



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:02 AM GMT

PDB ID : 2VPQ
Title : CRYSTAL STRUCTURE OF BIOTIN CARBOXYLASE FROM S. AUREUS
COMPLEXED WITH AMPPNP
Authors : Mochalkin, I.
Deposited on : 2008-03-03
Resolution : 2.10 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

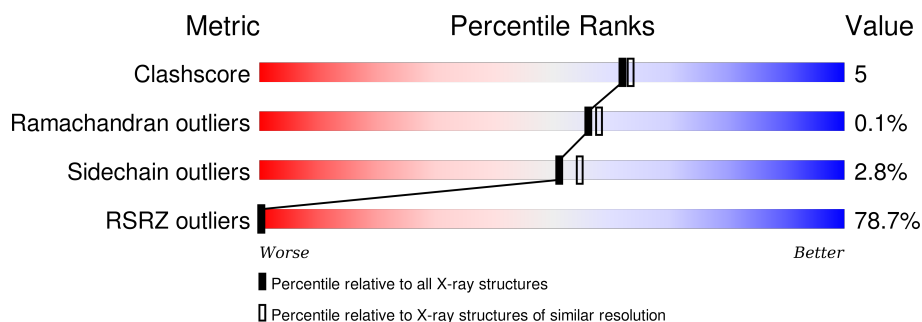
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	451	<div> <div>77%</div> <div>85%13%..</div> </div>
1	B	451	<div> <div>79%</div> <div>88%11%.</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
4	CL	A	1452	-	-	-	X
4	CL	B	1453	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7876 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 ACETYL-COA CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	1	0
			3486	2205	594	665	22			
1	B	448	Total	C	N	O	S	0	2	0
			3505	2218	599	666	22			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Mg 2	0	0
3	A	2	Total 2	Mg 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	A	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	419	Total 419	O 419	0	0
5	B	398	Total 398	O 398	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.25Å 63.32Å 105.14Å 90.00° 103.82° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 41.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.10) 84.4 (41.52-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.284 0.411 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.68$, $\langle L^2 \rangle = 0.56$	Xtriage
Outliers	28 of 55200 reflections (0.051%)	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7876	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, CL

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	$\# Z > 5$
1	A	0.47	0/3548	0.60	1/4791 (0.0%)
1	B	0.45	0/3573	0.58	0/4823
All	All	0.46	0/7121	0.59	1/9614 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ARG	NE-CZ-NH2	5.32	122.96	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3486	0	3479	48	0
1	B	3505	0	3513	28	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	419	0	0	4	0
5	B	398	0	0	4	1
All	All	7876	0	7018	76	1

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 5.

All (76) 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)
1:A:137:MET:CE	1:A:156:ILE:HD11	1.86	1.05
1:A:137:MET:HE3	1:A:156:ILE:HD11	1.41	0.98
1:A:137:MET:CE	1:A:156:ILE:CD1	2.57	0.82
1:B:265:VAL:HG12	1:B:265:VAL:O	1.83	0.79
1:A:137:MET:HE1	1:A:156:ILE:HD11	1.63	0.78
1:B:111:LYS:HD2	1:B:265:VAL:HG13	1.68	0.75
1:A:137:MET:HE1	1:A:156:ILE:CD1	2.16	0.75
1:A:428:ASN:HD22	1:A:431:PHE:H	1.37	0.72
1:B:137:MET:HE3	1:B:156:ILE:HD11	1.73	0.68
1:B:295:VAL:HG23	4:B:1453:CL:CL	2.31	0.68
1:A:357:GLN:HE21	1:A:413:LEU:HD12	1.64	0.62
1:A:265:VAL:O	1:A:265:VAL:HG12	1.99	0.62
1:A:41:THR:OG1	1:A:42:GLN:NE2	2.32	0.61
1:B:2:LYS:N	5:B:2001:HOH:O	2.32	0.61
1:A:111:LYS:HD2	1:A:265:VAL:HG13	1.82	0.61
1:A:26:GLN:HG3	5:A:2026:HOH:O	2.00	0.61
1:B:119:LYS:HE3	5:B:2194:HOH:O	2.01	0.59
1:A:26:GLN:OE1	5:A:2027:HOH:O	2.17	0.57
1:B:146:ILE:HG22	1:B:150:ILE:CD1	2.35	0.57
1:A:290:ASN:OD1	1:A:294:GLN:NE2	2.38	0.57
1:A:137:MET:HE3	1:A:156:ILE:CD1	2.23	0.56
1:B:221:ILE:HD12	1:B:328:ILE:HD11	1.89	0.55
1:A:112:MET:HE1	1:A:118:ALA:HA	1.88	0.55
1:A:28:VAL:HG22	1:A:46:GLU:HG3	1.89	0.54
1:A:102:ILE:HD12	1:A:316:ALA:CB	2.38	0.53
1:A:311:LEU:O	1:A:315:VAL:HG23	2.09	0.53
1:A:215:ASP:HA	1:A:315:VAL:HG13	1.89	0.53
1:A:204:ASN:HD22	1:A:280:ASN:ND2	2.07	0.52
1:B:299:VAL:CG1	1:B:336:GLU:HB2	2.40	0.51
1:A:295:VAL:HG23	4:A:1452:CL:CL	2.47	0.51
1:B:390:ILE:N	1:B:390:ILE:HD12	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:VAL:CG1	1:B:265:VAL:O	2.55	0.50
1:A:213:VAL:HG13	1:A:213:VAL:O	2.11	0.50
1:A:428:ASN:HD21	1:A:430:ILE:HB	1.76	0.50
1:A:299:VAL:CG1	1:A:336:GLU:HB2	2.42	0.49
1:B:283:LYS:NZ	5:B:2239:HOH:O	2.45	0.49
1:A:133:SER:HB3	1:A:146:ILE:HD13	1.94	0.49
1:A:222:HIS:HD2	1:A:224:GLY:H	1.60	0.49
1:B:92:GLU:HG2	1:B:106:TYR:CG	2.48	0.48
1:A:391:ILE:HD11	1:A:402:ALA:HB1	1.96	0.48
1:B:299:VAL:HG12	1:B:336:GLU:HB2	1.95	0.47
1:B:238:VAL:HG21	1:B:425:LEU:CD2	2.43	0.47
1:B:204:ASN:HD22	1:B:280:ASN:ND2	2.13	0.47
1:A:50:VAL:O	1:A:50:VAL:HG22	2.15	0.47
1:A:299:VAL:HG12	1:A:336:GLU:HB2	1.95	0.47
1:A:2:LYS:N	5:A:2002:HOH:O	2.48	0.47
1:A:150:ILE:HG22	1:A:200:LYS:HD2	1.96	0.46
1:B:11:GLU:OE2	1:B:81:TYR:OH	2.32	0.46
1:A:391:ILE:HG12	1:A:402:ALA:HB3	1.96	0.46
1:B:290:ASN:ND2	5:B:2243:HOH:O	2.43	0.46
1:B:28:VAL:HG22	1:B:46:GLU:HG3	1.98	0.45
1:A:383:ASP:HB3	5:A:2009:HOH:O	2.17	0.45
1:A:102:ILE:CD1	1:A:316:ALA:CB	2.95	0.44
1:B:357:GLN:OE1	1:B:413:LEU:HD12	2.17	0.44
1:B:297:HIS:N	1:B:298:PRO:CD	2.81	0.44
1:A:335:ILE:HG23	1:A:391:ILE:CG2	2.48	0.43
1:A:132:GLY:HA2	1:A:150:ILE:CD1	2.49	0.43
1:B:112:MET:SD	1:B:265:VAL:HG21	2.60	0.42
1:A:335:ILE:HG23	1:A:391:ILE:HG22	2.01	0.42
1:A:3:LYS:HG3	1:A:26:GLN:HB2	2.02	0.42
1:A:232:ARG:HB2	1:A:237:LEU:HD11	2.00	0.42
1:B:223:LEU:N	1:B:223:LEU:HD12	2.34	0.42
1:A:145:LYS:O	1:A:148:LYS:HG2	2.20	0.41
1:B:157:LYS:HG2	1:B:167:ILE:HG23	2.02	0.41
1:B:252[B]:ARG:HG3	1:B:253:GLU:N	2.35	0.41
1:A:212:ILE:C	1:A:212:ILE:HD13	2.41	0.41
1:A:102:ILE:CD1	1:A:316:ALA:HB1	2.51	0.41
1:A:81:TYR:CZ	1:A:295:VAL:HG22	2.55	0.41
1:B:206:ARG:HG3	1:B:229:THR:OG1	2.21	0.41
1:A:137:MET:HG2	1:A:146:ILE:HD12	2.02	0.41
1:A:297:HIS:N	1:A:298:PRO:CD	2.84	0.41
1:A:233:ARG:O	1:A:234:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ILE:HG22	1:B:150:ILE:HD12	2.03	0.40
1:A:157:LYS:HG2	1:A:167:ILE:HG23	2.04	0.40
1:B:361:PRO:HB3	1:B:409:GLU:HG3	2.04	0.40
1:A:60:LEU:HD21	1:A:83:PHE:HA	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2027:HOH:O	5:B:2172:HOH:O[2_545]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/451 (99%)	435 (98%)	11 (2%)	0	100	100
1	B	448/451 (99%)	436 (97%)	11 (2%)	1 (0%)	52	53
All	All	894/902 (99%)	871 (97%)	22 (2%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/375 (99%)	363 (98%)	9 (2%)	57	61
1	B	375/375 (100%)	363 (97%)	12 (3%)	46	48
All	All	747/750 (100%)	726 (97%)	21 (3%)	51	55

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	116	ASP
1	A	140	VAL
1	A	181	ARG
1	A	212	ILE
1	A	240	GLU
1	A	335	ILE
1	A	383	ASP
1	A	410	PHE
1	B	2	LYS
1	B	36	LYS
1	B	42	GLN
1	B	50	VAL
1	B	64	ASN
1	B	139	ASP
1	B	212	ILE
1	B	248	ASP
1	B	356	GLU
1	B	383	ASP
1	B	410	PHE
1	B	439	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	42	GLN
1	A	110	GLN
1	A	207	HIS
1	A	222	HIS
1	A	280	ASN
1	A	282	ASN

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Mol	Chain	Res	Type
1	A	357	GLN
1	A	375	ASN
1	A	422	HIS
1	A	428	ASN
1	A	448	ASN
1	B	222	HIS
1	B	280	ASN
1	B	375	ASN
1	B	422	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	1449	3	27,33,33	1.57	4 (14%)	30,52,52	2.22	7 (23%)
2	ANP	B	1450	3	27,33,33	1.69	6 (22%)	30,52,52	1.95	5 (16%)

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	1449	3	-	0/12/38/38	0/3/3/3
2	ANP	B	1450	3	-	0/12/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1450	ANP	PB-O2B	-2.53	1.49	1.56
2	A	1449	ANP	PB-O2B	-2.19	1.50	1.56
2	B	1450	ANP	PG-O3G	-2.05	1.51	1.56
2	B	1450	ANP	C5-C4	2.79	1.46	1.40
2	B	1450	ANP	PB-O3A	2.81	1.62	1.59
2	A	1449	ANP	C5-C4	2.96	1.47	1.40
2	A	1449	ANP	PG-O1G	4.15	1.50	1.46
2	A	1449	ANP	PB-O1B	4.16	1.50	1.46
2	B	1450	ANP	PG-O1G	4.37	1.51	1.46
2	B	1450	ANP	PB-O1B	4.66	1.51	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1449	ANP	N3-C2-N1	-8.06	122.72	128.89
2	B	1450	ANP	N3-C2-N1	-6.66	123.79	128.89
2	B	1450	ANP	C2'-C1'-N9	-4.17	107.92	114.29
2	A	1449	ANP	O1G-PG-N3B	-3.61	106.36	111.90
2	B	1450	ANP	C4-C5-N7	-3.16	106.57	109.48
2	A	1449	ANP	C2'-C1'-N9	-3.08	109.58	114.29
2	A	1449	ANP	C1'-N9-C4	-2.80	122.71	126.94
2	A	1449	ANP	C4-C5-N7	-2.48	107.20	109.48
2	B	1450	ANP	O3A-PB-N3B	2.15	112.34	106.44
2	A	1449	ANP	C2-N1-C6	2.20	122.70	118.77
2	B	1450	ANP	O2B-PB-O1B	3.62	117.57	110.00
2	A	1449	ANP	O2B-PB-O1B	4.14	118.63	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	447/451 (99%)	3.59	348 (77%) 0 0	14, 23, 34, 40	0
1	B	448/451 (99%)	3.79	356 (79%) 0 0	14, 24, 35, 38	0
All	All	895/902 (99%)	3.69	704 (78%) 0 0	14, 24, 35, 40	0

All (704) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	SER	22.7
1	B	384	SER	17.9
1	A	176	LEU	14.5
1	A	232	ARG	12.0
1	A	217	TYR	11.8
1	B	176	LEU	11.8
1	A	143	ALA	11.7
1	A	195	GLY	11.3
1	B	195	GLY	11.2
1	B	401	MET	11.2
1	B	163	GLY	11.1
1	A	43	ILE	11.0
1	B	179	GLY	10.9
1	B	47	ALA	10.7
1	B	232	ARG	10.7
1	B	143	ALA	10.4
1	B	445	SER	10.3
1	A	194	GLY	10.3
1	B	318	GLY	9.9
1	B	234	MET	9.7
1	B	82	GLY	9.5
1	B	150	ILE	9.3
1	A	48	TYR	9.3
1	A	440	PHE	9.3

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Mol	Chain	Res	Type	RSRZ
1	B	101	PHE	9.0
1	A	383	ASP	8.9
1	B	156	ILE	8.6
1	B	114	ILE	8.6
1	A	47	ALA	8.6
1	B	110	GLN	8.6
1	B	48	TYR	8.6
1	B	164	GLY	8.5
1	A	181	ARG	8.3
1	B	178	THR	8.2
1	A	101	PHE	8.2
1	A	165	LYS	8.1
1	B	216	SER	8.0
1	B	162	GLY	7.9
1	B	249	GLU	7.9
1	B	60	LEU	7.9
1	B	158	ALA	7.7
1	B	140	VAL	7.7
1	A	318	GLY	7.6
1	B	348	PHE	7.5
1	A	281	ASP	7.5
1	A	360	ALA	7.5
1	B	410	PHE	7.5
1	A	252	ARG	7.5
1	A	137	MET	7.5
1	A	114	ILE	7.5
1	A	234	MET	7.4
1	A	170	ALA	7.4
1	B	194	GLY	7.4
1	B	383	ASP	7.3
1	B	181	ARG	7.3
1	B	123	ILE	7.2
1	A	233	ARG	7.2
1	B	259	VAL	7.2
1	B	183	THR	7.2
1	A	190	ALA	7.1
1	B	389	LEU	7.1
1	B	43	ILE	7.1
1	A	183	THR	7.1
1	A	389	LEU	7.1
1	A	140	VAL	7.1
1	A	408	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	230	ILE	7.0
1	B	12	ILE	7.0
1	A	216	SER	7.0
1	B	8	ASN	7.0
1	B	126	ASN	7.0
1	B	50	VAL	6.9
1	B	217	TYR	6.9
1	B	113	GLY	6.9
1	A	68	ILE	6.8
1	B	281	ASP	6.8
1	A	277	TYR	6.7
1	A	150	ILE	6.7
1	A	259	VAL	6.7
1	B	359	LEU	6.7
1	A	182	MET	6.7
1	A	284	PHE	6.6
1	B	175	GLU	6.6
1	B	19	ALA	6.6
1	B	237	LEU	6.6
1	A	317	MET	6.5
1	A	60	LEU	6.5
1	A	167	ILE	6.5
1	B	167	ILE	6.5
1	A	368	ILE	6.5
1	A	249	GLU	6.5
1	A	193	ASN	6.4
1	A	155	ILE	6.4
1	A	208	ILE	6.4
1	B	407	LEU	6.4
1	B	170	ALA	6.4
1	B	381	TYR	6.4
1	B	441	LEU	6.4
1	B	245	ILE	6.3
1	B	133	SER	6.3
1	A	29	ALA	6.3
1	A	36	LYS	6.2
1	B	80	GLY	6.2
1	B	68	ILE	6.1
1	B	27	THR	6.1
1	B	330	LEU	6.1
1	A	71	SER	6.1
1	A	175	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	6.1
1	B	182	MET	6.1
1	B	85	ALA	6.1
1	A	230	ILE	6.0
1	B	160	ALA	6.0
1	B	81	TYR	5.9
1	B	191	PHE	5.9
1	B	71	SER	5.9
1	B	266	ASN	5.9
1	A	156	ILE	5.9
1	A	106	TYR	5.9
1	B	196	LEU	5.9
1	A	401	MET	5.9
1	A	434	GLY	5.9
1	A	178	THR	5.9
1	B	315	VAL	5.9
1	A	27	THR	5.8
1	B	247	ASP	5.8
1	B	408	SER	5.8
1	A	426	LEU	5.8
1	B	103	GLY	5.8
1	A	412	VAL	5.8
1	A	348	PHE	5.8
1	A	13	ALA	5.8
1	B	190	ALA	5.8
1	B	137	MET	5.8
1	A	238	VAL	5.7
1	A	237	LEU	5.7
1	B	201	PHE	5.7
1	B	319	ASP	5.7
1	B	267	TYR	5.7
1	A	55	SER	5.7
1	B	193	ASN	5.7
1	B	334	ALA	5.7
1	A	196	LEU	5.7
1	A	82	GLY	5.7
1	A	65	ILE	5.7
1	A	133	SER	5.6
1	A	220	VAL	5.6
1	A	300	THR	5.6
1	B	22	ASP	5.6
1	B	338[A]	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	295	VAL	5.5
1	A	315	VAL	5.5
1	A	366	VAL	5.5
1	A	161	GLY	5.5
1	A	54	LEU	5.5
1	B	421	PHE	5.5
1	A	80	GLY	5.5
1	B	238	VAL	5.5
1	A	268	GLU	5.5
1	B	168	ARG	5.5
1	A	179	GLY	5.4
1	B	254	MET	5.4
1	A	78	HIS	5.4
1	A	89	ASP	5.4
1	A	276	ILE	5.3
1	B	440	PHE	5.3
1	B	299	VAL	5.3
1	B	165	LYS	5.3
1	B	180	PHE	5.3
1	A	152	TYR	5.3
1	A	117	VAL	5.2
1	B	386	VAL	5.2
1	A	171	ARG	5.2
1	B	339	ILE	5.2
1	B	320	VAL	5.1
1	A	270	ALA	5.1
1	B	29	ALA	5.1
1	A	223	LEU	5.1
1	B	233	ARG	5.1
1	B	426	LEU	5.1
1	B	317	MET	5.1
1	A	57	ASP	5.0
1	B	161	GLY	5.0
1	A	359	LEU	5.0
1	A	19	ALA	5.0
1	A	387	ALA	5.0
1	B	155	ILE	5.0
1	B	97	CYS	5.0
1	A	441	LEU	5.0
1	A	158	ALA	5.0
1	B	235	GLN	5.0
1	B	36	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	52	PRO	4.9
1	A	282	ASN	4.9
1	A	110	GLN	4.9
1	B	425	LEU	4.9
1	A	381	TYR	4.9
1	B	106	TYR	4.9
1	B	280	ASN	4.9
1	A	107	GLN	4.9
1	B	390	ILE	4.9
1	B	297	HIS	4.9
1	A	130	VAL	4.9
1	A	410	PHE	4.8
1	A	303	VAL	4.8
1	A	362	GLY	4.8
1	B	257	ALA	4.8
1	B	424	LYS	4.8
1	B	406	ALA	4.8
1	A	12	ILE	4.8
1	B	306	ILE	4.8
1	A	126	ASN	4.8
1	A	337	PHE	4.8
1	B	429	ASP	4.8
1	B	368	ILE	4.8
1	B	223	LEU	4.8
1	B	331	THR	4.8
1	A	192	GLY	4.7
1	B	172	ASP	4.7
1	B	402	ALA	4.7
1	A	390	ILE	4.7
1	B	62	ILE	4.7
1	B	200	LYS	4.7
1	A	235	GLN	4.7
1	B	42	GLN	4.7
1	B	152	TYR	4.7
1	B	328	ILE	4.7
1	A	345	TYR	4.6
1	B	323	TYR	4.6
1	A	97	CYS	4.6
1	A	402	ALA	4.6
1	B	64	ASN	4.6
1	B	329	LYS	4.6
1	B	309	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	311	LEU	4.6
1	A	164	GLY	4.6
1	B	387	ALA	4.6
1	A	81	TYR	4.6
1	A	37	ASP	4.6
1	A	50	VAL	4.6
1	A	361	PRO	4.6
1	B	75	ASP	4.6
1	B	185	GLN	4.6
1	A	339	ILE	4.6
1	B	17	ILE	4.6
1	A	319	ASP	4.5
1	A	253	GLU	4.5
1	B	220	VAL	4.5
1	B	30	ILE	4.5
1	A	136	LEU	4.5
1	B	345	TYR	4.5
1	B	255	GLY	4.5
1	B	337	PHE	4.5
1	B	273	ILE	4.5
1	B	265	VAL	4.5
1	A	56	LYS	4.4
1	A	293	ILE	4.4
1	B	293	ILE	4.4
1	A	214	GLY	4.4
1	B	127	VAL	4.4
1	A	125	ALA	4.4
1	B	366	VAL	4.4
1	B	412	VAL	4.4
1	A	266[A]	ASN	4.3
1	B	327	ASP	4.3
1	A	17	ILE	4.3
1	B	187	ALA	4.3
1	B	208	ILE	4.3
1	B	446	ILE	4.3
1	B	54	LEU	4.3
1	B	352	PRO	4.3
1	B	302	MET	4.3
1	A	407	LEU	4.3
1	A	185	GLN	4.3
1	B	294	GLN	4.3
1	A	120	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	436	PHE	4.2
1	A	160	ALA	4.2
1	A	335	ILE	4.2
1	B	53	THR	4.2
1	B	253	GLU	4.2
1	B	67	SER	4.2
1	B	15	ARG	4.2
1	B	438	THR	4.2
1	A	30	ILE	4.2
1	B	28	VAL	4.2
1	B	213	VAL	4.2
1	A	229	THR	4.2
1	A	330	LEU	4.2
1	A	131	PRO	4.2
1	B	244	PRO	4.2
1	B	228	CYS	4.1
1	A	46	GLU	4.1
1	A	113	GLY	4.1
1	A	122	MET	4.1
1	B	202	ILE	4.1
1	B	372	CYS	4.1
1	A	151	GLY	4.1
1	A	299	VAL	4.1
1	B	258	ALA	4.1
1	A	163	GLY	4.1
1	B	149	LYS	4.1
1	A	218	GLY	4.1
1	A	174	LYS	4.1
1	B	295	VAL	4.1
1	A	391	ILE	4.1
1	B	419	ILE	4.1
1	B	125	ALA	4.1
1	B	447	MET	4.1
1	A	180	PHE	4.1
1	A	321	LEU	4.1
1	A	421	PHE	4.0
1	A	184	GLU	4.0
1	A	127	VAL	4.0
1	B	107	GLN	4.0
1	B	277	TYR	4.0
1	B	214	GLY	4.0
1	B	55	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	201	PHE	4.0
1	A	382	TYR	4.0
1	B	226	ARG	4.0
1	A	109	ILE	4.0
1	B	171	ARG	3.9
1	A	62	ILE	3.9
1	A	111	LYS	3.9
1	A	141	SER	3.9
1	B	91	ALA	3.9
1	A	352	PRO	3.9
1	B	111	LYS	3.9
1	B	290	ASN	3.9
1	A	287	MET	3.9
1	B	23	LEU	3.9
1	A	331	THR	3.9
1	B	360	ALA	3.9
1	B	83	PHE	3.9
1	A	446	ILE	3.8
1	B	26	GLN	3.8
1	B	413	LEU	3.8
1	B	252[A]	ARG	3.8
1	B	130	VAL	3.8
1	A	245	ILE	3.8
1	A	424	LYS	3.8
1	B	49	CYS	3.8
1	B	4	VAL	3.8
1	A	34	GLY	3.8
1	B	31	TYR	3.8
1	B	76	GLY	3.8
1	B	229	THR	3.8
1	A	413	LEU	3.8
1	B	311	LEU	3.8
1	B	376	TYR	3.8
1	B	326	GLU	3.8
1	A	290	ASN	3.8
1	B	99	LEU	3.8
1	B	117	VAL	3.8
1	A	308	LEU	3.8
1	B	86	GLU	3.8
1	A	258	ALA	3.7
1	B	304	THR	3.7
1	A	302	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	51	GLY	3.7
1	A	39	LEU	3.7
1	B	218	GLY	3.7
1	A	328	ILE	3.7
1	A	66	LEU	3.7
1	A	76	GLY	3.7
1	A	88	ALA	3.7
1	B	174	LYS	3.7
1	B	270	ALA	3.7
1	A	254	MET	3.7
1	A	365	GLY	3.6
1	B	192	GLY	3.6
1	A	38	ALA	3.6
1	B	95	GLU	3.6
1	A	429	ASP	3.6
1	A	367	ARG	3.6
1	B	210	ILE	3.6
1	A	83	PHE	3.6
1	B	434	GLY	3.6
1	A	96	ALA	3.6
1	B	416	ASP	3.6
1	B	268	GLU	3.6
1	A	64	ASN	3.6
1	A	286	PHE	3.5
1	A	341	ALA	3.5
1	B	144	LYS	3.5
1	B	365	GLY	3.5
1	A	31	TYR	3.5
1	A	159	THR	3.5
1	A	297	HIS	3.5
1	A	85	ALA	3.5
1	A	294	GLN	3.5
1	B	260	ARG	3.5
1	A	263	LYS	3.5
1	A	189	THR	3.5
1	B	78	HIS	3.5
1	B	248	ASP	3.5
1	A	210	ILE	3.5
1	B	287	MET	3.5
1	A	316	ALA	3.5
1	B	44	ALA	3.5
1	B	90	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	63	PRO	3.4
1	A	168	ARG	3.4
1	B	66	LEU	3.4
1	A	406	ALA	3.4
1	B	25	ILE	3.4
1	B	391	ILE	3.4
1	A	22	ASP	3.4
1	A	228	CYS	3.4
1	A	261	ALA	3.4
1	A	376	TYR	3.4
1	B	439	ASN	3.4
1	A	15	ARG	3.4
1	B	367	ARG	3.4
1	B	321	LEU	3.4
1	A	200	LYS	3.4
1	A	260	ARG	3.4
1	A	247	ASP	3.4
1	A	385	MET	3.4
1	A	204	ASN	3.4
1	A	59	TYR	3.4
1	A	203	GLU	3.4
1	A	265	VAL	3.3
1	A	420	PRO	3.3
1	B	63	PRO	3.3
1	B	120	ALA	3.3
1	B	65	ILE	3.3
1	B	432	ARG	3.3
1	B	58	SER	3.3
1	B	449	ASP	3.3
1	B	205	PHE	3.3
1	B	151	GLY	3.3
1	B	400	ILE	3.3
1	B	364	TYR	3.3
1	A	191	PHE	3.3
1	A	213	VAL	3.3
1	A	149	LYS	3.3
1	B	16	ILE	3.3
1	A	75	ASP	3.3
1	B	157	LYS	3.2
1	B	298	PRO	3.3
1	A	25	ILE	3.2
1	B	13	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	296	GLU	3.2
1	A	309	VAL	3.2
1	B	346	LYS	3.2
1	A	447	MET	3.2
1	B	289	MET	3.2
1	A	273	ILE	3.2
1	A	3	LYS	3.2
1	A	388	LYS	3.2
1	B	184	GLU	3.2
1	A	79	PRO	3.2
1	B	271	GLY	3.2
1	A	33	GLU	3.2
1	A	336	GLU	3.2
1	B	89	ASP	3.2
1	B	108	SER	3.2
1	B	427	ASN	3.2
1	A	374	THR	3.2
1	A	386	VAL	3.2
1	B	79	PRO	3.1
1	B	335	ILE	3.1
1	A	84	LEU	3.1
1	A	239	GLU	3.1
1	B	301	GLU	3.1
1	A	392	HIS	3.1
1	B	102	ILE	3.1
1	B	129	VAL	3.1
1	A	91	ALA	3.1
1	B	371	ALA	3.1
1	B	278	ASP	3.1
1	A	280	ASN	3.1
1	B	286	PHE	3.1
1	B	21	ARG	3.1
1	B	272	THR	3.1
1	B	11	GLU	3.1
1	A	51	GLY	3.1
1	A	42	GLN	3.1
1	B	211	GLN	3.1
1	B	239	GLU	3.1
1	B	428	ASN	3.0
1	B	418	THR	3.0
1	B	132	GLY	3.0
1	B	361	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	188	GLN	3.0
1	B	122	MET	3.0
1	A	207	HIS	3.0
1	A	162	GLY	3.0
1	B	282	ASN	3.0
1	B	3	LYS	3.0
1	A	52	PRO	3.0
1	B	59	TYR	3.0
1	B	336	GLU	3.0
1	A	135	GLY	3.0
1	B	9	ARG	3.0
1	B	61	ASN	3.0
1	A	23	LEU	2.9
1	B	92	GLU	2.9
1	A	370	SER	2.9
1	A	432	ARG	2.9
1	A	349	MET	2.9
1	A	236	LYS	2.9
1	B	124	LYS	2.9
1	A	26	GLN	2.9
1	B	347	ASN	2.9
1	B	378	ILE	2.9
1	B	20	CYS	2.9
1	A	112	MET	2.9
1	B	7	ALA	2.9
1	A	296	GLU	2.9
1	A	306	ILE	2.9
1	B	109	ILE	2.9
1	A	278	ASP	2.9
1	A	44	ALA	2.8
1	A	264	ALA	2.8
1	A	53	THR	2.8
1	A	267	TYR	2.8
1	A	95	GLU	2.8
1	A	427	ASN	2.8
1	A	428	ASN	2.8
1	A	350	PRO	2.8
1	B	344	PRO	2.8
1	B	394	PRO	2.8
1	A	119	LYS	2.8
1	A	304	THR	2.8
1	A	209	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	275	PHE	2.8
1	A	61	ASN	2.8
1	B	312	GLN	2.8
1	B	420	PRO	2.8
1	A	423	ILE	2.8
1	B	240	GLU	2.8
1	B	358	TYR	2.8
1	B	46	GLU	2.8
1	A	90	PHE	2.8
1	A	298	PRO	2.8
1	A	301	GLU	2.8
1	A	146	ILE	2.8
1	A	202	ILE	2.8
1	A	320	VAL	2.8
1	A	222	HIS	2.7
1	A	58	SER	2.7
1	B	188	GLN	2.7
1	A	118	ALA	2.7
1	A	399	ALA	2.7
1	B	415	ILE	2.7
1	B	423	ILE	2.7
1	B	138	LYS	2.7
1	B	392	HIS	2.7
1	A	323	TYR	2.7
1	A	358	TYR	2.7
1	B	262	ALA	2.7
1	B	300	THR	2.7
1	A	6	ILE	2.7
1	A	244	PRO	2.7
1	A	344	PRO	2.7
1	A	419	ILE	2.7
1	B	431	PHE	2.7
1	B	333	HIS	2.7
1	B	443	GLN	2.7
1	A	340	ASN	2.7
1	A	400	ILE	2.7
1	B	212	ILE	2.7
1	B	224	GLY	2.7
1	A	197	TYR	2.7
1	A	18	ARG	2.7
1	A	8	ASN	2.7
1	A	269	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	324	LYS	2.7
1	B	56	LYS	2.7
1	A	411	VAL	2.6
1	B	24	GLY	2.6
1	B	207	HIS	2.6
1	A	4	VAL	2.6
1	A	166	GLY	2.6
1	B	18	ARG	2.6
1	B	382	TYR	2.6
1	B	444	ASN	2.6
1	A	272	THR	2.6
1	B	70	THR	2.6
1	B	146	ILE	2.6
1	A	147	ALA	2.6
1	A	433	SER	2.6
1	B	189	THR	2.6
1	A	24	GLY	2.6
1	A	418	THR	2.6
1	B	236	LYS	2.6
1	A	231	GLN	2.6
1	B	231	GLN	2.6
1	A	338	ARG	2.6
1	A	256	ASN	2.5
1	B	350	PRO	2.5
1	A	371	ALA	2.5
1	B	88	ALA	2.5
1	B	209	GLU	2.5
1	A	312	GLN	2.5
1	B	136	LEU	2.5
1	A	430	ILE	2.5
1	A	346	LYS	2.5
1	B	145	LYS	2.5
1	B	159	THR	2.5
1	B	385	MET	2.5
1	B	284	PHE	2.5
1	A	226	ARG	2.5
1	A	444	ASN	2.5
1	A	123	ILE	2.5
1	A	187	ALA	2.5
1	B	357	GLN	2.5
1	A	439	ASN	2.4
1	B	353	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	84	LEU	2.4
1	A	169	VAL	2.4
1	B	112	MET	2.4
1	B	261	ALA	2.4
1	B	403	GLY	2.4
1	A	279	LEU	2.4
1	A	77	VAL	2.4
1	A	32	SER	2.4
1	A	105	SER	2.4
1	A	74	CYS	2.4
1	A	246	LEU	2.4
1	A	227	ASP	2.4
1	B	433	SER	2.4
1	A	333	HIS	2.4
1	A	186	GLU	2.4
1	B	388	LYS	2.4
1	B	325	GLN	2.4
1	B	166	GLY	2.4
1	A	285	TYR	2.4
1	B	283	LYS	2.3
1	B	370	SER	2.3
1	B	349	MET	2.3
1	B	94	CYS	2.3
1	B	206	ARG	2.3
1	B	316	ALA	2.3
1	A	28	VAL	2.3
1	A	129	VAL	2.3
1	A	108	SER	2.3
1	A	224	GLY	2.3
1	A	21	ARG	2.3
1	B	242	PRO	2.3
1	A	274	GLU	2.3
1	B	203	GLU	2.3
1	A	305	GLY	2.3
1	B	37	ASP	2.3
1	A	121	GLU	2.3
1	B	38	ALA	2.3
1	A	271	GLY	2.3
1	A	292	ARG	2.3
1	B	34	GLY	2.3
1	A	257	ALA	2.3
1	B	292	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	313	LEU	2.3
1	A	363	GLY	2.2
1	A	354	LYS	2.2
1	B	251	ARG	2.2
1	A	116	ASP	2.2
1	B	57	ASP	2.2
1	A	177	GLU	2.2
1	A	100	LYS	2.2
1	A	377	THR	2.2
1	A	310	LYS	2.2
1	A	289	MET	2.2
1	A	364	TYR	2.2
1	B	291	THR	2.2
1	B	354	LYS	2.2
1	A	442	GLU	2.2
1	A	414	GLY	2.2
1	A	379	PRO	2.2
1	B	279	LEU	2.2
1	B	197	TYR	2.2
1	B	169	VAL	2.2
1	B	96	ALA	2.2
1	A	132	GLY	2.1
1	A	291	THR	2.1
1	A	372	CYS	2.1
1	A	334	ALA	2.1
1	A	16	ILE	2.1
1	B	221	ILE	2.1
1	B	324	LYS	2.1
1	A	138	LYS	2.1
1	A	332	GLY	2.1
1	B	39	LEU	2.1
1	A	326	GLU	2.1
1	A	20	CYS	2.1
1	B	241	ALA	2.1
1	B	322	PRO	2.1
1	B	332	GLY	2.1
1	A	11	GLU	2.1
1	B	246	LEU	2.1
1	B	177	GLU	2.1
1	B	308	LEU	2.1
1	A	288	GLU	2.1
1	B	269	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	222	HIS	2.0
1	B	379	PRO	2.0
1	A	73	GLY	2.0
1	A	41	THR	2.0
1	B	411	VAL	2.0
1	B	74	CYS	2.0
1	B	256	ASN	2.0
1	B	422	HIS	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
4	CL	A	1452	1/1	0.79	0.61	9.05	32,32,32,32	0
4	CL	B	1453	1/1	0.53	0.52	3.51	36,36,36,36	0
2	ANP	A	1449	31/31	0.66	0.25	-0.86	15,21,24,25	0
2	ANP	B	1450	31/31	0.72	0.23	-1.05	21,23,24,25	0
3	MG	A	1451	1/1	0.71	0.20	-1.80	18,18,18,18	0
3	MG	B	1452	1/1	0.58	0.16	-2.04	27,27,27,27	0
3	MG	B	1451	1/1	0.63	0.17	-2.92	29,29,29,29	0
3	MG	A	1450	1/1	0.80	0.10	-	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.