5.3
1	C	214	HIS	5.2
1	C	76	ILE	5.2
1	C	223	GLN	5.2
1	C	112	PRO	5.2
1	D	160	MET	5.2
1	D	482	SER	5.2
1	C	18	PRO	5.2
1	D	27	LEU	5.2
1	A	555	ILE	5.2
1	B	409	GLU	5.2
1	C	308	PHE	5.2
1	A	476	GLU	5.2
1	A	187	LYS	5.2
1	A	465	LYS	5.2
1	D	237	MET	5.2
1	C	101	ARG	5.1
1	C	38	ALA	5.1
1	B	304	VAL	5.1
1	C	477	ASN	5.1
1	D	116	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	440	ALA	5.0
1	D	112	PRO	5.0
1	D	445	TYR	5.0
1	B	221	GLY	5.0
1	D	450	ILE	5.0
1	C	73	GLY	5.0
1	D	200	MET	5.0
1	D	351	TYR	5.0
1	D	369	GLY	5.0
1	D	575	LEU	5.0
1	D	290	SER	4.9
1	A	472	THR	4.9
1	C	25	ALA	4.9
1	B	25	ALA	4.9
1	C	249	SER	4.9
1	C	260	SER	4.9
1	D	525	GLU	4.9
1	B	136	ALA	4.9
1	A	146	VAL	4.9
1	C	410	TYR	4.9
1	A	339	THR	4.9
1	B	170	ILE	4.9
1	A	521	ALA	4.9
1	D	520	GLN	4.9
1	A	410	TYR	4.9
1	B	526	LEU	4.9
1	C	454	ALA	4.9
1	A	21	ALA	4.9
1	A	311	GLY	4.9
1	B	138	SER	4.8
1	C	405	HIS	4.8
1	C	254	ILE	4.8
1	C	246	SER	4.8
1	A	513	THR	4.8
1	D	191	SER	4.8
1	B	19	THR	4.8
1	A	425	ASN	4.8
1	C	430	ASN	4.8
1	B	557	VAL	4.8
1	D	574	GLN	4.8
1	D	223	GLN	4.8
1	B	579	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	141	GLY	4.8
1	B	348	THR	4.8
1	A	295	MET	4.8
1	D	54	ASP	4.7
1	D	22	PRO	4.7
1	D	199	THR	4.7
1	A	331	GLY	4.7
1	B	131	ASP	4.7
1	B	447	ARG	4.7
1	C	355	GLU	4.7
1	B	345	ARG	4.7
1	A	173	VAL	4.7
1	D	317	THR	4.7
1	D	184	VAL	4.7
1	C	360	ARG	4.7
1	D	210	MET	4.6
1	C	204	THR	4.6
1	A	293	ALA	4.6
1	A	22	PRO	4.6
1	A	409	GLU	4.6
1	C	425	ASN	4.6
1	D	83	TYR	4.6
1	D	523	LEU	4.6
1	C	402	MET	4.6
1	A	432	THR	4.6
1	C	198	ASN	4.6
1	D	468	ASN	4.6
1	A	434	ALA	4.6
1	D	394	ASP	4.6
1	B	429	PHE	4.6
1	B	181	ALA	4.5
1	A	427	HIS	4.5
1	D	408	ARG	4.5
1	A	378	SER	4.5
1	A	123	THR	4.5
1	D	281	ALA	4.5
1	D	577	LYS	4.5
1	A	59	THR	4.5
1	A	140	SER	4.5
1	D	405	HIS	4.5
1	A	31	GLY	4.5
1	C	378	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	471	ASP	4.5
1	C	154	ILE	4.5
1	C	200	MET	4.5
1	D	387	SER	4.5
1	A	561	THR	4.5
1	D	438	ALA	4.5
1	C	540	SER	4.4
1	D	28	ILE	4.4
1	B	180	ILE	4.4
1	A	403	ASP	4.4
1	C	63	VAL	4.4
1	B	242	MET	4.4
1	C	49	LYS	4.4
1	D	484	GLY	4.4
1	C	282	GLY	4.4
1	D	234	SER	4.4
1	B	210	MET	4.4
1	D	40	SER	4.4
1	A	58	LYS	4.3
1	C	161	PHE	4.3
1	A	396	ASP	4.3
1	C	169	ILE	4.3
1	A	180	ILE	4.3
1	A	517	ARG	4.3
1	A	500	PRO	4.3
1	A	79	GLY	4.3
1	B	187	LYS	4.3
1	B	68	PRO	4.3
1	A	212	LYS	4.3
1	D	518	ALA	4.3
1	C	576	HIS	4.3
1	D	381	GLY	4.3
1	D	383	SER	4.3
1	B	117	ASP	4.3
1	B	315	CYS	4.3
1	C	394	ASP	4.3
1	A	540	SER	4.3
1	B	471	ASP	4.3
1	B	493	ARG	4.3
1	B	406	ASP	4.3
1	C	30	ALA	4.3
1	C	131	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	328	LYS	4.3
1	C	232	LYS	4.3
1	A	214	HIS	4.2
1	A	357	PRO	4.2
1	A	549	VAL	4.2
1	C	350	THR	4.2
1	C	289	SER	4.2
1	A	61	ARG	4.2
1	A	305	ASN	4.2
1	D	72	ILE	4.2
1	D	389	ILE	4.2
1	C	434	ALA	4.2
1	B	67	MET	4.2
1	A	445	TYR	4.2
1	D	42	THR	4.2
1	A	105	PHE	4.2
1	C	150	GLY	4.2
1	B	460	MET	4.2
1	A	376	GLY	4.2
1	D	96	VAL	4.2
1	B	467	ASP	4.2
1	A	516	GLU	4.2
1	A	41	ASP	4.2
1	B	539	LEU	4.1
1	C	443	GLU	4.1
1	B	127	ARG	4.1
1	C	118	LYS	4.1
1	D	270	ALA	4.1
1	D	329	ASP	4.1
1	C	346	ASN	4.1
1	A	380	SER	4.1
1	D	88	CYS	4.1
1	B	37	ASN	4.1
1	C	251	SER	4.1
1	D	579	GLN	4.1
1	C	90	SER	4.1
1	D	311	GLY	4.1
1	C	465	LYS	4.1
1	D	378	SER	4.0
1	A	209	GLN	4.0
1	C	143	LEU	4.0
1	D	494	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	427	HIS	4.0
1	B	251	SER	4.0
1	B	162	TYR	4.0
1	A	534	VAL	4.0
1	B	381	GLY	4.0
1	A	544	GLN	4.0
1	D	168	SER	4.0
1	C	221	GLY	4.0
1	B	235	ASN	4.0
1	A	514	GLU	4.0
1	C	129	THR	4.0
1	B	524	ASP	4.0
1	D	106	GLY	4.0
1	B	204	THR	4.0
1	B	351	TYR	3.9
1	D	12	THR	3.9
1	B	199	THR	3.9
1	D	260	SER	3.9
1	C	274	SER	3.9
1	A	336	ASP	3.9
1	B	306	ALA	3.9
1	C	382	LYS	3.9
1	C	568	GLN	3.9
1	D	296	ARG	3.9
1	C	567	ALA	3.9
1	D	457	ALA	3.9
1	C	330	GLU	3.9
1	D	204	THR	3.9
1	A	120	SER	3.9
1	D	101	ARG	3.8
1	A	271	SER	3.8
1	B	543	GLU	3.8
1	A	38	ALA	3.8
1	A	379	GLY	3.8
1	C	370	LYS	3.8
1	A	208	GLU	3.8
1	C	252	ASP	3.8
1	B	227	THR	3.8
1	A	111	MET	3.8
1	B	248	SER	3.8
1	A	307	GLN	3.8
1	C	351	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	354	ARG	3.8
1	A	217	VAL	3.8
1	A	529	ASN	3.8
1	B	418	GLN	3.8
1	D	353	GLY	3.8
1	C	17	TRP	3.8
1	C	438	ALA	3.8
1	C	471	ASP	3.8
1	A	350	THR	3.8
1	A	505	ASP	3.8
1	D	314	ALA	3.8
1	B	326	GLN	3.8
1	A	446	SER	3.7
1	D	333	ARG	3.7
1	B	450	ILE	3.7
1	D	118	LYS	3.7
1	D	320	ALA	3.7
1	D	164	SER	3.7
1	A	335	ILE	3.7
1	C	469	GLY	3.7
1	D	155	GLY	3.7
1	D	403	ASP	3.7
1	B	458	TYR	3.7
1	B	540	SER	3.7
1	A	402	MET	3.7
1	D	361	ASN	3.7
1	D	51	LEU	3.7
1	B	108	MET	3.7
1	B	12	THR	3.7
1	D	509	SER	3.7
1	B	15	ARG	3.7
1	D	220	PHE	3.7
1	D	475	GLY	3.7
1	D	434	ALA	3.7
1	A	322	LEU	3.7
1	A	231	ASP	3.7
1	B	97	VAL	3.7
1	B	172	VAL	3.7
1	C	302	THR	3.7
1	C	231	ASP	3.6
1	C	384	THR	3.6
1	C	311	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	254	ILE	3.6
1	A	282	GLY	3.6
1	B	230	PHE	3.6
1	B	208	GLU	3.6
1	D	209	GLN	3.6
1	A	107	HIS	3.6
1	B	376	GLY	3.6
1	D	20	ILE	3.6
1	A	304	VAL	3.6
1	B	112	PRO	3.6
1	B	217	VAL	3.6
1	C	407	LEU	3.6
1	C	580	PHE	3.6
1	C	449	GLN	3.6
1	A	469	GLY	3.6
1	A	485	GLN	3.6
1	B	464	ASN	3.6
1	C	319	PHE	3.6
1	B	352	PRO	3.6
1	C	461	ASP	3.6
1	B	363	ASN	3.6
1	D	563	SER	3.6
1	C	440	ALA	3.5
1	D	304	VAL	3.5
1	C	321	ILE	3.5
1	A	82	SER	3.5
1	C	145	THR	3.5
1	C	398	GLY	3.5
1	D	48	LEU	3.5
1	B	380	SER	3.5
1	B	518	ALA	3.5
1	B	369	GLY	3.5
1	D	45	LEU	3.5
1	D	71	VAL	3.5
1	A	141	GLY	3.5
1	A	530	ARG	3.5
1	B	382	LYS	3.5
1	C	381	GLY	3.5
1	D	30	ALA	3.5
1	A	19	THR	3.5
1	A	205	THR	3.5
1	C	508	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	476	GLU	3.5
1	A	199	THR	3.5
1	D	487	GLN	3.5
1	A	318	LEU	3.4
1	D	144	ILE	3.4
1	D	511	LEU	3.4
1	A	269	ALA	3.4
1	A	268	TYR	3.4
1	D	132	SER	3.4
1	D	176	PRO	3.4
1	B	255	ILE	3.4
1	A	382	LYS	3.4
1	D	366	ILE	3.4
1	D	400	ILE	3.4
1	D	360	ARG	3.4
1	D	70	VAL	3.4
1	A	256	GLN	3.4
1	C	487	GLN	3.4
1	B	330	GLU	3.4
1	C	491	ILE	3.4
1	D	150	GLY	3.4
1	D	561	THR	3.4
1	C	527	GLN	3.4
1	C	333	ARG	3.4
1	B	256	GLN	3.4
1	A	464	ASN	3.4
1	C	380	SER	3.4
1	B	99	THR	3.3
1	A	219	ILE	3.3
1	B	531	THR	3.3
1	A	394	ASP	3.3
1	C	396	ASP	3.3
1	B	427	HIS	3.3
1	A	579	GLN	3.3
1	B	166	GLN	3.3
1	D	252	ASP	3.3
1	B	232	LYS	3.3
1	A	519	ILE	3.3
1	D	467	ASP	3.3
1	B	236	LYS	3.3
1	C	482	SER	3.3
1	D	94	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	231	ASP	3.3
1	D	397	GLU	3.3
1	A	55	GLY	3.3
1	A	203	VAL	3.3
1	B	454	ALA	3.3
1	A	317	THR	3.3
1	D	480	LEU	3.3
1	D	17	TRP	3.3
1	A	573	ALA	3.3
1	B	361	ASN	3.3
1	C	331	GLY	3.3
1	C	555	ILE	3.3
1	A	467	ASP	3.3
1	A	389	ILE	3.3
1	D	426	VAL	3.3
1	B	158	ILE	3.3
1	B	563	SER	3.3
1	C	147	VAL	3.3
1	C	317	THR	3.3
1	C	408	ARG	3.3
1	D	331	GLY	3.3
1	D	377	ARG	3.3
1	D	328	LYS	3.3
1	A	387	SER	3.3
1	C	304	VAL	3.2
1	D	38	ALA	3.2
1	C	272	PHE	3.2
1	C	526	LEU	3.2
1	B	186	SER	3.2
1	A	435	ASN	3.2
1	C	353	GLY	3.2
1	B	514	GLU	3.2
1	A	124	LEU	3.2
1	B	394	ASP	3.2
1	A	438	ALA	3.2
1	D	147	VAL	3.2
1	D	196	MET	3.2
1	A	286	VAL	3.2
1	D	122	GLY	3.2
1	C	215	LYS	3.2
1	A	27	LEU	3.2
1	B	222	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	383	SER	3.2
1	D	131	ASP	3.2
1	C	250	ILE	3.2
1	B	478	GLY	3.2
1	B	513	THR	3.2
1	A	449	GLN	3.2
1	C	494	ALA	3.2
1	A	363	ASN	3.2
1	B	190	ARG	3.2
1	B	328	LYS	3.2
1	A	571	VAL	3.2
1	C	130	TYR	3.2
1	C	31	GLY	3.1
1	C	152	SER	3.1
1	D	357	PRO	3.1
1	A	126	SER	3.1
1	A	383	SER	3.1
1	C	339	THR	3.1
1	B	511	LEU	3.1
1	D	325	GLU	3.1
1	C	517	ARG	3.1
1	D	127	ARG	3.1
1	C	523	LEU	3.1
1	B	333	ARG	3.1
1	D	286	VAL	3.1
1	A	347	VAL	3.1
1	C	495	LEU	3.1
1	B	576	HIS	3.1
1	D	256	GLN	3.1
1	D	443	GLU	3.1
1	C	368	ALA	3.1
1	D	478	GLY	3.1
1	A	276	MET	3.1
1	C	208	GLU	3.1
1	D	236	LYS	3.1
1	A	426	VAL	3.1
1	A	163	TYR	3.1
1	B	423	SER	3.1
1	B	444	GLU	3.0
1	C	273	PRO	3.0
1	A	113	VAL	3.0
1	A	290	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	221	GLY	3.0
1	D	308	PHE	3.0
1	A	515	SER	3.0
1	B	298	LEU	3.0
1	D	557	VAL	3.0
1	C	176	PRO	3.0
1	B	435	ASN	3.0
1	A	155	GLY	3.0
1	A	306	ALA	3.0
1	A	440	ALA	3.0
1	C	348	THR	3.0
1	D	335	ILE	3.0
1	A	441	ARG	3.0
1	C	277	ASP	3.0
1	C	386	ALA	3.0
1	B	234	SER	3.0
1	B	383	SER	3.0
1	C	456	MET	3.0
1	B	436	ASN	3.0
1	D	535	ILE	3.0
1	B	289	SER	3.0
1	C	16	LEU	3.0
1	B	160	MET	3.0
1	D	123	THR	3.0
1	A	215	LYS	3.0
1	A	475	GLY	3.0
1	C	104	LEU	3.0
1	C	29	VAL	3.0
1	C	411	THR	3.0
1	D	79	GLY	3.0
1	A	468	ASN	3.0
1	C	123	THR	3.0
1	A	241	GLY	2.9
1	D	497	ARG	2.9
1	C	248	SER	2.9
1	B	379	GLY	2.9
1	C	192	ILE	2.9
1	C	431	ASP	2.9
1	D	102	ARG	2.9
1	D	416	ARG	2.9
1	B	211	LEU	2.9
1	B	159	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	197	GLN	2.9
1	B	104	LEU	2.9
1	D	336	ASP	2.9
1	B	224	GLU	2.9
1	D	513	THR	2.9
1	A	169	ILE	2.9
1	A	346	ASN	2.9
1	D	29	VAL	2.9
1	C	403	ASP	2.9
1	D	297	PRO	2.9
1	B	168	SER	2.9
1	C	554	GLY	2.9
1	D	86	SER	2.9
1	B	102	ARG	2.9
1	B	441	ARG	2.9
1	C	116	PHE	2.9
1	D	74	LEU	2.9
1	C	219	ILE	2.9
1	D	224	GLU	2.9
1	A	298	LEU	2.9
1	D	313	ALA	2.9
1	D	371	THR	2.9
1	C	139	SER	2.9
1	B	359	LEU	2.9
1	D	498	ASP	2.9
1	D	257	LEU	2.9
1	D	435	ASN	2.9
1	A	191	SER	2.8
1	B	64	LEU	2.8
1	B	484	GLY	2.8
1	C	58	LYS	2.8
1	C	242	MET	2.8
1	A	386	ALA	2.8
1	D	433	VAL	2.8
1	B	331	GLY	2.8
1	C	42	THR	2.8
1	C	564	GLU	2.8
1	B	194	LYS	2.8
1	D	217	VAL	2.8
1	D	578	MET	2.8
1	A	90	SER	2.8
1	B	66	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	424	GLN	2.8
1	C	132	SER	2.8
1	D	235	ASN	2.8
1	B	468	ASN	2.8
1	D	358	ALA	2.8
1	A	351	TYR	2.8
1	D	391	ARG	2.8
1	B	477	ASN	2.8
1	C	326	GLN	2.8
1	C	344	PHE	2.8
1	D	197	GLN	2.8
1	D	192	ILE	2.8
1	A	229	ARG	2.8
1	A	223	GLN	2.8
1	B	73	GLY	2.8
1	C	463	ILE	2.8
1	A	265	PHE	2.8
1	D	53	ASP	2.8
1	A	226	GLU	2.8
1	C	61	ARG	2.8
1	D	559	ARG	2.8
1	D	356	VAL	2.8
1	D	485	GLN	2.8
1	A	63	VAL	2.8
1	A	526	LEU	2.8
1	D	240	GLN	2.8
1	B	293	ALA	2.8
1	A	69	LEU	2.8
1	B	572	TYR	2.8
1	C	377	ARG	2.8
1	A	133	GLU	2.8
1	C	444	GLU	2.7
1	C	71	VAL	2.7
1	B	347	VAL	2.7
1	C	107	HIS	2.7
1	D	362	ILE	2.7
1	C	244	MET	2.7
1	C	475	GLY	2.7
1	D	26	GLY	2.7
1	B	295	MET	2.7
1	C	445	TYR	2.7
1	A	523	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	503	ILE	2.7
1	A	522	ALA	2.7
1	D	18	PRO	2.7
1	A	430	ASN	2.7
1	C	216	GLU	2.7
1	A	14	ARG	2.7
1	C	230	PHE	2.7
1	B	358	ALA	2.7
1	C	68	PRO	2.7
1	A	143	LEU	2.7
1	C	309	GLN	2.7
1	C	342	LEU	2.7
1	B	141	GLY	2.7
1	D	300	SER	2.7
1	C	498	ASP	2.7
1	D	472	THR	2.7
1	C	478	GLY	2.7
1	B	223	GLN	2.7
1	D	538	ARG	2.7
1	A	418	GLN	2.7
1	A	283	THR	2.7
1	D	115	PHE	2.7
1	B	121	THR	2.7
1	D	541	THR	2.7
1	A	359	LEU	2.7
1	B	53	ASP	2.7
1	B	205	THR	2.7
1	A	34	LEU	2.6
1	B	411	THR	2.6
1	D	211	LEU	2.6
1	A	451	GLU	2.6
1	D	546	ASP	2.6
1	C	211	LEU	2.6
1	C	300	SER	2.6
1	A	116	PHE	2.6
1	A	194	LYS	2.6
1	A	360	ARG	2.6
1	C	111	MET	2.6
1	C	53	ASP	2.6
1	C	379	GLY	2.6
1	B	270	ALA	2.6
1	C	235	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	195	ASN	2.6
1	D	491	ILE	2.6
1	B	62	SER	2.6
1	D	279	LEU	2.6
1	B	386	ALA	2.6
1	D	108	MET	2.6
1	D	550	VAL	2.6
1	A	62	SER	2.6
1	A	135	VAL	2.6
1	B	559	ARG	2.6
1	A	332	LYS	2.6
1	C	490	ALA	2.6
1	D	504	LEU	2.6
1	D	169	ILE	2.6
1	D	212	LYS	2.6
1	B	565	LEU	2.6
1	D	52	LEU	2.6
1	D	229	ARG	2.6
1	A	12	THR	2.6
1	B	105	PHE	2.6
1	A	172	VAL	2.6
1	D	135	VAL	2.6
1	C	376	GLY	2.6
1	B	480	LEU	2.6
1	C	514	GLU	2.6
1	A	160	MET	2.6
1	B	377	ARG	2.6
1	C	480	LEU	2.6
1	D	455	ARG	2.6
1	B	323	ASP	2.6
1	B	482	SER	2.6
1	D	85	SER	2.6
1	A	324	SER	2.6
1	B	473	ILE	2.6
1	C	158	ILE	2.6
1	C	362	ILE	2.6
1	D	219	ILE	2.5
1	D	355	GLU	2.5
1	C	565	LEU	2.5
1	A	366	ILE	2.5
1	C	113	VAL	2.5
1	C	276	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	107	HIS	2.5
1	C	418	GLN	2.5
1	D	326	GLN	2.5
1	D	341	ASP	2.5
1	B	556	ILE	2.5
1	C	295	MET	2.5
1	D	262	ALA	2.5
1	B	14	ARG	2.5
1	B	549	VAL	2.5
1	C	162	TYR	2.5
1	C	492	ALA	2.5
1	B	147	VAL	2.5
1	D	174	LEU	2.5
1	A	195	ASN	2.5
1	C	544	GLN	2.5
1	C	559	ARG	2.5
1	B	537	HIS	2.5
1	C	22	PRO	2.5
1	B	212	LYS	2.5
1	D	69	LEU	2.5
1	B	568	GLN	2.5
1	D	245	VAL	2.5
1	A	262	ALA	2.5
1	D	225	VAL	2.5
1	A	267	LEU	2.5
1	C	363	ASN	2.5
1	B	525	GLU	2.5
1	C	187	LYS	2.5
1	D	283	THR	2.5
1	D	63	VAL	2.5
1	A	323	ASP	2.5
1	B	488	ARG	2.5
1	A	15	ARG	2.5
1	B	515	SER	2.5
1	D	414	SER	2.5
1	C	286	VAL	2.5
1	D	495	LEU	2.5
1	C	269	ALA	2.5
1	C	373	ALA	2.5
1	A	88	CYS	2.4
1	A	482	SER	2.4
1	B	56	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	390	THR	2.4
1	C	165	TRP	2.4
1	D	411	THR	2.4
1	D	469	GLY	2.4
1	D	527	GLN	2.4
1	D	39	ALA	2.4
1	D	347	VAL	2.4
1	D	90	SER	2.4
1	A	73	GLY	2.4
1	C	226	GLU	2.4
1	D	441	ARG	2.4
1	C	180	ILE	2.4
1	A	365	LYS	2.4
1	D	531	THR	2.4
1	B	150	GLY	2.4
1	D	521	ALA	2.4
1	A	184	VAL	2.4
1	A	558	GLU	2.4
1	C	423	SER	2.4
1	A	83	TYR	2.4
1	A	577	LYS	2.4
1	C	26	GLY	2.4
1	D	396	ASP	2.4
1	B	79	GLY	2.4
1	B	34	LEU	2.4
1	B	219	ILE	2.4
1	C	366	ILE	2.4
1	B	272	PHE	2.4
1	A	118	LYS	2.4
1	A	568	GLN	2.4
1	D	418	GLN	2.4
1	C	40	SER	2.4
1	C	203	VAL	2.4
1	B	496	LEU	2.4
1	D	189	PHE	2.4
1	A	527	GLN	2.4
1	A	528	LYS	2.4
1	C	349	PHE	2.4
1	C	413	ALA	2.4
1	A	423	SER	2.4
1	B	228	LYS	2.4
1	D	569	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	307	GLN	2.4
1	D	500	PRO	2.4
1	A	37	ASN	2.3
1	A	508	THR	2.3
1	B	461	ASP	2.3
1	C	79	GLY	2.3
1	B	10	TRP	2.3
1	A	334	VAL	2.3
1	C	507	ALA	2.3
1	B	486	ARG	2.3
1	D	166	GLN	2.3
1	B	249	SER	2.3
1	C	189	PHE	2.3
1	A	168	SER	2.3
1	B	46	SER	2.3
1	D	78	ARG	2.3
1	A	377	ARG	2.3
1	B	27	LEU	2.3
1	D	483	GLY	2.3
1	D	87	TYR	2.3
1	A	553	ASP	2.3
1	C	447	ARG	2.3
1	B	237	MET	2.3
1	C	484	GLY	2.3
1	C	466	MET	2.3
1	C	64	LEU	2.3
1	D	517	ARG	2.3
1	A	384	THR	2.3
1	D	345	ARG	2.3
1	D	534	VAL	2.3
1	B	40	SER	2.3
1	D	440	ALA	2.3
1	B	512	ASP	2.3
1	B	178	VAL	2.3
1	C	391	ARG	2.3
1	D	50	PRO	2.3
1	B	31	GLY	2.3
1	B	314	ALA	2.3
1	B	385	ILE	2.3
1	C	299	LYS	2.3
1	C	134	GLN	2.3
1	D	137	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLY	2.3
1	D	143	LEU	2.3
1	B	378	SER	2.3
1	A	381	GLY	2.3
1	B	90	SER	2.2
1	B	132	SER	2.2
1	B	276	MET	2.2
1	B	459	ALA	2.2
1	D	82	SER	2.2
1	D	386	ALA	2.2
1	A	24	LYS	2.2
1	D	167	LEU	2.2
1	D	503	ILE	2.2
1	A	454	ALA	2.2
1	D	554	GLY	2.2
1	C	354	ARG	2.2
1	D	339	THR	2.2
1	D	46	SER	2.2
1	C	538	ARG	2.2
1	C	388	LEU	2.2
1	B	438	ALA	2.2
1	C	437	ILE	2.2
1	D	133	GLU	2.2
1	C	581	GLY	2.2
1	D	175	ALA	2.2
1	D	255	ILE	2.2
1	A	198	ASN	2.2
1	B	280	THR	2.2
1	B	179	SER	2.2
1	A	72	ILE	2.2
1	B	334	VAL	2.2
1	C	485	GLN	2.2
1	A	132	SER	2.2
1	A	254	ILE	2.2
1	B	33	ALA	2.2
1	C	210	MET	2.2
1	D	368	ALA	2.2
1	D	73	GLY	2.2
1	D	103	ARG	2.2
1	A	17	TRP	2.2
1	A	390	THR	2.2
1	D	201	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	133	GLU	2.2
1	C	264	ALA	2.2
1	B	173	VAL	2.2
1	B	13	PHE	2.2
1	D	75	MET	2.2
1	C	10	TRP	2.2
1	C	483	GLY	2.2
1	B	245	VAL	2.2
1	B	269	ALA	2.2
1	D	156	LEU	2.2
1	D	228	LYS	2.2
1	D	31	GLY	2.1
1	A	496	LEU	2.1
1	B	338	ALA	2.1
1	C	228	LYS	2.1
1	B	322	LEU	2.1
1	B	83	TYR	2.1
1	C	528	LYS	2.1
1	B	426	VAL	2.1
1	B	489	ILE	2.1
1	B	398	GLY	2.1
1	A	473	ILE	2.1
1	D	316	GLN	2.1
1	D	282	GLY	2.1
1	B	367	PRO	2.1
1	B	368	ALA	2.1
1	D	226	GLU	2.1
1	A	277	ASP	2.1
1	B	570	GLY	2.1
1	A	176	PRO	2.1
1	D	572	TYR	2.1
1	B	561	THR	2.1
1	B	431	ASP	2.1
1	D	117	ASP	2.1
1	D	173	VAL	2.1
1	D	277	ASP	2.1
1	B	384	THR	2.1
1	D	110	GLY	2.1
1	A	97	VAL	2.1
1	C	21	ALA	2.1
1	C	262	ALA	2.1
1	D	198	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	429	PHE	2.1
1	B	114	ALA	2.1
1	C	110	GLY	2.1
1	B	156	LEU	2.1
1	C	28	ILE	2.1
1	C	563	SER	2.1
1	D	76	ILE	2.1
1	D	330	GLU	2.1
1	B	175	ALA	2.1
1	A	361	ASN	2.1
1	D	421	LEU	2.1
1	B	87	TYR	2.1
1	C	247	ALA	2.1
1	C	325	GLU	2.1
1	A	429	PHE	2.1
1	D	295	MET	2.1
1	D	126	SER	2.1
1	A	489	ILE	2.1
1	B	58	LYS	2.1
1	A	148	ARG	2.0
1	B	207	ALA	2.0
1	D	165	TRP	2.0
1	A	224	GLU	2.0
1	C	358	ALA	2.0
1	C	519	ILE	2.0
1	B	470	LEU	2.0
1	A	292	ILE	2.0
1	A	314	ALA	2.0
1	B	195	ASN	2.0
1	B	528	LYS	2.0
1	D	179	SER	2.0
1	D	496	LEU	2.0
1	C	265	PHE	2.0
1	A	352	PRO	2.0
1	A	278	SER	2.0
1	D	499	SER	2.0
1	A	216	GLU	2.0
1	D	382	LYS	2.0
1	D	205	THR	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	ADP	B	601	26/27	0.63	0.83	0.32	156,156,156,156	0
2	ADP	A	5001	26/27	0.64	0.82	-0.48	156,156,156,156	0
2	ADP	C	601	26/27	0.74	0.81	-0.70	156,156,156,156	0
2	ADP	D	601	26/27	0.69	0.81	-0.81	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	0.75	-	156,156,156,156	0
3	VO4	C	602	2/5	0.82	0.73	-	156,156,156,156	0
3	VO4	B	602	2/5	0.73	0.86	-	156,156,156,156	0

6.5 Other polymers [i](#)

There are no such residues in this entry.