



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:29 AM UTC

PDB ID : 4B1Z / pdb_00004b1z
Title : Structure of the Phactr1 RPEL domain bound to G-actin
Authors : Mouilleron, S.; Wielek, M.; O'Reilly, N.; Treisman, R.; McDonald, N.Q.
Deposited on : 2012-07-12
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

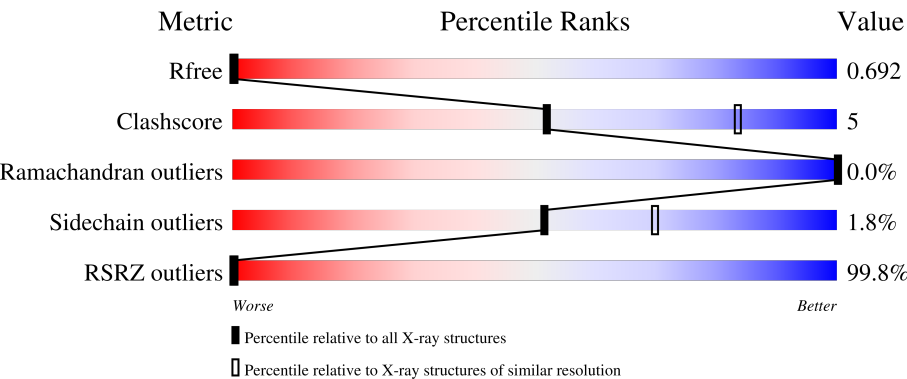
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	376	89% 78%10%•11%
1	B	376	95% 84%10%•5%
1	C	376	98% 87%10%••
1	D	376	95% 82%12%•5%
1	E	376	95% 83%12%•5%

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Mol	Chain	Length	Quality of chain
1	F	376	95% 81% 13% • 5%
2	M	115	96% 74% 18% • •
2	N	115	93% 76% 15% • 7%

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
3	ATP	D	1376	-	-	-	X
5	GOL	A	1379	-	-	-	X
5	GOL	B	1378	-	-	-	X
5	GOL	C	1379	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17941 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.

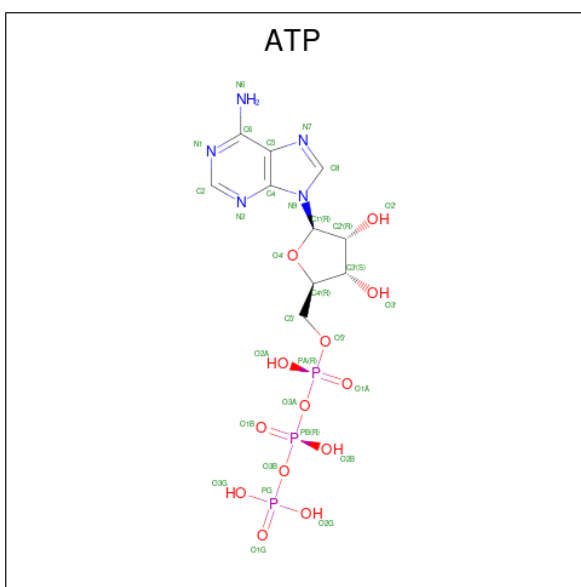
- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2495	1588	415	474	18			
1	B	357	Total	C	N	O	S	0	0	0
			2711	1721	448	523	19			
1	C	370	Total	C	N	O	S	0	0	0
			2815	1787	476	532	20			
1	D	356	Total	C	N	O	S	0	0	0
			2648	1675	446	508	19			
1	E	359	Total	C	N	O	S	0	0	0
			2682	1701	450	512	19			
1	F	357	Total	C	N	O	S	0	0	0
			2682	1706	444	513	19			

- Molecule 2 is a protein called PHOSPHATASE AND ACTIN REGULATOR 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	110	Total	C	N	O	0	0	0
			846	517	166	163			
2	N	107	Total	C	N	O	0	0	0
			821	505	159	157			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		

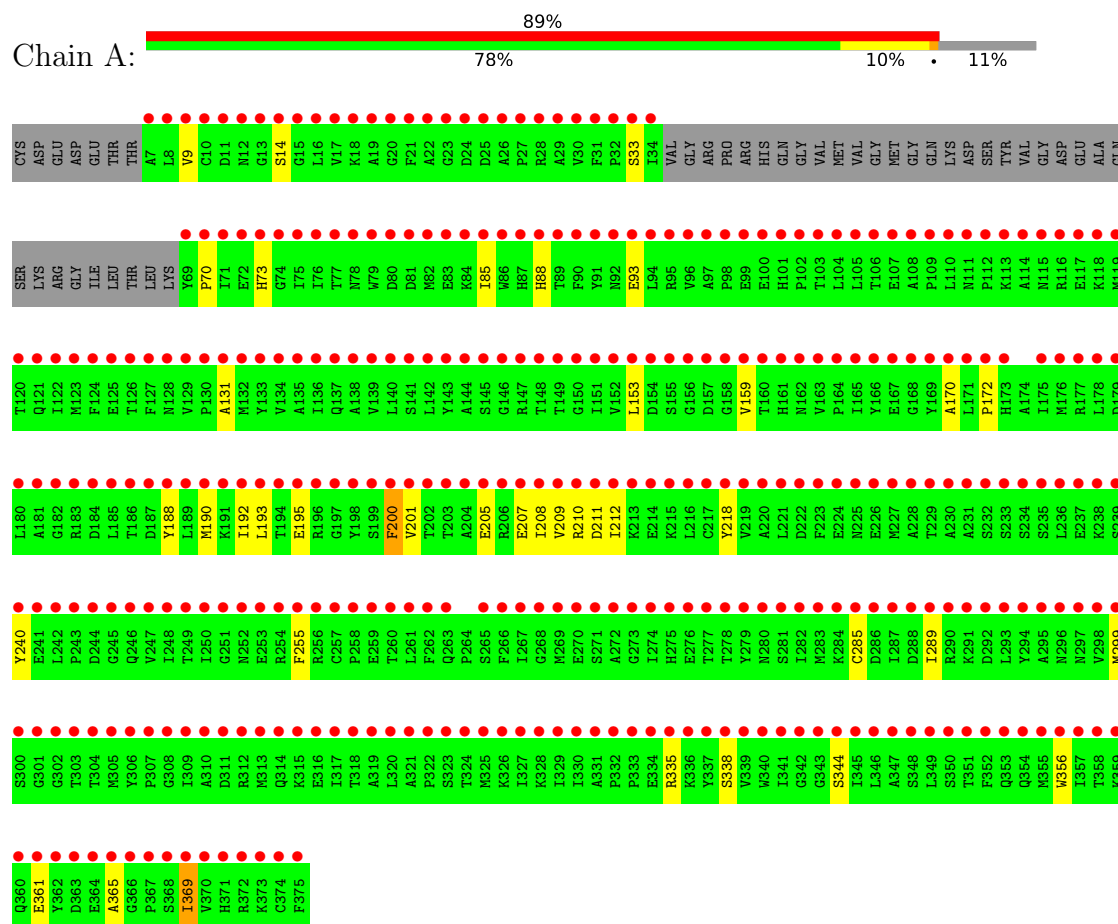
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	O	0	0
			1	1		

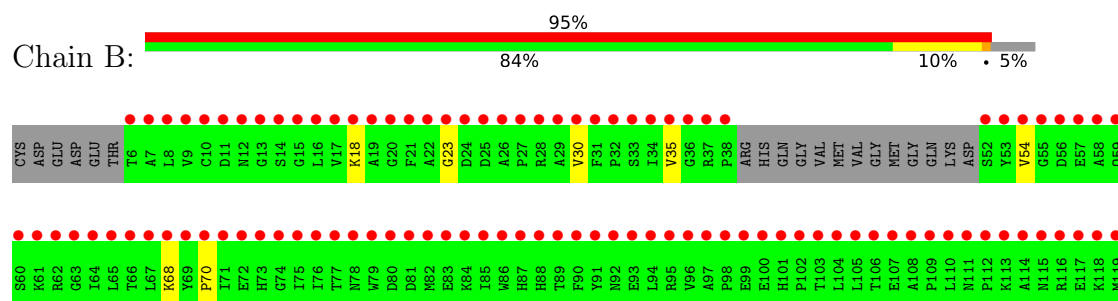
3 Residue-property plots

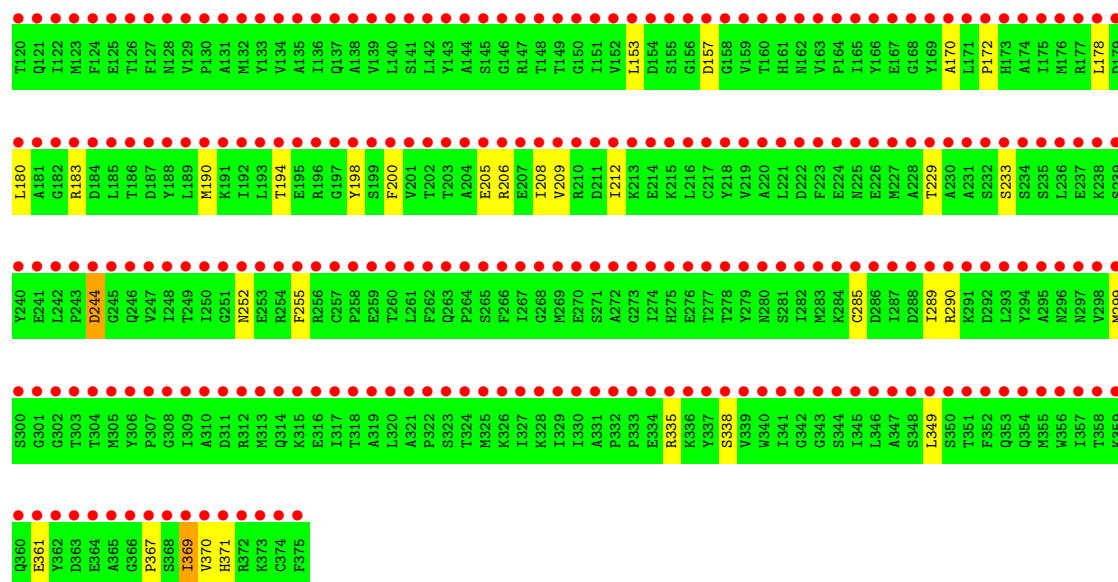
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ACTIN, ALPHA SKELETAL MUSCLE



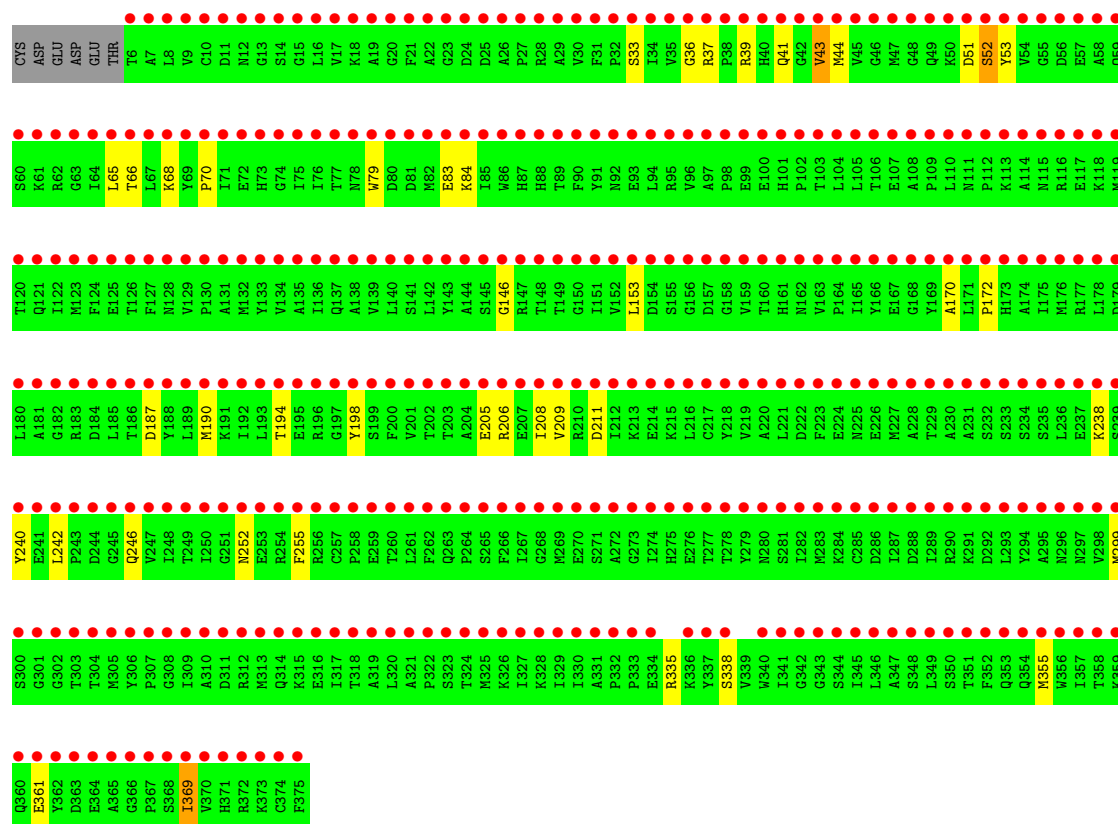
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE





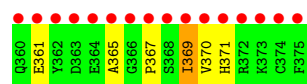
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain C: 98% 87% 10% ..

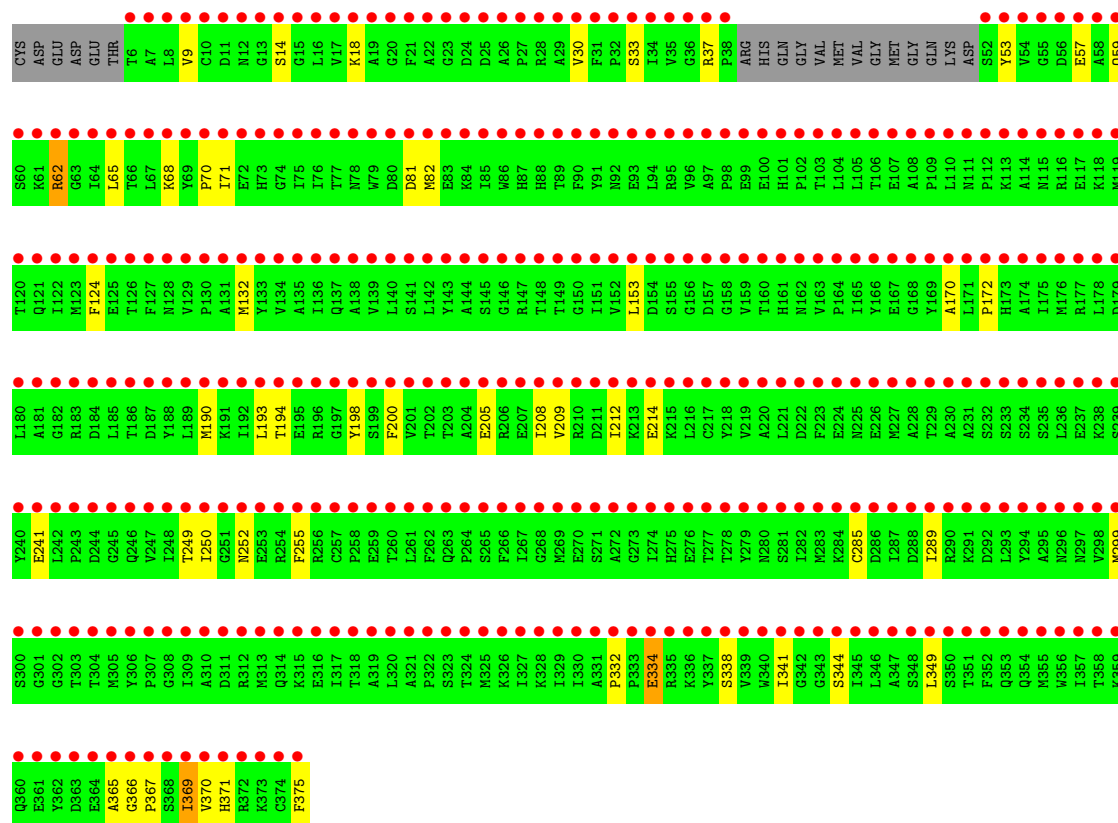
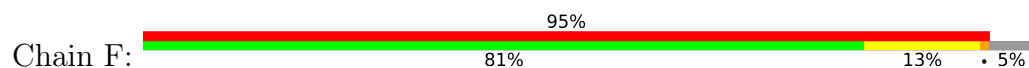


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

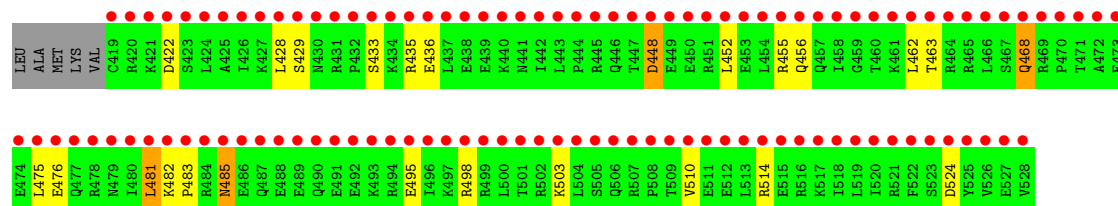
Chain D: 95% 82% 12% • 5%



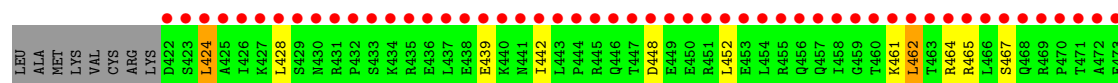
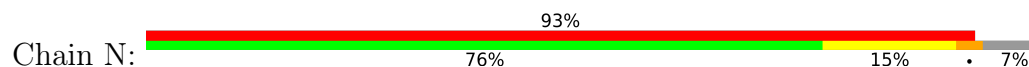
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1



• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1



E474	E475	E476	Q477	R478	R479	I480	L481	K482	P483	R484	M485	E486	Q487	E488	E489	Q490	E491	E492	K493	R494	E495	I496	K497	R498	R499	L500	T501	R502	K503	L504	S505	Q506	R507	P508	T509	V510	E511	E512	L513	R514	E515	R516	K517	I518	L519	I520	R521	F522	S523	D524	Y525	V526	E527	V528
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.06Å 142.89Å 184.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.62 – 3.30 74.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (74.62-3.30) 96.7 (74.62-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.213 , 0.236 0.685 , 0.692	Depositor DCC
R_{free} test set	2580 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.57	EDS
Total number of atoms	17941	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: GOL, ATP, MG

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	0.33	0/2552	0.83	2/3480 (0.1%)
1	B	0.33	0/2772	0.79	1/3774 (0.0%)
1	C	0.32	0/2878	0.80	0/3911
1	D	0.32	0/2706	0.84	4/3685 (0.1%)
1	E	0.34	0/2742	0.82	0/3738
1	F	0.34	0/2742	0.82	1/3736 (0.0%)
2	M	0.27	0/851	0.79	0/1148
2	N	0.26	0/827	0.77	0/1115
All	All	0.33	0/18070	0.81	8/24587 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	366	GLY	CA-C-N	6.57	126.26	119.56
1	D	366	GLY	C-N-CA	6.57	126.26	119.56
1	D	200	PHE	N-CA-C	5.68	117.32	109.54
1	A	200	PHE	N-CA-C	5.45	117.48	108.49
1	D	202	THR	N-CA-C	5.42	117.87	110.55
1	F	200	PHE	N-CA-C	5.18	116.64	109.54
1	B	200	PHE	N-CA-C	5.12	116.56	109.54
1	A	201	VAL	N-CA-C	5.11	119.56	112.35

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	2495	0	2353	21	0
1	B	2711	0	2582	27	0
1	C	2815	0	2724	30	0
1	D	2648	0	2476	30	0
1	E	2682	0	2525	35	0
1	F	2682	0	2550	35	0
2	M	846	0	814	13	0
2	N	821	0	787	12	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	3	0
3	E	31	0	12	1	0
3	F	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	E	6	0	8	1	0
5	F	6	0	8	0	0
5	N	6	0	8	0	0
6	E	1	0	0	0	0
All	All	17941	0	16947	179	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 5.

All (179) 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:E:146:GLY:O	2:N:465:ARG:NH1	2.04	0.89
1:F:371:HIS:HB3	2:N:527:GLU:HG3	1.58	0.84
1:D:62:ARG:HB2	1:D:67:LEU:HD11	1.63	0.80
1:C:41:GLN:O	1:E:28:ARG:NH2	2.14	0.80
1:C:39:ARG:HG2	1:C:66:THR:HG23	1.67	0.77
1:A:153:LEU:HD23	1:A:299:MET:HE3	1.76	0.67
1:D:157:ASP:OD2	1:D:183:ARG:NH2	2.27	0.66
1:E:70:PRO:HG3	1:E:81:ASP:HB3	1.77	0.65
1:E:39:ARG:HG2	1:E:66:THR:HG23	1.77	0.65
1:C:153:LEU:HD23	1:C:299:MET:HE3	1.79	0.65
1:C:246:GLN:HG3	1:F:249:THR:OG1	1.97	0.65
1:B:370:VAL:HG13	1:B:371:HIS:HD2	1.62	0.64
1:A:211:ASP:OD2	1:A:240:TYR:OH	2.16	0.63
2:M:433:SER:HB3	2:M:436:GLU:HG3	1.82	0.61
1:F:53:TYR:HD2	1:F:65:LEU:HD21	1.65	0.60
1:F:153:LEU:HD23	1:F:299:MET:HE3	1.84	0.60
1:D:335:ARG:HA	1:D:338:SER:HB3	1.84	0.60
1:E:370:VAL:HG13	1:E:371:HIS:HD2	1.66	0.59
1:F:53:TYR:CD2	1:F:65:LEU:HD21	2.37	0.59
1:F:190:MET:HG2	1:F:209:VAL:HG21	1.83	0.59
1:D:59:GLN:O	1:D:62:ARG:HB3	2.03	0.58
1:E:199:SER:N	5:E:1378:GOL:O1	2.37	0.58
1:A:335:ARG:HA	1:A:338:SER:HB3	1.85	0.58
1:D:153:LEU:HD23	1:D:299:MET:HE3	1.88	0.56
1:A:190:MET:HE3	1:A:200:PHE:O	2.06	0.56
1:E:180:LEU:HD21	1:E:260:THR:HG22	1.88	0.56
1:A:14:SER:N	3:A:1376:ATP:O1G	2.26	0.56
1:E:205:GLU:HA	1:E:208:ILE:HG22	1.88	0.55
1:F:59:GLN:O	1:F:62:ARG:HB3	2.07	0.55
1:B:23:GLY:HA2	2:M:455:ARG:NH2	2.22	0.54
1:D:287:ILE:HG12	1:D:290:ARG:NH1	2.23	0.54
1:E:324:THR:HG21	1:F:57:GLU:HA	1.89	0.54
1:B:190:MET:HG2	1:B:209:VAL:HG21	1.89	0.54
1:D:9:VAL:HG21	1:D:344:SER:HA	1.90	0.54
1:F:365:ALA:HB3	1:F:369:ILE:HB	1.89	0.54
1:E:153:LEU:HD23	1:E:299:MET:HE3	1.89	0.54
1:E:183:ARG:HG2	1:E:206:ARG:HH22	1.72	0.54
2:M:485:ASN:N	2:M:485:ASN:OD1	2.39	0.54
1:D:146:GLY:HA2	2:N:424:LEU:HD23	1.90	0.54
1:E:207:GLU:HG2	1:E:210:ARG:HH21	1.72	0.54
1:F:14:SER:N	3:F:1376:ATP:O1G	2.34	0.54
1:C:53:TYR:HD2	1:C:65:LEU:CD2	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:PRO:HG3	1:F:81:ASP:HB3	1.91	0.53
1:F:241:GLU:OE1	2:N:464:ARG:NH2	2.41	0.53
1:F:194:THR:HA	1:F:198:TYR:O	2.09	0.53
2:M:510:VAL:HG12	2:M:514:ARG:HE	1.74	0.53
1:A:70:PRO:HG2	1:A:85:ILE:HD11	1.89	0.53
1:D:324:THR:HG21	1:E:57:GLU:HA	1.91	0.53
1:C:211:ASP:OD2	1:C:240:TYR:OH	2.22	0.52
1:F:332:PRO:HB2	1:F:334:GLU:OE2	2.10	0.52
1:C:36:GLY:O	1:C:52:SER:HA	2.09	0.52
1:D:367:PRO:O	1:D:370:VAL:HG12	2.10	0.52
1:A:365:ALA:HB3	1:A:369:ILE:HB	1.92	0.52
1:D:33:SER:O	1:D:33:SER:OG	2.28	0.52
1:F:170:ALA:O	1:F:172:PRO:HD3	2.11	0.51
1:C:194:THR:HA	1:C:198:TYR:O	2.10	0.51
1:E:306:TYR:CE1	3:E:1376:ATP:H2	2.29	0.51
1:B:349:LEU:HD13	2:M:463:THR:HG23	1.92	0.51
1:F:205:GLU:O	1:F:209:VAL:HG23	2.10	0.51
1:B:68:LYS:O	1:B:70:PRO:HD3	2.11	0.50
1:D:157:ASP:OD1	3:D:1376:ATP:O3'	2.29	0.50
1:E:194:THR:HA	1:E:198:TYR:O	2.10	0.50
1:C:205:GLU:O	1:C:209:VAL:HG23	2.12	0.50
1:B:153:LEU:HD23	1:B:299:MET:HE3	1.93	0.50
1:E:39:ARG:HG3	1:E:65:LEU:HA	1.94	0.50
1:F:33:SER:O	1:F:33:SER:OG	2.28	0.50
1:A:33:SER:O	1:A:33:SER:OG	2.29	0.49
1:E:146:GLY:HA2	2:N:462:LEU:HD23	1.95	0.49
1:C:170:ALA:O	1:C:172:PRO:HD3	2.11	0.49
2:M:495:GLU:OE2	2:M:498:ARG:NH1	2.45	0.49
1:B:194:THR:HA	1:B:198:TYR:O	2.13	0.49
1:E:170:ALA:O	1:E:172:PRO:HD3	2.13	0.49
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.95	0.48
1:B:18:LYS:HG3	1:B:30:VAL:HG22	1.94	0.48
1:F:18:LYS:HG3	1:F:30:VAL:HG22	1.94	0.48
2:N:464:ARG:O	2:N:467:SER:OG	2.25	0.48
1:E:33:SER:O	1:E:33:SER:OG	2.28	0.48
1:D:289:ILE:HD11	2:N:442:ILE:HG12	1.94	0.48
1:F:214:GLU:O	2:N:478:ARG:NH1	2.39	0.48
1:D:70:PRO:HG3	1:D:81:ASP:HB3	1.95	0.48
1:E:252:ASN:HA	1:E:255:PHE:CE1	2.49	0.48
1:B:170:ALA:O	1:B:172:PRO:HD3	2.14	0.48
1:D:14:SER:N	3:D:1376:ATP:O1G	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:MET:HG2	1:C:209:VAL:HG21	1.94	0.47
1:F:349:LEU:HD11	2:N:500:LEU:HD23	1.95	0.47
1:D:188:TYR:O	1:D:192:ILE:HG12	2.14	0.47
1:C:146:GLY:O	2:M:503:LYS:NZ	2.47	0.47
1:E:183:ARG:HG2	1:E:206:ARG:NH2	2.29	0.47
1:E:208:ILE:O	1:E:212:ILE:HG13	2.14	0.47
1:F:193:LEU:HD21	1:F:250:ILE:HG13	1.97	0.47
2:M:452:LEU:O	2:M:456:GLN:HG2	2.14	0.47
1:D:68:LYS:O	1:D:70:PRO:HD3	2.15	0.47
1:A:170:ALA:O	1:A:172:PRO:HD3	2.15	0.46
1:B:157:ASP:OD1	3:B:1376:ATP:O3'	2.30	0.46
1:B:229:THR:HG23	1:D:367:PRO:HD2	1.96	0.46
2:N:485:ASN:ND2	2:N:488:GLU:OE1	2.48	0.46
1:E:285:CYS:HB3	1:E:289:ILE:HD11	1.97	0.46
1:E:370:VAL:HG13	1:E:371:HIS:CD2	2.49	0.46
1:E:205:GLU:O	1:E:209:VAL:HG23	2.15	0.46
1:F:367:PRO:O	1:F:370:VAL:HG12	2.16	0.46
2:M:482:LYS:HA	2:M:483:PRO:HD3	1.84	0.46
1:A:207:GLU:CD	1:A:210:ARG:HH21	2.24	0.46
1:C:36:GLY:HA3	1:C:65:LEU:HD13	1.98	0.46
1:F:252:ASN:HA	1:F:255:PHE:CE1	2.50	0.46
1:A:205:GLU:O	1:A:209:VAL:HG23	2.15	0.46
1:D:53:TYR:HD2	1:D:65:LEU:HD21	1.81	0.46
1:A:208:ILE:O	1:A:212:ILE:HG13	2.16	0.45
1:F:71:ILE:HD11	1:F:82:MET:SD	2.55	0.45
1:B:361:GLU:HB3	1:B:369:ILE:HD13	1.97	0.45
1:D:205:GLU:O	1:D:209:VAL:HG23	2.16	0.45
1:B:370:VAL:HG13	1:B:371:HIS:CD2	2.47	0.45
1:C:68:LYS:O	1:C:70:PRO:HD3	2.16	0.45
1:F:68:LYS:O	1:F:70:PRO:HD3	2.17	0.45
1:B:367:PRO:O	1:B:370:VAL:HG12	2.17	0.45
1:D:170:ALA:O	1:D:172:PRO:HD3	2.16	0.45
1:F:208:ILE:O	1:F:212:ILE:HG13	2.16	0.45
1:B:178:LEU:HG	1:B:180:LEU:HB3	1.98	0.45
1:F:366:GLY:O	1:F:369:ILE:HG22	2.17	0.45
2:M:448:ASP:OD1	2:M:448:ASP:N	2.49	0.45
1:A:73:HIS:HA	1:A:159:VAL:HB	1.97	0.45
1:A:131:ALA:HB1	1:A:356:TRP:HB3	1.99	0.45
1:D:252:ASN:HA	1:D:255:PHE:CE1	2.52	0.44
1:B:233:SER:HB2	1:D:363:ASP:HA	1.99	0.44
1:C:361:GLU:HB3	1:C:369:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG21	1:A:344:SER:HA	1.99	0.44
1:C:33:SER:O	1:C:33:SER:OG	2.29	0.44
1:C:238:LYS:HD3	2:M:468:GLN:NE2	2.33	0.44
2:M:476:GLU:HG2	2:M:481:LEU:HB3	1.99	0.44
1:D:275:HIS:CE1	1:D:276:GLU:HG3	2.53	0.44
1:F:37:ARG:O	1:F:65:LEU:HB2	2.18	0.44
1:B:335:ARG:HA	1:B:338:SER:HB3	1.99	0.44
1:C:37:ARG:HH22	1:C:84:LYS:HE3	1.83	0.44
1:C:51:ASP:O	1:C:52:SER:OG	2.26	0.44
1:C:53:TYR:HD2	1:C:65:LEU:HD21	1.83	0.43
1:C:187:ASP:OD1	1:C:206:ARG:NH2	2.40	0.43
1:E:189:LEU:HD13	1:E:257:CYS:HB2	1.99	0.43
1:E:71:ILE:HD11	1:E:82:MET:SD	2.59	0.43
1:B:35:VAL:HG22	1:B:54:VAL:HG22	2.00	0.43
1:C:208:ILE:HG21	1:C:242:LEU:HD22	1.99	0.43
1:E:324:THR:HG21	1:F:57:GLU:CA	2.48	0.43
1:F:285:CYS:HB3	1:F:289:ILE:HD11	2.02	0.42
1:C:252:ASN:HA	1:C:255:PHE:CE1	2.53	0.42
1:E:226:GLU:HB3	1:E:255:PHE:CE2	2.54	0.42
1:C:44:MET:HE3	1:D:280:ASN:HB3	2.02	0.42
1:E:335:ARG:HA	1:E:338:SER:HB3	2.01	0.42
1:D:116:ARG:HH12	1:D:371:HIS:HA	1.84	0.42
1:B:205:GLU:O	1:B:209:VAL:HG23	2.19	0.42
1:B:285:CYS:HB3	1:B:289:ILE:HD11	2.02	0.42
1:C:44:MET:HE1	1:D:284:LYS:HE2	2.00	0.42
1:B:252:ASN:HA	1:B:255:PHE:CE1	2.54	0.42
1:B:349:LEU:HD11	2:M:462:LEU:HD23	2.02	0.42
1:C:335:ARG:HA	1:C:338:SER:HB3	2.01	0.42
1:F:9:VAL:HG21	1:F:344:SER:HA	2.02	0.42
1:F:375:PHE:C	2:N:507:ARG:HH22	2.26	0.42
1:A:88:HIS:CD2	1:A:93:GLU:HG2	2.55	0.42
1:F:124:PHE:CZ	1:F:132:MET:HG3	2.55	0.42
1:D:366:GLY:O	1:D:369:ILE:HG22	2.20	0.41
1:E:68:LYS:O	1:E:70:PRO:HD3	2.20	0.41
1:C:79:TRP:O	1:C:83:GLU:HG3	2.20	0.41
1:E:365:ALA:HB3	1:E:369:ILE:HB	2.02	0.41
1:D:18:LYS:HG3	1:D:30:VAL:HG22	2.02	0.41
1:B:190:MET:HG3	1:B:209:VAL:HG11	2.01	0.41
1:D:306:TYR:CE1	3:D:1376:ATP:H2	2.38	0.41
1:E:367:PRO:O	1:E:370:VAL:HG12	2.20	0.41
1:B:285:CYS:O	1:B:290:ARG:NH2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:SER:HA	1:F:341:ILE:HD12	2.03	0.41
1:C:65:LEU:HD12	1:C:65:LEU:O	2.20	0.41
1:F:193:LEU:HD23	1:F:193:LEU:HA	1.95	0.41
1:A:193:LEU:HD13	1:A:200:PHE:CE2	2.56	0.41
1:A:218:TYR:O	1:A:255:PHE:HA	2.21	0.41
1:B:208:ILE:O	1:B:212:ILE:HG13	2.21	0.41
1:B:244:ASP:N	1:B:244:ASP:OD1	2.53	0.41
1:C:43:VAL:HG22	1:E:28:ARG:HD2	2.01	0.41
1:E:361:GLU:HB3	1:E:369:ILE:HD13	2.03	0.41
2:N:491:GLU:CD	2:N:494:ARG:HH12	2.28	0.41
1:A:361:GLU:HB3	1:A:369:ILE:HD13	2.02	0.41
1:C:53:TYR:CD2	1:C:65:LEU:HD21	2.56	0.41
1:A:188:TYR:O	1:A:192:ILE:HG12	2.20	0.40
1:B:183:ARG:HG2	1:B:206:ARG:NH2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	331/376 (88%)	326 (98%)	5 (2%)	0	100	100
1	B	353/376 (94%)	347 (98%)	6 (2%)	0	100	100
1	C	368/376 (98%)	359 (98%)	8 (2%)	1 (0%)	36	65
1	D	352/376 (94%)	346 (98%)	6 (2%)	0	100	100
1	E	355/376 (94%)	348 (98%)	7 (2%)	0	100	100
1	F	353/376 (94%)	346 (98%)	7 (2%)	0	100	100
2	M	108/115 (94%)	105 (97%)	3 (3%)	0	100	100
2	N	105/115 (91%)	102 (97%)	3 (3%)	0	100	100
All	All	2325/2486 (94%)	2279 (98%)	45 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	SER

5.3.2 Protein sidechains ⓘ

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	251/319 (79%)	249 (99%)	2 (1%)	73	79
1	B	281/319 (88%)	279 (99%)	2 (1%)	76	80
1	C	292/319 (92%)	289 (99%)	3 (1%)	68	76
1	D	264/319 (83%)	263 (100%)	1 (0%)	84	84
1	E	270/319 (85%)	267 (99%)	3 (1%)	65	76
1	F	274/319 (86%)	271 (99%)	3 (1%)	65	76
2	M	83/111 (75%)	73 (88%)	10 (12%)	5	20
2	N	80/111 (72%)	71 (89%)	9 (11%)	5	21
All	All	1795/2136 (84%)	1762 (98%)	33 (2%)	51	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	369	ILE
1	B	244	ASP
1	B	369	ILE
1	C	43	VAL
1	C	355	MET
1	C	369	ILE
1	D	62	ARG
1	E	208	ILE
1	E	297	ASN
1	E	369	ILE
1	F	62	ARG
1	F	334	GLU

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Mol	Chain	Res	Type
1	F	369	ILE
2	M	422	ASP
2	M	428	LEU
2	M	429	SER
2	M	435	ARG
2	M	448	ASP
2	M	468	GLN
2	M	475	LEU
2	M	481	LEU
2	M	485	ASN
2	M	524	ASP
2	N	424	LEU
2	N	428	LEU
2	N	439	GLU
2	N	448	ASP
2	N	452	LEU
2	N	461	LYS
2	N	462	LEU
2	N	475	LEU
2	N	527	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	88	HIS
1	B	161	HIS
1	B	162	ASN
1	B	371	HIS
1	C	73	HIS
1	D	162	ASN
1	D	297	ASN
1	E	263	GLN
1	E	353	GLN
1	E	371	HIS
1	F	162	ASN
1	F	297	ASN
1	F	353	GLN
2	N	446	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\# Z > 2$
5	GOL	C	1379	-	5,5,5	0.37	0	5,5,5	0.33	0
3	ATP	F	1376	4	32,33,33	1.41	5 (15%)	48,52,52	1.72	9 (18%)
3	ATP	E	1376	4	32,33,33	1.42	5 (15%)	48,52,52	1.68	8 (16%)
5	GOL	A	1378	-	5,5,5	0.39	0	5,5,5	0.23	0
5	GOL	C	1378	-	5,5,5	0.38	0	5,5,5	0.34	0
3	ATP	D	1376	4	32,33,33	1.42	5 (15%)	48,52,52	1.70	9 (18%)
5	GOL	A	1379	-	5,5,5	0.38	0	5,5,5	0.32	0
3	ATP	C	1376	4	32,33,33	1.39	5 (15%)	48,52,52	1.72	9 (18%)
5	GOL	N	1529	-	5,5,5	0.38	0	5,5,5	0.33	0
5	GOL	B	1378	-	5,5,5	0.37	0	5,5,5	0.25	0
3	ATP	A	1376	4	32,33,33	1.40	5 (15%)	48,52,52	1.72	9 (18%)
3	ATP	B	1376	4	32,33,33	1.38	5 (15%)	48,52,52	1.74	10 (20%)
5	GOL	F	1378	-	5,5,5	0.38	0	5,5,5	0.25	0
5	GOL	E	1378	-	5,5,5	0.37	0	5,5,5	0.35	0

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
5	GOL	C	1379	-	-	4/4/4/4	-
3	ATP	F	1376	4	-	0/22/38/38	0/3/3/3
3	ATP	E	1376	4	-	3/22/38/38	0/3/3/3
5	GOL	A	1378	-	-	2/4/4/4	-
5	GOL	C	1378	-	-	2/4/4/4	-
3	ATP	D	1376	4	-	0/22/38/38	0/3/3/3
5	GOL	A	1379	-	-	0/4/4/4	-
3	ATP	C	1376	4	-	1/22/38/38	0/3/3/3
5	GOL	N	1529	-	-	2/4/4/4	-
5	GOL	B	1378	-	-	2/4/4/4	-
3	ATP	A	1376	4	-	0/22/38/38	0/3/3/3
3	ATP	B	1376	4	-	2/22/38/38	0/3/3/3
5	GOL	F	1378	-	-	2/4/4/4	-
5	GOL	E	1378	-	-	2/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1376	ATP	C5-C4	4.75	1.47	1.39
3	D	1376	ATP	C5-C4	4.72	1.47	1.39
3	C	1376	ATP	C5-C4	4.71	1.47	1.39
3	A	1376	ATP	C5-C4	4.69	1.47	1.39
3	F	1376	ATP	C5-C4	4.67	1.47	1.39
3	B	1376	ATP	C5-C4	4.64	1.47	1.39
3	E	1376	ATP	C5-C6	2.82	1.48	1.41
3	D	1376	ATP	C5-C6	2.81	1.48	1.41
3	C	1376	ATP	C5-C6	2.78	1.48	1.41
3	A	1376	ATP	C5-C6	2.77	1.48	1.41
3	F	1376	ATP	C5-C6	2.76	1.48	1.41
3	B	1376	ATP	C5-C6	2.74	1.48	1.41
3	D	1376	ATP	C8-N7	2.41	1.36	1.31
3	E	1376	ATP	C8-N7	2.40	1.36	1.31
3	A	1376	ATP	C8-N7	2.39	1.36	1.31
3	C	1376	ATP	C8-N7	2.38	1.36	1.31
3	B	1376	ATP	C8-N7	2.35	1.36	1.31
3	F	1376	ATP	C8-N7	2.34	1.36	1.31
3	D	1376	ATP	PB-O3B	2.28	1.62	1.59
3	E	1376	ATP	PB-O3B	2.25	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1376	ATP	C5-N7	-2.22	1.35	1.39
3	C	1376	ATP	C5-N7	-2.22	1.35	1.39
3	A	1376	ATP	C5-N7	-2.19	1.35	1.39
3	F	1376	ATP	C5-N7	-2.17	1.35	1.39
3	B	1376	ATP	PB-O3B	2.16	1.61	1.59
3	E	1376	ATP	C5-N7	-2.15	1.35	1.39
3	D	1376	ATP	C5-N7	-2.14	1.35	1.39
3	F	1376	ATP	PB-O3B	2.14	1.61	1.59
3	C	1376	ATP	PB-O3B	2.07	1.61	1.59
3	A	1376	ATP	PB-O3B	2.03	1.61	1.59

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1376	ATP	C5-C4-N3	-5.84	118.68	126.72
3	B	1376	ATP	C5-C4-N3	-5.82	118.70	126.72
3	C	1376	ATP	C5-C4-N3	-5.68	118.89	126.72
3	A	1376	ATP	C5-C4-N3	-5.65	118.94	126.72
3	D	1376	ATP	C5-C4-N3	-5.55	119.07	126.72
3	F	1376	ATP	C5-C4-N3	-5.51	119.13	126.72
3	E	1376	ATP	N3-C4-N9	4.52	134.86	127.17
3	A	1376	ATP	N3-C4-N9	4.50	134.83	127.17
3	B	1376	ATP	N3-C4-N9	4.48	134.78	127.17
3	C	1376	ATP	N3-C4-N9	4.47	134.77	127.17
3	D	1376	ATP	N3-C4-N9	4.47	134.77	127.17
3	F	1376	ATP	N3-C4-N9	4.41	134.67	127.17
3	B	1376	ATP	C2-N3-C4	3.76	121.01	111.83
3	C	1376	ATP	C2-N3-C4	3.70	120.87	111.83
3	B	1376	ATP	C4-C5-N7	-3.65	106.41	110.58
3	A	1376	ATP	C2-N3-C4	3.64	120.71	111.83
3	F	1376	ATP	C2-N3-C4	3.64	120.71	111.83
3	E	1376	ATP	C4-C5-N7	-3.59	106.47	110.58
3	D	1376	ATP	C2-N3-C4	3.56	120.53	111.83
3	C	1376	ATP	C4-C5-N7	-3.53	106.54	110.58
3	E	1376	ATP	C2-N3-C4	3.49	120.36	111.83
3	F	1376	ATP	C4-C5-N7	-3.48	106.61	110.58
3	D	1376	ATP	C4-C5-N7	-3.43	106.66	110.58
3	A	1376	ATP	C4-C5-N7	-3.41	106.68	110.58
3	F	1376	ATP	N3-C2-N1	-3.34	123.52	128.58
3	B	1376	ATP	N3-C2-N1	-3.30	123.58	128.58
3	C	1376	ATP	N3-C2-N1	-3.27	123.63	128.58
3	A	1376	ATP	N3-C2-N1	-3.20	123.73	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1376	ATP	N3-C2-N1	-3.10	123.89	128.58
3	D	1376	ATP	C4-N9-C8	2.96	108.84	105.74
3	F	1376	ATP	C4-N9-C8	2.93	108.81	105.74
3	A	1376	ATP	C4-N9-C8	2.80	108.68	105.74
3	C	1376	ATP	C4-N9-C8	2.74	108.61	105.74
3	E	1376	ATP	N3-C2-N1	-2.71	124.48	128.58
3	B	1376	ATP	C5-N7-C8	2.66	107.64	103.45
3	F	1376	ATP	C5-N7-C8	2.59	107.51	103.45
3	E	1376	ATP	C4-N9-C8	2.58	108.45	105.74
3	B	1376	ATP	C4-N9-C8	2.57	108.44	105.74
3	C	1376	ATP	C5-N7-C8	2.56	107.47	103.45
3	E	1376	ATP	C5-N7-C8	2.56	107.47	103.45
3	D	1376	ATP	C5-N7-C8	2.53	107.43	103.45
3	A	1376	ATP	C5-N7-C8	2.53	107.42	103.45
3	F	1376	ATP	C6-C5-N7	2.24	136.42	132.09
3	C	1376	ATP	C6-C5-N7	2.24	136.41	132.09
3	B	1376	ATP	C6-C5-N7	2.19	136.31	132.09
3	F	1376	ATP	N9-C8-N7	-2.16	110.88	113.94
3	D	1376	ATP	C6-C5-N7	2.14	136.22	132.09
3	D	1376	ATP	N9-C8-N7	-2.13	110.91	113.94
3	A	1376	ATP	C6-C5-N7	2.11	136.17	132.09
3	A	1376	ATP	N9-C8-N7	-2.08	110.98	113.94
3	B	1376	ATP	N9-C8-N7	-2.07	111.01	113.94
3	B	1376	ATP	C3'-C2'-C1'	2.05	105.35	101.46
3	C	1376	ATP	N9-C8-N7	-2.05	111.03	113.94
3	E	1376	ATP	C6-C5-N7	2.04	136.02	132.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1376	ATP	C5'-O5'-PA-O2A
5	A	1378	GOL	C1-C2-C3-O3
5	C	1378	GOL	C1-C2-C3-O3
5	C	1379	GOL	C1-C2-C3-O3
5	F	1378	GOL	C1-C2-C3-O3
5	B	1378	GOL	C1-C2-C3-O3
5	N	1529	GOL	C1-C2-C3-O3
5	A	1378	GOL	O2-C2-C3-O3
5	C	1378	GOL	O2-C2-C3-O3
5	C	1379	GOL	O2-C2-C3-O3
5	F	1378	GOL	O2-C2-C3-O3

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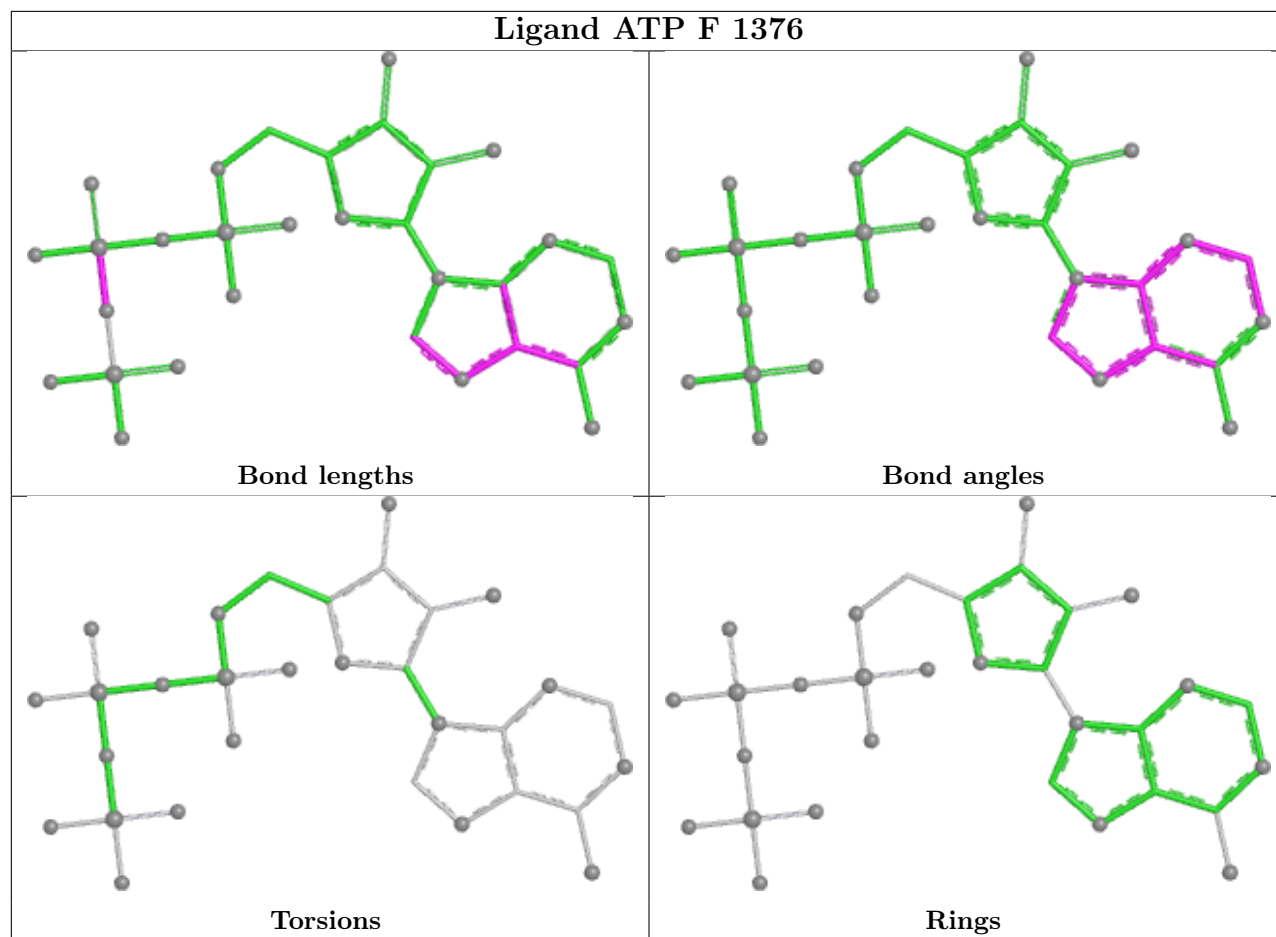
Mol	Chain	Res	Type	Atoms
5	N	1529	GOL	O2-C2-C3-O3
5	C	1379	GOL	O1-C1-C2-O2
5	E	1378	GOL	O2-C2-C3-O3
3	B	1376	ATP	PG-O3B-PB-O1B
5	B	1378	GOL	O2-C2-C3-O3
5	E	1378	GOL	C1-C2-C3-O3
3	E	1376	ATP	C3'-C4'-C5'-O5'
3	B	1376	ATP	PG-O3B-PB-O2B
5	C	1379	GOL	O1-C1-C2-C3
3	C	1376	ATP	PG-O3B-PB-O2B
3	E	1376	ATP	PG-O3B-PB-O2B

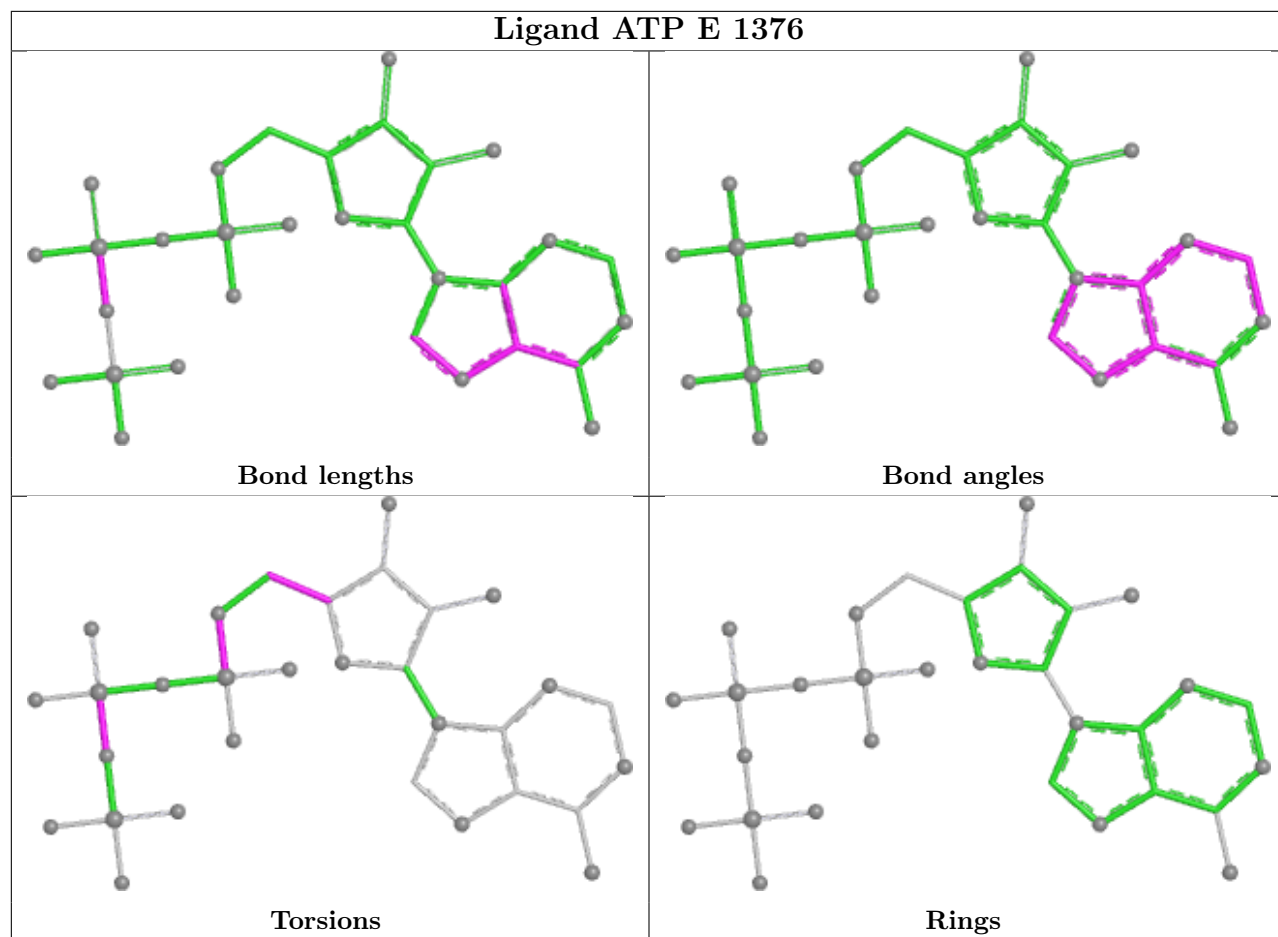
There are no ring outliers.

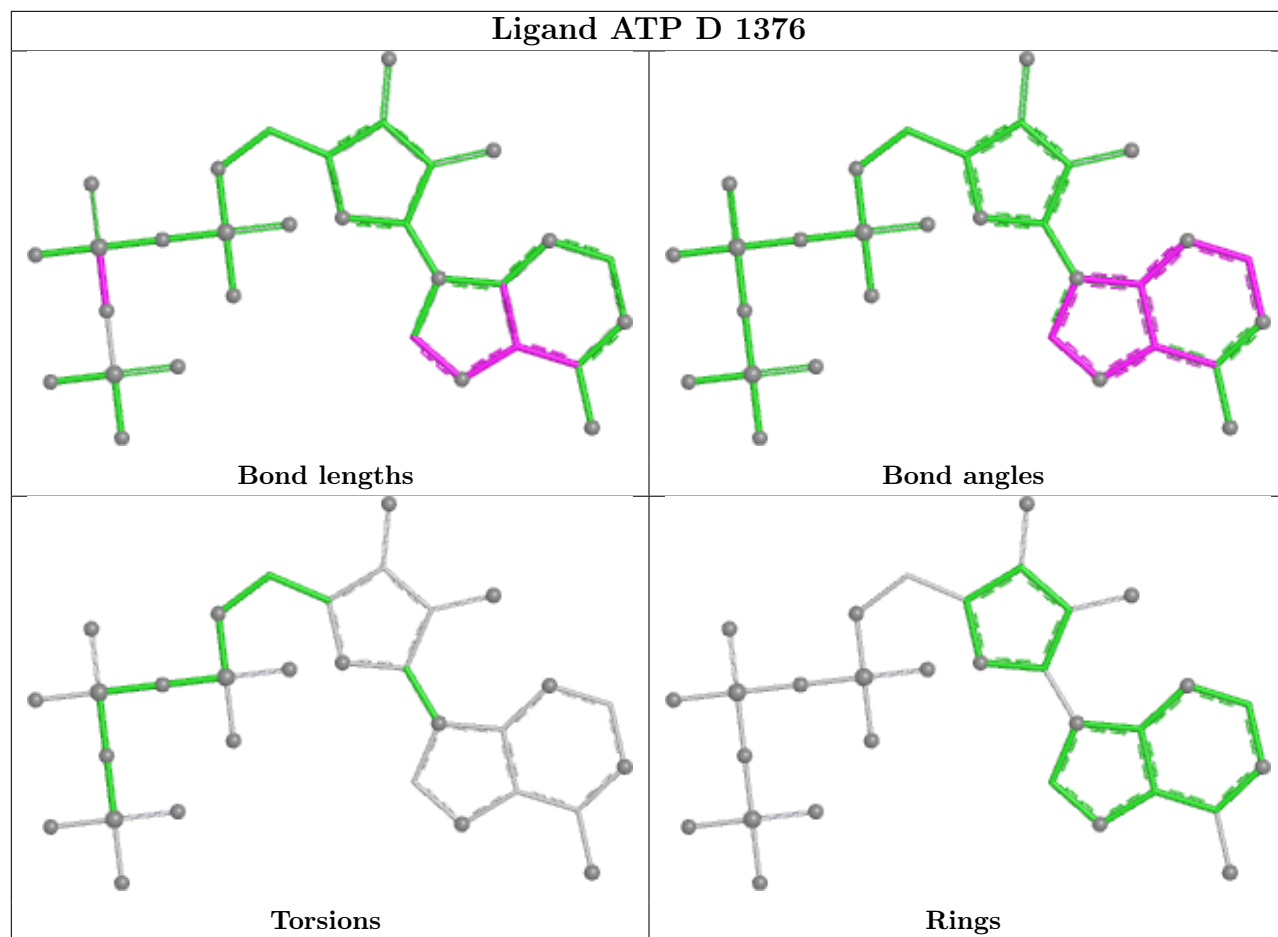
6 monomers are involved in 8 short contacts:

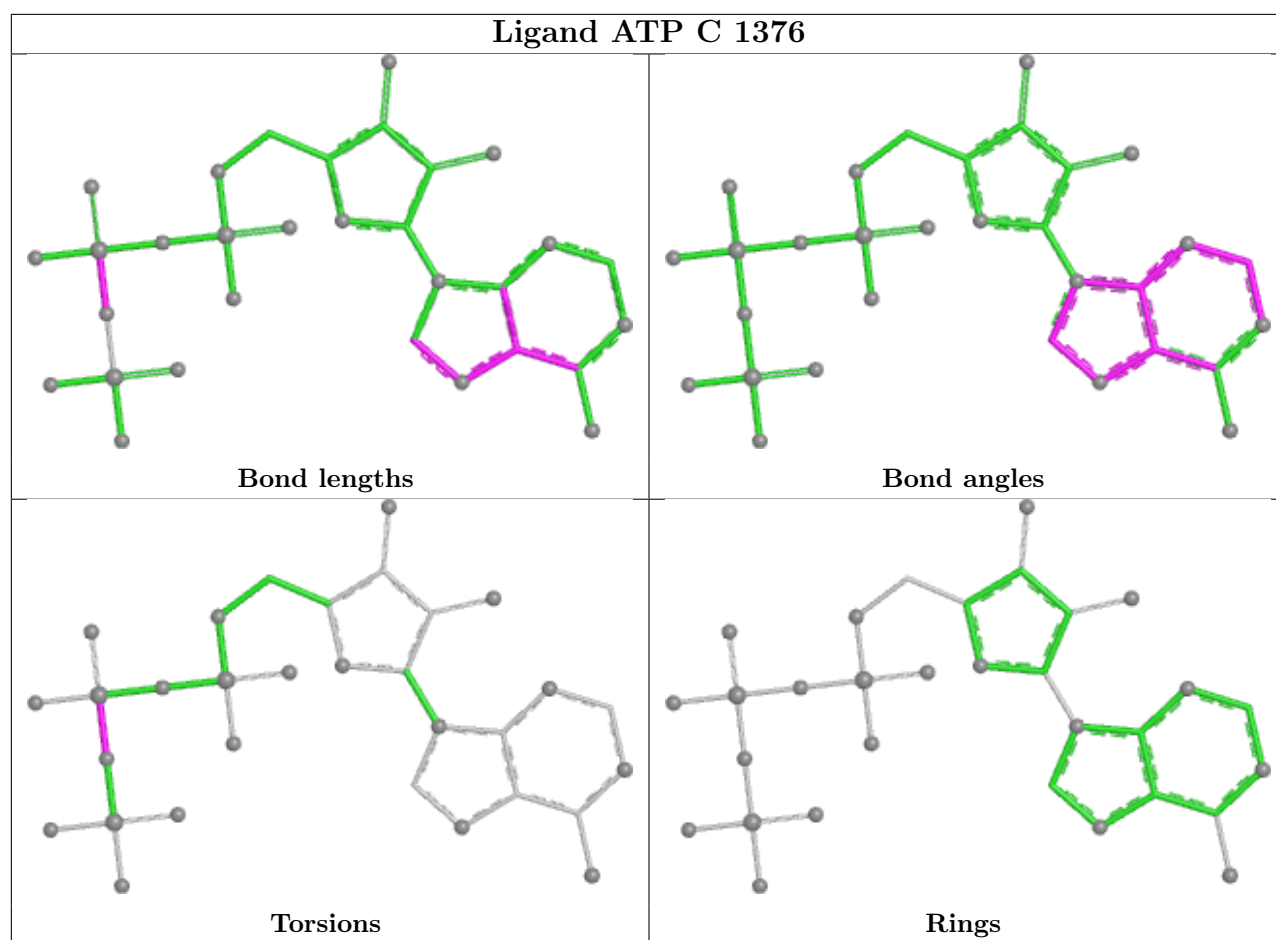
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1376	ATP	1	0
3	E	1376	ATP	1	0
3	D	1376	ATP	3	0
3	A	1376	ATP	1	0
3	B	1376	ATP	1	0
5	E	1378	GOL	1	0

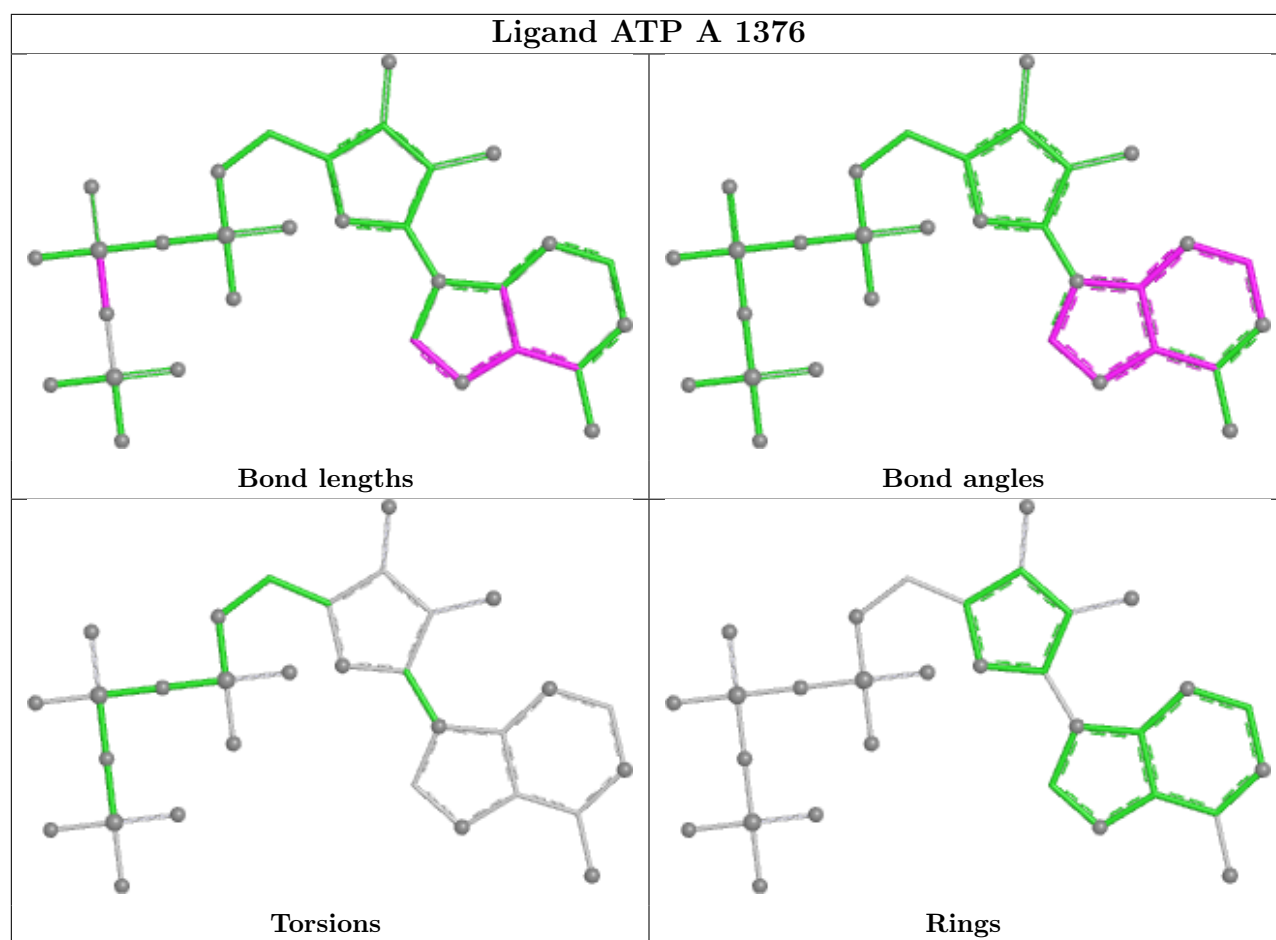
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

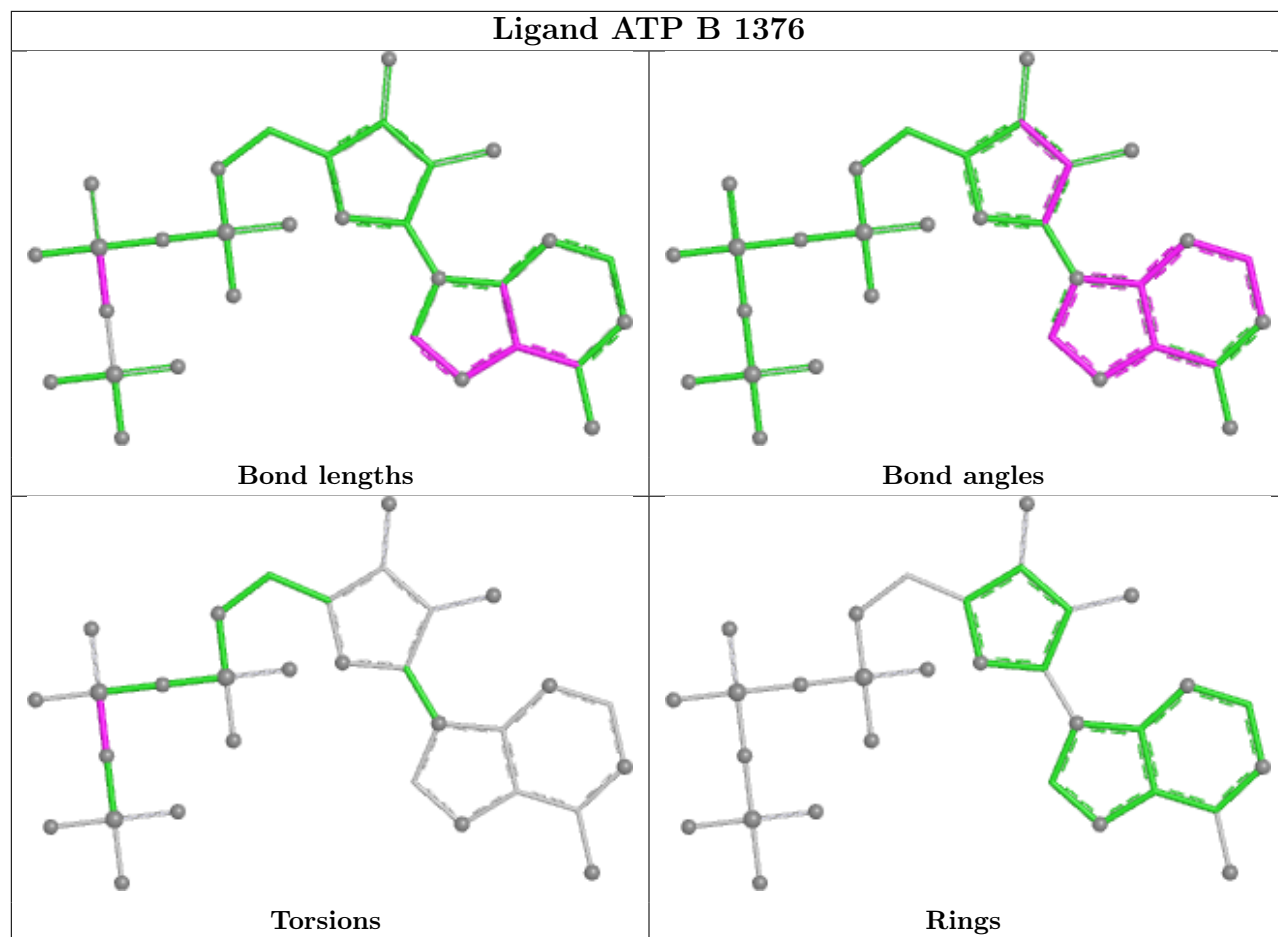












5.7 Other polymers [i](#)

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	335/376 (89%)	5.89	333 (99%) 0 0	57, 83, 142, 192	0
1	B	357/376 (94%)	5.73	357 (100%) 0 0	49, 78, 120, 162	0
1	C	370/376 (98%)	5.39	368 (99%) 0 0	55, 74, 107, 137	0
1	D	356/376 (94%)	6.19	356 (100%) 0 0	70, 98, 133, 162	0
1	E	359/376 (95%)	5.58	358 (99%) 0 0	58, 82, 118, 151	0
1	F	357/376 (94%)	5.54	357 (100%) 0 0	55, 82, 128, 166	0
2	M	110/115 (95%)	5.87	110 (100%) 0 0	61, 84, 128, 150	0
2	N	107/115 (93%)	5.83	107 (100%) 0 0	67, 88, 119, 133	0
All	All	2351/2486 (94%)	5.73	2346 (99%) 0 0	49, 84, 128, 192	0

All (2346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	15	GLY	17.8
1	D	25	ASP	15.5
2	M	487	GLN	14.8
1	F	354	GLN	14.4
2	M	436	GLU	13.5
1	C	202	THR	13.5
1	D	160	THR	13.4
1	F	155	SER	13.4
1	B	310	ALA	13.3
1	E	354	GLN	13.0
1	A	273	GLY	12.9
1	A	25	ASP	12.9
1	D	292	ASP	12.6
2	M	489	GLU	12.5
1	B	97	ALA	12.4
1	A	348	SER	12.4

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Mol	Chain	Res	Type	RSRZ
1	F	372	ARG	12.2
1	B	246	GLN	12.1
1	A	115	ASN	12.0
1	F	75	ILE	11.9
1	F	16	LEU	11.8
1	B	234	SER	11.7
1	B	333	PRO	11.7
1	E	78	ASN	11.6
1	C	292	ASP	11.5
1	A	90	PHE	11.4
1	B	103	THR	11.1
1	E	334	GLU	11.1
1	D	115	ASN	10.9
1	F	286	ASP	10.9
1	F	93	GLU	10.9
1	A	187	ASP	10.9
1	B	9	VAL	10.9
1	D	7	ALA	10.8
1	B	244	ASP	10.8
1	C	365	ALA	10.7
1	A	203	THR	10.7
1	E	244	ASP	10.6
1	C	248	ILE	10.6
1	A	314	GLN	10.6
1	E	80	ASP	10.6
2	M	523	SER	10.6
1	A	316	GLU	10.5
1	C	232	SER	10.5
1	A	344	SER	10.5
1	C	239	SER	10.4
1	C	323	SER	10.4
1	B	193	LEU	10.4
1	B	363	ASP	10.4
1	B	77	THR	10.4
1	B	65	LEU	10.4
1	D	145	SER	10.4
1	C	162	ASN	10.3
1	D	322	PRO	10.3
2	M	515	GLU	10.3
1	D	199	SER	10.3
2	M	419	CYS	10.3
1	E	134	VAL	10.3

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Mol	Chain	Res	Type	RSRZ
1	A	241	GLU	10.2
1	D	286	ASP	10.2
1	A	351	THR	10.2
1	A	19	ALA	10.2
1	D	155	SER	10.2
1	D	348	SER	10.2
1	C	80	ASP	10.1
1	B	98	PRO	10.1
1	B	111	ASN	10.1
1	D	370	VAL	10.1
1	E	14	SER	10.0
1	A	26	ALA	10.0
1	D	233	SER	10.0
2	M	423	SER	10.0
1	F	253	GLU	10.0
1	D	325	MET	10.0
1	A	292	ASP	10.0
2	M	465	ARG	10.0
1	B	128	ASN	9.9
1	E	237	GLU	9.9
1	B	145	SER	9.9
1	B	72	GLU	9.9
1	D	371	HIS	9.9
1	A	80	ASP	9.8
2	N	479	ASN	9.8
1	E	168	GLY	9.7
1	F	25	ASP	9.7
1	C	135	ALA	9.7
1	D	86	TRP	9.7
1	B	176	MET	9.7
1	C	24	ASP	9.7
2	M	492	GLU	9.7
1	A	17	VAL	9.6
1	F	22	ALA	9.6
1	D	173	HIS	9.6
1	A	163	VAL	9.6
1	D	297	ASN	9.6
1	C	56	ASP	9.6
1	D	350	SER	9.6
1	E	332	PRO	9.5
1	A	363	ASP	9.5
2	N	505	SER	9.5

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Mol	Chain	Res	Type	RSRZ
1	B	37	ARG	9.5
1	D	26	ALA	9.4
1	E	344	SER	9.4
1	F	70	PRO	9.4
1	B	187	ASP	9.4
1	A	341	ILE	9.4
1	B	67	LEU	9.4
1	F	224	GLU	9.4
1	E	220	ALA	9.3
1	B	6	THR	9.3
1	C	103	THR	9.3
1	C	78	ASN	9.3
1	A	91	TYR	9.2
1	A	32	PRO	9.2
1	B	344	SER	9.2
1	E	296	ASN	9.2
2	N	506	GLN	9.2
1	C	10	CYS	9.2
1	D	217	CYS	9.2
1	E	374	CYS	9.2
1	B	173	HIS	9.2
1	C	33	SER	9.2
1	D	194	THR	9.1
1	F	352	PHE	9.1
2	N	447	THR	9.1
1	C	289	ILE	9.1
1	B	66	THR	9.1
1	C	126	THR	9.1
1	D	161	HIS	9.1
1	D	61	LYS	9.1
2	M	429	SER	9.1
1	E	310	ALA	9.0
1	B	59	GLN	9.0
2	M	468	GLN	9.0
1	F	21	PHE	9.0
1	F	203	THR	9.0
1	D	354	GLN	9.0
1	A	334	GLU	9.0
1	F	241	GLU	9.0
1	D	32	PRO	9.0
1	D	232	SER	9.0
1	D	351	THR	9.0

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Mol	Chain	Res	Type	RSRZ
1	F	7	ALA	9.0
1	B	334	GLU	9.0
2	N	449	GLU	8.9
1	A	95	ARG	8.9
1	A	155	SER	8.9
1	D	357	ILE	8.9
1	A	364	GLU	8.9
1	B	70	PRO	8.9
1	C	354	GLN	8.9
1	A	239	SER	8.8
1	F	194	THR	8.8
1	D	284	LYS	8.8
1	B	357	ILE	8.8
1	E	34	ILE	8.8
1	F	343	GLY	8.8
1	B	225	ASN	8.8
2	M	430	ASN	8.8
1	C	14	SER	8.8
1	D	308	GLY	8.8
1	B	69	TYR	8.8
1	B	80	ASP	8.8
2	M	522	PHE	8.8
1	D	182	GLY	8.8
1	D	179	ASP	8.8
1	A	315	LYS	8.7
1	E	108	ALA	8.7
1	C	100	GLU	8.7
1	B	224	GLU	8.7
1	D	356	TRP	8.7
1	D	12	ASN	8.7
1	A	118	LYS	8.7
1	A	78	ASN	8.6
1	C	9	VAL	8.6
1	A	156	GLY	8.6
1	B	38	PRO	8.6
1	E	321	ALA	8.6
1	F	157	ASP	8.6
1	F	351	THR	8.6
1	D	355	MET	8.6
1	E	241	GLU	8.6
2	N	483	PRO	8.5
1	A	249	THR	8.5

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Mol	Chain	Res	Type	RSRZ
1	A	72	GLU	8.5
1	C	72	GLU	8.5
1	E	71	ILE	8.5
1	A	135	ALA	8.5
1	F	148	THR	8.5
2	M	426	ILE	8.5
1	C	169	TYR	8.5
1	E	53	TYR	8.5
1	B	268	GLY	8.5
1	A	358	THR	8.5
1	F	160	THR	8.5
1	F	60	SER	8.5
1	D	360	GLN	8.5
1	E	240	TYR	8.5
1	C	201	VAL	8.5
1	D	22	ALA	8.4
2	M	525	TYR	8.4
1	C	286	ASP	8.4
1	D	69	TYR	8.4
1	B	36	GLY	8.4
1	D	80	ASP	8.4
1	A	221	LEU	8.4
1	A	114	ALA	8.4
1	D	309	ILE	8.4
1	B	81	ASP	8.4
1	C	50	LYS	8.4
1	D	114	ALA	8.4
2	N	443	LEU	8.4
1	E	290	ARG	8.3
1	A	166	TYR	8.3
1	E	359	LYS	8.3
1	F	304	THR	8.3
1	F	94	LEU	8.3
1	E	159	VAL	8.3
1	E	184	ASP	8.3
2	M	422	ASP	8.3
1	C	41	GLN	8.3
1	D	283	MET	8.3
1	D	91	TYR	8.3
1	A	101	HIS	8.3
1	D	204	ALA	8.3
1	F	350	SER	8.3

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Mol	Chain	Res	Type	RSRZ
1	D	242	LEU	8.2
1	D	288	ASP	8.2
1	C	298	VAL	8.2
1	B	78	ASN	8.2
1	B	156	GLY	8.2
1	A	186	THR	8.2
1	C	179	ASP	8.2
1	E	187	ASP	8.2
1	A	268	GLY	8.2
1	A	184	ASP	8.2
1	E	252	ASN	8.2
1	C	205	GLU	8.2
1	B	52	SER	8.2
1	F	348	SER	8.2
1	A	318	THR	8.2
1	A	372	ARG	8.2
1	D	192	ILE	8.2
1	D	65	LEU	8.1
1	E	372	ARG	8.1
1	C	115	ASN	8.1
1	C	65	LEU	8.1
1	A	81	ASP	8.1
1	C	139	VAL	8.1
1	A	29	ALA	8.1
1	C	57	GLU	8.1
1	F	108	ALA	8.1
2	N	502	ARG	8.1
1	A	126	THR	8.1
1	E	287	ILE	8.1
2	N	442	ILE	8.1
2	N	423	SER	8.1
1	C	364	GLU	8.1
1	C	13	GLY	8.0
1	E	63	GLY	8.0
1	E	343	GLY	8.0
1	D	58	ALA	8.0
1	D	144	ALA	8.0
1	E	353	GLN	8.0
1	D	243	PRO	8.0
1	D	323	SER	8.0
1	E	210	ARG	8.0
1	B	134	VAL	8.0

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Mol	Chain	Res	Type	RSRZ
1	F	101	HIS	8.0
1	C	59	GLN	8.0
1	D	66	THR	8.0
1	A	271	SER	8.0
1	F	234	SER	8.0
1	B	367	PRO	7.9
1	D	72	GLU	7.9
1	C	215	LYS	7.9
1	B	374	CYS	7.9
2	M	483	PRO	7.9
1	A	94	LEU	7.9
1	A	97	ALA	7.9
1	D	151	ILE	7.9
1	C	134	VAL	7.9
1	B	155	SER	7.9
1	F	52	SER	7.9
1	A	31	PHE	7.9
1	E	90	PHE	7.9
1	E	203	THR	7.9
1	F	90	PHE	7.9
1	F	308	GLY	7.9
2	N	501	THR	7.9
1	F	340	TRP	7.9
2	M	526	VAL	7.9
1	D	241	GLU	7.9
2	N	527	GLU	7.9
1	F	344	SER	7.9
1	E	311	ASP	7.9
1	E	279	TYR	7.9
1	E	82	MET	7.9
1	A	84	LYS	7.8
1	B	366	GLY	7.8
1	B	309	ILE	7.8
1	B	324	THR	7.8
1	D	249	THR	7.8
2	N	503	LYS	7.8
1	B	217	CYS	7.8
1	A	229	THR	7.8
1	D	154	ASP	7.8
1	D	260	THR	7.8
2	N	430	ASN	7.8
2	N	453	GLU	7.8

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Mol	Chain	Res	Type	RSRZ
1	D	365	ALA	7.8
2	N	429	SER	7.8
1	C	244	ASP	7.8
1	E	295	ALA	7.7
1	C	110	LEU	7.7
1	F	249	THR	7.7
1	A	164	PRO	7.7
1	B	347	ALA	7.7
1	F	66	THR	7.7
1	B	228	ALA	7.7
1	F	72	GLU	7.7
2	M	486	GLU	7.7
1	B	314	GLN	7.7
1	C	69	TYR	7.7
1	A	87	HIS	7.7
1	B	101	HIS	7.7
2	M	460	THR	7.7
2	N	467	SER	7.7
1	E	211	ASP	7.7
1	C	270	GLU	7.7
1	C	285	CYS	7.7
1	F	128	ASN	7.7
1	D	375	PHE	7.6
1	B	68	LYS	7.6
2	N	485	ASN	7.6
1	F	333	PRO	7.6
1	C	344	SER	7.6
1	D	368	SER	7.6
2	M	433	SER	7.6
1	C	374	CYS	7.6
1	A	28	ARG	7.6
1	E	104	LEU	7.6
1	C	370	VAL	7.6
1	F	55	GLY	7.6
1	B	205	GLU	7.6
1	D	207	GLU	7.6
1	B	71	ILE	7.6
1	B	57	GLU	7.6
1	E	69	TYR	7.6
1	D	77	THR	7.6
1	F	202	THR	7.6
1	A	296	ASN	7.5

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Mol	Chain	Res	Type	RSRZ
1	C	352	PHE	7.5
1	F	232	SER	7.5
1	B	189	LEU	7.5
1	C	171	LEU	7.5
1	B	131	ALA	7.5
1	D	143	TYR	7.5
1	B	56	ASP	7.5
2	M	482	LYS	7.5
1	E	270	GLU	7.5
1	B	353	GLN	7.5
1	F	54	VAL	7.5
1	A	144	ALA	7.5
1	D	240	TYR	7.5
1	E	32	PRO	7.5
1	B	92	ASN	7.5
1	E	288	ASP	7.5
2	N	524	ASP	7.5
1	D	152	VAL	7.5
1	D	97	ALA	7.5
1	D	347	ALA	7.5
1	B	115	ASN	7.5
1	C	363	ASP	7.5
1	A	148	THR	7.4
1	A	360	GLN	7.4
1	C	359	LYS	7.4
1	A	343	GLY	7.4
1	F	56	ASP	7.4
1	D	17	VAL	7.4
1	D	215	LYS	7.4
1	B	319	ALA	7.4
1	F	69	TYR	7.4
1	F	103	THR	7.4
1	B	182	GLY	7.4
1	A	287	ILE	7.4
1	C	219	VAL	7.4
1	D	339	VAL	7.4
2	M	524	ASP	7.4
1	B	89	THR	7.3
1	D	358	THR	7.3
1	A	92	ASN	7.3
2	M	485	ASN	7.3
1	A	244	ASP	7.3

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Mol	Chain	Res	Type	RSRZ
1	E	258	PRO	7.3
1	D	274	ILE	7.3
1	E	88	HIS	7.3
1	D	279	TYR	7.3
1	F	198	TYR	7.3
1	D	181	ALA	7.3
1	F	58	ALA	7.3
1	C	43	VAL	7.3
1	F	53	TYR	7.3
1	A	127	PHE	7.3
1	C	346	LEU	7.3
1	B	165	ILE	7.3
1	B	345	ILE	7.3
1	D	258	PRO	7.3
1	D	203	THR	7.3
1	B	368	SER	7.3
1	D	234	SER	7.3
1	E	207	GLU	7.3
1	E	243	PRO	7.3
1	F	252	ASN	7.3
1	C	45	VAL	7.3
1	D	349	LEU	7.3
1	F	65	LEU	7.3
1	B	202	THR	7.2
1	E	186	THR	7.2
2	N	460	THR	7.2
1	A	98	PRO	7.2
1	D	13	GLY	7.2
1	B	219	VAL	7.2
1	F	17	VAL	7.2
1	A	291	LYS	7.2
1	D	128	ASN	7.2
1	F	184	ASP	7.2
1	E	362	TYR	7.2
1	C	87	HIS	7.2
1	C	51	ASP	7.2
1	D	187	ASP	7.2
1	E	154	ASP	7.2
1	A	260	THR	7.2
1	B	160	THR	7.2
1	C	186	THR	7.2
1	F	355	MET	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	134	VAL	7.2
1	E	185	LEU	7.2
1	D	138	ALA	7.2
1	D	310	ALA	7.2
1	A	337	TYR	7.2
1	B	25	ASP	7.2
1	B	329	ILE	7.2
1	C	48	GLY	7.2
1	D	30	VAL	7.2
1	D	163	VAL	7.2
1	E	247	VAL	7.2
1	E	127	PHE	7.2
1	D	338	SER	7.2
1	F	88	HIS	7.2
1	B	143	TYR	7.1
1	A	195	GLU	7.1
1	B	102	PRO	7.1
1	C	66	THR	7.1
1	C	367	PRO	7.1
2	M	425	ALA	7.1
1	A	179	ASP	7.1
1	E	283	MET	7.1
1	A	30	VAL	7.1
1	A	99	GLU	7.1
1	D	364	GLU	7.1
1	E	226	GLU	7.1
1	B	200	PHE	7.1
1	A	350	SER	7.1
1	E	297	ASN	7.1
1	B	311	ASP	7.1
2	N	448	ASP	7.1
1	E	221	LEU	7.1
1	E	309	ILE	7.1
1	D	53	TYR	7.1
1	A	202	THR	7.1
1	B	360	GLN	7.1
1	A	133	TYR	7.1
1	A	323	SER	7.1
1	B	96	VAL	7.0
1	A	128	ASN	7.0
1	D	333	PRO	7.0
1	D	324	THR	7.0

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Mol	Chain	Res	Type	RSRZ
1	E	24	ASP	7.0
2	M	472	ALA	7.0
2	M	518	ILE	7.0
2	N	426	ILE	7.0
1	A	73	HIS	7.0
1	F	159	VAL	7.0
1	F	339	VAL	7.0
1	D	293	LEU	7.0
1	F	91	TYR	7.0
1	E	38	PRO	7.0
1	B	351	THR	7.0
1	E	6	THR	7.0
1	E	122	ILE	7.0
1	B	222	ASP	7.0
1	D	352	PHE	7.0
1	A	338	SER	7.0
1	B	235	SER	7.0
1	E	115	ASN	7.0
1	D	6	THR	7.0
1	D	159	VAL	7.0
1	B	371	HIS	7.0
1	D	346	LEU	7.0
1	E	102	PRO	7.0
1	B	231	ALA	7.0
2	N	433	SER	7.0
1	C	240	TYR	6.9
1	B	32	PRO	6.9
1	D	76	ILE	6.9
1	D	99	GLU	6.9
1	E	192	ILE	6.9
2	M	511	GLU	6.9
1	B	199	SER	6.9
1	D	277	THR	6.9
1	F	77	THR	6.9
1	E	198	TYR	6.9
1	D	307	PRO	6.9
1	A	170	ALA	6.9
1	D	341	ILE	6.9
1	E	170	ALA	6.9
1	D	252	ASN	6.9
1	F	11	ASP	6.9
1	B	64	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
1	F	321	ALA	6.9
1	C	207	GLU	6.9
1	A	79	TRP	6.9
1	A	373	LYS	6.9
2	M	476	GLU	6.9
1	C	351	THR	6.9
1	E	12	ASN	6.9
1	B	198	TYR	6.9
1	D	345	ILE	6.9
1	E	215	LYS	6.9
1	A	167	GLU	6.9
1	D	132	MET	6.9
1	B	14	SER	6.9
1	C	235	SER	6.9
1	C	338	SER	6.9
1	D	278	THR	6.9
1	E	199	SER	6.9
1	E	202	THR	6.9
1	E	235	SER	6.9
1	D	225	ASN	6.9
1	E	289	ILE	6.9
1	C	307	PRO	6.9
1	D	29	ALA	6.9
1	D	110	LEU	6.9
1	E	224	GLU	6.9
1	C	199	SER	6.8
1	D	52	SER	6.8
1	E	121	GLN	6.8
2	M	421	LYS	6.8
1	D	321	ALA	6.8
1	E	109	PRO	6.8
1	A	105	LEU	6.8
1	B	183	ARG	6.8
1	B	60	SER	6.8
1	E	246	GLN	6.8
1	F	197	GLY	6.8
1	B	365	ALA	6.8
1	F	177	ARG	6.8
1	B	362	TYR	6.8
1	D	139	VAL	6.8
1	B	241	GLU	6.8
1	B	208	ILE	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	6.8
1	F	158	GLY	6.8
1	C	128	ASN	6.8
1	A	311	ASP	6.8
1	C	25	ASP	6.8
1	D	157	ASP	6.8
1	E	195	GLU	6.8
1	C	22	ALA	6.8
1	B	12	ASN	6.8
1	E	347	ALA	6.8
1	C	173	HIS	6.8
1	A	117	GLU	6.7
1	B	83	GLU	6.7
1	A	177	ARG	6.7
1	A	11	ASP	6.7
1	C	311	ASP	6.7
1	D	64	ILE	6.7
1	E	327	ILE	6.7
1	D	180	LEU	6.7
1	F	298	VAL	6.7
1	A	235	SER	6.7
1	A	293	LEU	6.7
1	A	345	ILE	6.7
1	B	318	THR	6.7
1	D	361	GLU	6.7
1	F	356	TRP	6.7
1	D	247	VAL	6.7
1	F	130	PRO	6.7
2	N	435	ARG	6.7
1	E	162	ASN	6.7
1	A	140	LEU	6.7
1	D	105	LEU	6.7
1	E	346	LEU	6.7
1	A	146	GLY	6.7
1	C	343	GLY	6.7
1	D	54	VAL	6.7
2	N	422	ASP	6.7
1	D	101	HIS	6.7
1	C	129	VAL	6.7
1	A	130	PRO	6.6
1	B	130	PRO	6.6
1	F	307	PRO	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	244	ASP	6.6
1	A	362	TYR	6.6
1	B	188	TYR	6.6
1	D	136	ILE	6.6
1	A	355	MET	6.6
1	A	243	PRO	6.6
2	N	471	THR	6.6
1	E	178	LEU	6.6
2	N	481	LEU	6.6
1	A	306	TYR	6.6
2	N	440	LYS	6.6
1	A	214	GLU	6.6
1	F	78	ASN	6.6
1	C	149	THR	6.6
1	D	374	CYS	6.6
1	D	125	GLU	6.6
1	E	209	VAL	6.6
1	A	181	ALA	6.6
1	D	298	VAL	6.6
1	F	347	ALA	6.6
1	F	12	ASN	6.6
1	B	242	LEU	6.6
1	C	216	LEU	6.6
1	F	235	SER	6.6
1	A	240	TYR	6.6
1	B	63	GLY	6.6
1	D	107	GLU	6.6
1	C	118	LYS	6.5
1	A	70	PRO	6.5
1	F	115	ASN	6.5
1	C	203	THR	6.5
1	F	176	MET	6.5
1	A	15	GLY	6.5
1	A	197	GLY	6.5
1	D	168	GLY	6.5
1	F	156	GLY	6.5
2	N	511	GLU	6.5
1	C	327	ILE	6.5
1	B	233	SER	6.5
1	D	170	ALA	6.5
1	D	373	LYS	6.5
1	D	178	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	311	ASP	6.5
2	N	491	GLU	6.5
1	B	349	LEU	6.5
1	C	164	PRO	6.5
1	A	149	THR	6.5
1	B	129	VAL	6.5
1	B	181	ALA	6.5
2	M	517	LYS	6.5
1	D	93	GLU	6.5
1	A	86	TRP	6.5
1	D	250	ILE	6.5
1	A	368	SER	6.5
1	F	228	ALA	6.5
1	A	288	ASP	6.5
1	D	222	ASP	6.5
1	E	352	PHE	6.5
1	E	152	VAL	6.5
2	M	471	THR	6.4
2	N	463	THR	6.4
1	A	302	GLY	6.4
1	D	74	GLY	6.4
1	D	183	ARG	6.4
1	E	83	GLU	6.4
1	F	367	PRO	6.4
1	E	56	ASP	6.4
1	F	363	ASP	6.4
1	A	374	CYS	6.4
1	B	370	VAL	6.4
1	C	291	LYS	6.4
1	C	355	MET	6.4
1	E	54	VAL	6.4
1	E	129	VAL	6.4
1	C	295	ALA	6.4
1	F	97	ALA	6.4
1	A	280	ASN	6.4
1	B	104	LEU	6.4
1	D	111	ASN	6.4
1	A	150	GLY	6.4
1	F	145	SER	6.4
1	B	364	GLU	6.4
1	B	201	VAL	6.4
1	D	56	ASP	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	321	ALA	6.4
1	C	94	LEU	6.4
1	C	189	LEU	6.4
1	F	59	GLN	6.4
2	M	490	GLN	6.4
1	C	12	ASN	6.4
1	D	36	GLY	6.4
1	C	127	PHE	6.4
1	D	270	GLU	6.4
1	A	333	PRO	6.4
1	A	367	PRO	6.4
1	A	178	LEU	6.4
1	D	230	ALA	6.4
1	E	101	HIS	6.4
2	M	420	ARG	6.4
1	C	360	GLN	6.4
2	M	456	GLN	6.4
1	B	13	GLY	6.4
1	D	71	ILE	6.4
1	E	151	ILE	6.4
2	N	496	ILE	6.4
1	E	291	LYS	6.4
1	D	372	ARG	6.4
1	E	183	ARG	6.4
1	A	104	LEU	6.4
1	D	10	CYS	6.4
1	A	18	LYS	6.4
1	B	250	ILE	6.4
1	C	192	ILE	6.4
1	B	207	GLU	6.4
1	C	337	TYR	6.4
2	M	510	VAL	6.4
1	A	359	LYS	6.3
1	E	274	ILE	6.3
1	F	122	ILE	6.3
1	F	370	VAL	6.3
2	N	476	GLU	6.3
2	M	435	ARG	6.3
1	D	102	PRO	6.3
1	E	130	PRO	6.3
1	E	350	SER	6.3
1	F	208	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	375	PHE	6.3
1	B	283	MET	6.3
1	C	123	MET	6.3
1	D	169	TYR	6.3
1	F	219	VAL	6.3
1	D	83	GLU	6.3
1	D	98	PRO	6.3
1	D	112	PRO	6.3
1	D	200	PHE	6.3
1	E	77	THR	6.3
1	F	126	THR	6.3
1	D	214	GLU	6.3
1	E	94	LEU	6.3
1	F	226	GLU	6.3
2	M	512	GLU	6.3
2	N	519	LEU	6.3
1	C	217	CYS	6.3
1	A	113	LYS	6.3
1	E	181	ALA	6.3
1	C	145	SER	6.3
1	C	23	GLY	6.3
1	D	73	HIS	6.3
1	B	90	PHE	6.3
1	A	106	THR	6.3
2	M	500	LEU	6.3
1	E	166	TYR	6.3
1	D	285	CYS	6.3
1	A	182	GLY	6.3
1	B	87	HIS	6.3
1	C	74	GLY	6.3
1	D	245	GLY	6.3
1	A	246	GLN	6.3
1	E	358	THR	6.2
1	A	286	ASP	6.2
1	F	154	ASP	6.2
1	D	133	TYR	6.2
1	D	313	MET	6.2
1	E	355	MET	6.2
2	N	504	LEU	6.2
1	D	68	LYS	6.2
1	B	358	THR	6.2
1	E	260	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	107	GLU	6.2
1	D	231	ALA	6.2
1	D	253	GLU	6.2
1	E	19	ALA	6.2
1	F	100	GLU	6.2
1	B	206	ARG	6.2
1	D	67	LEU	6.2
1	E	16	LEU	6.2
1	F	242	LEU	6.2
1	F	246	GLN	6.2
1	B	237	GLU	6.2
1	B	240	TYR	6.2
1	D	287	ILE	6.2
1	C	168	GLY	6.2
1	D	63	GLY	6.2
1	A	257	CYS	6.2
1	E	284	LYS	6.2
1	D	14	SER	6.2
1	D	229	THR	6.2
2	N	498	ARG	6.2
1	D	248	ILE	6.2
1	D	369	ILE	6.2
1	F	76	ILE	6.2
1	B	308	GLY	6.2
1	D	104	LEU	6.2
1	E	18	LYS	6.2
1	A	161	HIS	6.2
1	C	275	HIS	6.2
1	C	52	SER	6.2
1	C	38	PRO	6.2
1	C	172	PRO	6.2
1	B	117	GLU	6.2
1	D	149	THR	6.2
1	B	166	TYR	6.2
1	E	276	GLU	6.2
1	F	284	LYS	6.2
1	A	24	ASP	6.2
1	C	21	PHE	6.2
1	F	292	ASP	6.2
1	A	119	MET	6.1
1	F	87	HIS	6.1
1	B	10	CYS	6.1

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Mol	Chain	Res	Type	RSRZ
1	E	10	CYS	6.1
1	B	232	SER	6.1
1	C	345	ILE	6.1
1	B	91	TYR	6.1
1	C	218	TYR	6.1
1	E	84	LYS	6.1
2	M	424	LEU	6.1
1	C	302	GLY	6.1
1	D	134	VAL	6.1
1	B	116	ARG	6.1
1	F	297	ASN	6.1
1	B	19	ALA	6.1
1	D	85	ILE	6.1
1	F	38	PRO	6.1
1	F	274	ILE	6.1
1	F	276	GLU	6.1
2	M	474	GLU	6.1
1	F	223	PHE	6.1
1	B	355	MET	6.1
1	C	247	VAL	6.1
2	N	499	ARG	6.1
1	E	81	ASP	6.1
1	E	179	ASP	6.1
1	B	34	ILE	6.1
1	F	258	PRO	6.1
1	E	323	SER	6.1
1	C	182	GLY	6.1
1	F	146	GLY	6.1
1	A	173	HIS	6.1
1	D	24	ASP	6.1
1	C	97	ALA	6.1
1	A	175	ILE	6.1
2	M	462	LEU	6.1
2	M	513	LEU	6.1
1	C	141	SER	6.1
1	A	304	THR	6.1
1	A	361	GLU	6.1
1	B	33	SER	6.1
1	C	334	GLU	6.1
1	F	6	THR	6.1
1	F	195	GLU	6.1
1	B	133	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	204	ALA	6.1
1	D	184	ASP	6.1
1	D	272	ALA	6.1
1	F	80	ASP	6.1
1	B	354	GLN	6.1
1	D	172	PRO	6.1
2	N	441	ASN	6.1
2	N	500	LEU	6.1
1	C	82	MET	6.0
1	C	200	PHE	6.0
1	A	233	SER	6.0
1	C	20	GLY	6.0
1	B	327	ILE	6.0
1	D	108	ALA	6.0
1	E	73	HIS	6.0
2	N	425	ALA	6.0
1	D	314	GLN	6.0
1	A	112	PRO	6.0
1	A	172	PRO	6.0
1	B	112	PRO	6.0
1	C	112	PRO	6.0
1	A	124	PHE	6.0
1	A	139	VAL	6.0
1	B	17	VAL	6.0
1	B	54	VAL	6.0
1	B	107	GLU	6.0
1	F	23	GLY	6.0
1	F	141	SER	6.0
1	F	279	TYR	6.0
2	N	509	THR	6.0
1	D	315	LYS	6.0
1	C	8	LEU	6.0
2	M	470	PRO	6.0
1	D	211	ASP	6.0
1	E	21	PHE	6.0
1	A	198	TYR	6.0
1	E	76	ILE	6.0
1	F	371	HIS	6.0
2	N	424	LEU	6.0
1	D	59	GLN	6.0
1	E	200	PHE	6.0
1	D	280	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	8	LEU	6.0
1	F	331	ALA	6.0
1	E	119	MET	6.0
1	A	103	THR	6.0
1	B	337	TYR	6.0
1	D	166	TYR	6.0
1	A	369	ILE	6.0
1	B	212	ILE	6.0
1	E	110	LEU	6.0
1	F	34	ILE	6.0
1	A	7	ALA	6.0
1	C	347	ALA	6.0
1	E	52	SER	6.0
1	D	79	TRP	5.9
1	A	152	VAL	5.9
1	A	298	VAL	5.9
1	C	35	VAL	5.9
1	F	35	VAL	5.9
1	F	375	PHE	5.9
2	N	444	PRO	5.9
1	E	137	GLN	5.9
1	C	288	ASP	5.9
1	A	330	ILE	5.9
1	E	133	TYR	5.9
1	E	250	ILE	5.9
1	A	365	ALA	5.9
1	B	7	ALA	5.9
1	A	9	VAL	5.9
1	E	72	GLU	5.9
2	M	507	ARG	5.9
1	A	317	ILE	5.9
1	A	278	THR	5.9
1	E	277	THR	5.9
1	C	375	PHE	5.9
1	E	172	PRO	5.9
1	E	312	ARG	5.9
1	C	75	ILE	5.9
1	E	212	ILE	5.9
1	F	67	LEU	5.9
1	F	99	GLU	5.9
2	M	481	LEU	5.9
1	C	53	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	328	LYS	5.9
1	E	25	ASP	5.9
1	F	278	THR	5.9
1	D	264	PRO	5.9
1	D	28	ARG	5.9
1	B	110	LEU	5.9
1	E	293	LEU	5.9
1	A	357	ILE	5.9
1	D	327	ILE	5.9
1	A	100	GLU	5.9
1	F	135	ALA	5.9
1	B	152	VAL	5.9
1	B	86	TRP	5.9
1	B	372	ARG	5.9
1	F	32	PRO	5.9
1	A	265	SER	5.9
1	B	300	SER	5.9
1	A	8	LEU	5.9
1	A	193	LEU	5.9
1	C	49	GLN	5.9
1	D	158	GLY	5.9
1	D	246	GLN	5.9
1	C	122	ILE	5.9
1	D	122	ILE	5.9
1	D	289	ILE	5.9
1	F	131	ALA	5.9
1	E	139	VAL	5.8
1	F	132	MET	5.8
1	B	266	PHE	5.8
1	A	199	SER	5.8
1	B	359	LYS	5.8
1	C	234	SER	5.8
1	C	330	ILE	5.8
1	E	330	ILE	5.8
1	D	135	ALA	5.8
1	F	231	ALA	5.8
1	B	99	GLU	5.8
1	F	96	VAL	5.8
2	M	528	VAL	5.8
1	B	194	THR	5.8
1	E	160	THR	5.8
1	F	211	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	322	PRO	5.8
1	B	84	LYS	5.8
1	F	336	LYS	5.8
1	D	251	GLY	5.8
1	F	323	SER	5.8
1	F	204	ALA	5.8
1	A	279	TYR	5.8
1	D	147	ARG	5.8
2	M	494	ARG	5.8
1	B	203	THR	5.8
1	B	229	THR	5.8
1	B	184	ASP	5.8
1	C	371	HIS	5.8
1	D	216	LEU	5.8
1	C	212	ILE	5.8
1	E	342	GLY	5.8
1	F	199	SER	5.8
1	F	123	MET	5.8
1	E	148	THR	5.8
1	A	307	PRO	5.8
1	D	367	PRO	5.8
1	D	175	ILE	5.8
1	F	267	ILE	5.8
1	B	292	ASP	5.8
1	D	366	GLY	5.8
1	D	129	VAL	5.8
1	F	14	SER	5.8
1	D	255	PHE	5.8
1	F	215	LYS	5.8
1	F	180	LEU	5.8
1	A	76	ILE	5.8
1	C	46	GLY	5.8
1	E	256	ARG	5.7
1	C	44	MET	5.7
1	A	270	GLU	5.7
1	D	57	GLU	5.7
1	C	348	SER	5.7
1	A	169	TYR	5.7
1	D	218	TYR	5.7
1	B	277	THR	5.7
1	E	89	THR	5.7
1	D	228	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	26	ALA	5.7
1	E	356	TRP	5.7
2	M	455	ARG	5.7
1	B	132	MET	5.7
1	C	17	VAL	5.7
1	C	187	ASP	5.7
1	F	137	GLN	5.7
2	M	506	GLN	5.7
1	D	31	PHE	5.7
1	E	99	GLU	5.7
1	E	100	GLU	5.7
1	E	167	GLU	5.7
1	E	205	GLU	5.7
2	N	515	GLU	5.7
1	D	236	LEU	5.7
1	B	348	SER	5.7
1	D	337	TYR	5.7
1	A	71	ILE	5.7
1	D	282	ILE	5.7
1	A	308	GLY	5.7
1	B	15	GLY	5.7
1	B	210	ARG	5.7
1	C	88	HIS	5.7
1	D	340	TRP	5.7
1	D	137	GLN	5.7
1	B	24	ASP	5.7
1	D	141	SER	5.7
1	E	60	SER	5.7
1	F	337	TYR	5.7
2	M	458	ILE	5.7
2	N	518	ILE	5.7
1	E	177	ARG	5.7
1	F	95	ARG	5.7
2	N	465	ARG	5.7
1	C	251	GLY	5.7
1	D	15	GLY	5.7
1	B	58	ALA	5.7
1	D	174	ALA	5.7
1	C	119	MET	5.7
1	B	142	LEU	5.7
1	B	297	ASN	5.7
1	F	136	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	341	ILE	5.7
2	N	445	ARG	5.7
1	D	306	TYR	5.7
1	E	294	TYR	5.7
1	A	232	SER	5.7
1	D	273	GLY	5.7
1	F	273	GLY	5.7
1	A	123	MET	5.7
1	F	247	VAL	5.7
1	C	86	TRP	5.7
1	E	86	TRP	5.7
1	D	257	CYS	5.7
1	A	12	ASN	5.7
1	A	157	ASP	5.7
1	A	75	ILE	5.7
1	E	85	ILE	5.7
1	E	147	ARG	5.7
1	F	166	TYR	5.6
2	N	434	LYS	5.6
1	D	146	GLY	5.6
1	E	234	SER	5.6
1	F	281	SER	5.6
1	F	302	GLY	5.6
1	B	123	MET	5.6
1	D	299	MET	5.6
1	E	173	HIS	5.6
2	N	454	LEU	5.6
1	F	374	CYS	5.6
1	C	64	ILE	5.6
1	F	287	ILE	5.6
1	F	364	GLU	5.6
2	M	491	GLU	5.6
2	M	496	ILE	5.6
1	F	191	LYS	5.6
2	N	427	LYS	5.6
1	E	233	SER	5.6
2	N	466	LEU	5.6
1	B	127	PHE	5.6
1	C	183	ARG	5.6
1	D	267	ILE	5.6
1	F	225	ASN	5.6
1	F	237	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	292	ASP	5.6
1	A	301	GLY	5.6
1	A	305	MET	5.6
1	C	138	ALA	5.6
1	F	358	THR	5.6
1	F	265	SER	5.6
1	E	206	ARG	5.6
1	B	79	TRP	5.6
1	B	35	VAL	5.6
1	E	366	GLY	5.6
2	M	428	LEU	5.6
1	D	89	THR	5.6
1	D	275	HIS	5.6
1	B	350	SER	5.6
1	C	79	TRP	5.6
1	C	267	ILE	5.6
1	E	345	ILE	5.6
1	F	85	ILE	5.6
1	F	357	ILE	5.6
1	C	170	ALA	5.6
1	E	339	VAL	5.6
2	M	475	LEU	5.6
1	F	24	ASP	5.6
2	N	451	ARG	5.6
1	D	223	PHE	5.6
1	F	127	PHE	5.6
1	A	141	SER	5.6
1	E	368	SER	5.6
1	E	105	LEU	5.5
2	M	519	LEU	5.5
1	E	128	ASN	5.5
2	N	478	ARG	5.5
2	N	461	LYS	5.5
1	C	73	HIS	5.5
1	D	126	THR	5.5
1	E	103	THR	5.5
1	E	165	ILE	5.5
1	D	33	SER	5.5
1	D	100	GLU	5.5
1	A	16	LEU	5.5
1	B	180	LEU	5.5
1	F	346	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	13	GLY	5.5
1	F	68	LYS	5.5
1	F	113	LYS	5.5
1	A	69	TYR	5.5
1	E	169	TYR	5.5
1	B	223	PHE	5.5
1	A	85	ILE	5.5
1	F	187	ASP	5.5
1	C	314	GLN	5.5
1	E	265	SER	5.5
2	N	494	ARG	5.5
1	B	55	GLY	5.5
1	C	245	GLY	5.5
1	F	102	PRO	5.5
1	D	188	TYR	5.5
1	F	200	PHE	5.5
2	N	522	PHE	5.5
1	C	151	ILE	5.5
1	A	154	ASP	5.5
1	F	89	THR	5.5
2	M	484	ARG	5.5
2	N	456	GLN	5.5
1	E	144	ALA	5.5
1	A	171	LEU	5.5
1	D	94	LEU	5.5
1	A	230	ALA	5.5
1	B	178	LEU	5.4
1	F	293	LEU	5.4
2	N	493	LYS	5.4
1	E	222	ASP	5.4
2	N	528	VAL	5.4
1	A	295	ALA	5.4
1	A	27	PRO	5.4
1	B	322	PRO	5.4
1	E	322	PRO	5.4
1	F	74	GLY	5.4
1	F	300	SER	5.4
1	A	151	ILE	5.4
2	N	482	LYS	5.4
1	A	189	LEU	5.4
1	C	252	ASN	5.4
1	D	92	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	261	LEU	5.4
1	E	8	LEU	5.4
1	A	159	VAL	5.4
1	E	17	VAL	5.4
1	F	30	VAL	5.4
2	N	526	VAL	5.4
1	E	269	MET	5.4
1	F	313	MET	5.4
1	D	266	PHE	5.4
1	E	367	PRO	5.4
1	A	165	ILE	5.4
2	M	520	ILE	5.4
1	A	147	ARG	5.4
1	C	326	LYS	5.4
2	M	461	LYS	5.4
1	A	320	LEU	5.4
1	F	349	LEU	5.4
1	F	190	MET	5.4
1	A	354	GLN	5.4
1	C	342	GLY	5.4
1	E	20	GLY	5.4
1	D	109	PRO	5.4
1	B	75	ILE	5.4
1	D	317	ILE	5.4
1	E	357	ILE	5.4
1	E	281	SER	5.4
1	D	96	VAL	5.4
1	F	353	GLN	5.4
2	N	446	GLN	5.4
1	A	183	ARG	5.4
1	B	335	ARG	5.4
1	C	290	ARG	5.4
1	B	179	ASP	5.4
1	B	259	GLU	5.4
1	D	208	ILE	5.4
1	D	316	GLU	5.4
1	E	136	ILE	5.4
1	F	117	GLU	5.4
1	F	214	GLU	5.4
1	F	285	CYS	5.4
1	B	185	LEU	5.4
1	D	265	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	155	SER	5.4
2	N	437	LEU	5.4
2	N	475	LEU	5.4
1	F	144	ALA	5.4
1	B	85	ILE	5.4
2	N	487	GLN	5.4
2	N	436	GLU	5.3
2	N	473	GLU	5.3
2	N	492	GLU	5.3
1	C	293	LEU	5.3
1	D	239	SER	5.3
1	C	40	HIS	5.3
1	E	5	THR	5.3
1	F	277	THR	5.3
1	F	303	THR	5.3
1	A	223	PHE	5.3
1	B	356	TRP	5.3
1	C	111	ASN	5.3
1	C	301	GLY	5.3
1	E	273	GLY	5.3
1	A	93	GLU	5.3
1	C	195	GLU	5.3
1	D	334	GLU	5.3
1	E	117	GLU	5.3
1	B	293	LEU	5.3
1	B	288	ASP	5.3
1	F	28	ARG	5.3
1	F	73	HIS	5.3
1	B	114	ALA	5.3
1	E	131	ALA	5.3
1	B	317	ILE	5.3
1	C	71	ILE	5.3
1	E	225	ASN	5.3
1	A	346	LEU	5.3
1	B	221	LEU	5.3
1	E	193	LEU	5.3
1	C	30	VAL	5.3
1	F	240	TYR	5.3
1	C	310	ALA	5.3
1	F	326	LYS	5.3
1	B	124	PHE	5.3
1	E	229	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	341	ILE	5.3
1	E	70	PRO	5.3
1	E	253	GLU	5.3
1	E	280	ASN	5.3
2	N	489	GLU	5.3
1	B	190	MET	5.3
1	F	119	MET	5.3
1	C	206	ARG	5.3
1	A	218	TYR	5.3
1	D	113	LYS	5.3
1	D	363	ASP	5.3
1	E	188	TYR	5.3
1	E	114	ALA	5.3
1	B	88	HIS	5.3
1	F	271	SER	5.3
1	F	327	ILE	5.3
1	B	23	GLY	5.3
1	B	260	THR	5.3
1	F	104	LEU	5.3
2	N	428	LEU	5.3
1	C	121	GLN	5.3
1	A	132	MET	5.3
1	B	204	ALA	5.3
1	C	282	ILE	5.3
1	E	197	GLY	5.2
1	E	106	THR	5.2
2	M	501	THR	5.2
1	B	167	GLU	5.2
1	D	190	MET	5.2
1	C	91	TYR	5.2
1	A	222	ASP	5.2
1	B	21	PHE	5.2
1	F	212	ILE	5.2
2	N	452	LEU	5.2
1	C	39	ARG	5.2
1	E	37	ARG	5.2
1	F	324	THR	5.2
1	A	212	ILE	5.2
1	B	113	LYS	5.2
1	B	323	SER	5.2
1	C	233	SER	5.2
1	C	358	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	35	VAL	5.2
1	D	119	MET	5.2
1	C	180	LEU	5.2
1	F	110	LEU	5.2
1	A	88	HIS	5.2
1	A	275	HIS	5.2
1	D	196	ARG	5.2
2	N	459	GLY	5.2
1	C	155	SER	5.2
1	C	167	GLU	5.2
1	A	236	LEU	5.2
1	A	250	ILE	5.2
1	B	105	LEU	5.2
1	B	341	ILE	5.2
1	B	375	PHE	5.2
1	D	177	ARG	5.2
1	E	91	TYR	5.2
1	B	168	GLY	5.2
1	E	161	HIS	5.2
1	E	238	LYS	5.2
1	B	211	ASP	5.2
1	C	81	ASP	5.2
1	D	103	THR	5.2
1	E	66	THR	5.2
1	D	60	SER	5.2
2	N	512	GLU	5.2
1	A	297	ASN	5.1
1	B	343	GLY	5.1
1	B	163	VAL	5.1
1	E	163	VAL	5.1
1	E	298	VAL	5.1
1	B	258	PRO	5.1
1	B	11	ASP	5.1
1	A	194	THR	5.1
1	A	324	THR	5.1
1	C	83	GLU	5.1
1	C	137	GLN	5.1
1	A	33	SER	5.1
1	A	352	PHE	5.1
1	E	375	PHE	5.1
1	B	74	GLY	5.1
1	D	87	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	70	PRO	5.1
1	D	27	PRO	5.1
1	D	130	PRO	5.1
1	C	324	THR	5.1
1	A	237	GLU	5.1
1	B	8	LEU	5.1
1	C	84	LYS	5.1
1	C	99	GLU	5.1
1	C	185	LEU	5.1
1	C	136	ILE	5.1
1	C	55	GLY	5.1
1	F	366	GLY	5.1
1	B	294	TYR	5.1
2	N	508	PRO	5.1
1	A	289	ILE	5.1
1	A	319	ALA	5.1
1	E	59	GLN	5.1
1	F	317	ILE	5.1
2	N	472	ALA	5.1
1	C	184	ASP	5.1
1	D	81	ASP	5.1
1	E	31	PHE	5.1
1	D	156	GLY	5.1
1	E	182	GLY	5.1
1	B	53	TYR	5.1
1	C	296	ASN	5.1
1	B	320	LEU	5.1
1	A	310	ALA	5.1
1	F	165	ILE	5.1
1	A	253	GLU	5.1
1	A	251	GLY	5.1
2	N	510	VAL	5.1
1	D	198	TYR	5.1
1	E	371	HIS	5.1
2	N	470	PRO	5.1
1	E	135	ALA	5.0
1	C	340	TRP	5.0
1	D	202	THR	5.0
2	N	468	GLN	5.0
1	D	176	MET	5.0
1	A	300	SER	5.0
1	C	281	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	362	TYR	5.0
1	C	193	LEU	5.0
1	D	193	LEU	5.0
1	E	189	LEU	5.0
2	M	508	PRO	5.0
1	B	252	ASN	5.0
1	F	151	ILE	5.0
1	A	120	THR	5.0
1	B	121	GLN	5.0
1	B	270	GLU	5.0
1	C	120	THR	5.0
1	C	241	GLU	5.0
1	C	276	GLU	5.0
1	E	120	THR	5.0
2	N	490	GLN	5.0
1	B	209	VAL	5.0
1	A	211	ASP	5.0
1	C	227	MET	5.0
1	D	37	ARG	5.0
1	B	218	TYR	5.0
1	F	368	SER	5.0
1	C	333	PRO	5.0
1	A	267	ILE	5.0
1	C	58	ALA	5.0
1	D	78	ASN	5.0
1	B	249	THR	5.0
1	E	79	TRP	5.0
1	E	364	GLU	5.0
1	A	96	VAL	5.0
1	C	210	ARG	5.0
1	D	140	LEU	5.0
1	B	239	SER	5.0
1	D	294	TYR	5.0
1	F	26	ALA	5.0
1	A	303	THR	5.0
1	B	339	VAL	5.0
1	C	89	THR	5.0
1	D	191	LYS	5.0
1	E	107	GLU	5.0
1	F	106	THR	5.0
2	N	464	ARG	5.0
1	B	192	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	248	ILE	5.0
1	D	34	ILE	5.0
1	F	192	ILE	5.0
1	C	321	ALA	5.0
1	E	338	SER	5.0
1	F	33	SER	5.0
1	A	196	ARG	5.0
1	F	147	ARG	5.0
2	M	509	THR	5.0
1	E	36	GLY	5.0
1	F	189	LEU	5.0
1	A	34	ILE	4.9
1	C	175	ILE	4.9
1	C	231	ALA	4.9
1	D	21	PHE	4.9
1	D	312	ARG	4.9
1	A	207	GLU	4.9
1	A	285	CYS	4.9
1	B	137	GLN	4.9
1	A	20	GLY	4.9
1	C	229	THR	4.9
1	C	366	GLY	4.9
1	E	268	GLY	4.9
1	F	120	THR	4.9
1	F	261	LEU	4.9
1	F	329	ILE	4.9
1	F	109	PRO	4.9
1	F	169	TYR	4.9
2	N	497	LYS	4.9
1	A	234	SER	4.9
1	A	247	VAL	4.9
1	C	60	SER	4.9
1	A	185	LEU	4.9
1	D	84	LYS	4.9
1	D	336	LYS	4.9
1	E	138	ALA	4.9
1	E	272	ALA	4.9
1	F	37	ARG	4.9
2	M	431	ARG	4.9
1	F	221	LEU	4.9
1	A	13	GLY	4.9
1	C	15	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	182	GLY	4.9
2	N	474	GLU	4.9
1	A	356	TRP	4.9
1	C	160	THR	4.9
1	B	326	LYS	4.9
1	C	191	LYS	4.9
1	B	164	PRO	4.9
1	D	95	ARG	4.9
1	D	254	ARG	4.9
1	E	29	ALA	4.9
1	F	332	PRO	4.9
1	F	306	TYR	4.9
1	E	30	VAL	4.9
1	C	47	MET	4.9
1	F	244	ASP	4.9
2	N	523	SER	4.9
1	F	259	GLU	4.9
1	D	75	ILE	4.9
1	F	369	ILE	4.9
1	A	336	LYS	4.9
2	M	464	ARG	4.9
1	B	230	ALA	4.9
1	E	87	HIS	4.9
1	C	159	VAL	4.9
1	E	370	VAL	4.9
1	D	320	LEU	4.9
1	B	157	ASP	4.9
1	C	329	ILE	4.8
1	E	75	ILE	4.8
1	E	141	SER	4.8
1	E	145	SER	4.8
2	M	527	GLU	4.8
1	F	360	GLN	4.8
1	A	204	ALA	4.8
1	F	295	ALA	4.8
1	B	73	HIS	4.8
1	D	201	VAL	4.8
1	E	123	MET	4.8
1	D	326	LYS	4.8
1	B	369	ILE	4.8
2	N	450	GLU	4.8
1	B	141	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	331	ALA	4.8
1	C	26	ALA	4.8
1	E	98	PRO	4.8
1	D	16	LEU	4.8
1	D	209	VAL	4.8
1	D	256	ARG	4.8
1	A	274	ILE	4.8
1	D	268	GLY	4.8
1	B	316	GLU	4.8
1	C	214	GLU	4.8
1	C	224	GLU	4.8
1	F	288	ASP	4.8
1	A	200	PHE	4.8
1	F	181	ALA	4.8
1	F	9	VAL	4.8
1	F	161	HIS	4.8
1	E	218	TYR	4.8
1	B	146	GLY	4.8
1	D	90	PHE	4.8
1	C	236	LEU	4.8
1	A	326	LYS	4.8
1	C	269	MET	4.8
1	D	291	LYS	4.8
1	B	62	ARG	4.8
1	E	111	ASN	4.8
2	M	502	ARG	4.8
2	N	431	ARG	4.8
1	A	217	CYS	4.8
1	C	76	ILE	4.8
1	F	248	ILE	4.8
1	F	316	GLU	4.8
1	C	19	ALA	4.8
1	C	114	ALA	4.8
1	C	228	ALA	4.8
1	B	120	THR	4.8
1	E	27	PRO	4.8
1	E	271	SER	4.8
1	A	255	PHE	4.7
1	B	321	ALA	4.7
1	C	361	GLU	4.7
2	M	449	GLU	4.7
1	B	16	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	142	LEU	4.7
1	C	61	LYS	4.7
1	A	269	MET	4.7
1	B	196	ARG	4.7
1	D	148	THR	4.7
1	D	235	SER	4.7
1	F	143	TYR	4.7
1	B	125	GLU	4.7
1	B	195	GLU	4.7
1	C	67	LEU	4.7
1	E	142	LEU	4.7
1	E	230	ALA	4.7
1	C	238	LYS	4.7
1	A	353	GLN	4.7
1	C	96	VAL	4.7
1	B	82	MET	4.7
1	F	283	MET	4.7
1	E	126	THR	4.7
1	A	225	ASN	4.7
1	A	366	GLY	4.7
1	C	36	GLY	4.7
1	B	135	ALA	4.7
1	C	242	LEU	4.7
1	F	29	ALA	4.7
2	N	521	ARG	4.7
1	B	100	GLU	4.7
1	E	93	GLU	4.7
2	N	438	GLU	4.7
1	A	102	PRO	4.7
1	F	263	GLN	4.7
1	F	79	TRP	4.7
1	E	149	THR	4.7
1	E	11	ASP	4.7
1	B	275	HIS	4.7
1	F	13	GLY	4.7
1	A	216	LEU	4.7
1	B	236	LEU	4.7
1	F	185	LEU	4.7
1	C	272	ALA	4.7
1	E	28	ARG	4.7
1	E	231	ALA	4.7
1	C	54	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	269	MET	4.7
2	N	486	GLU	4.7
1	D	70	PRO	4.7
1	F	172	PRO	4.7
1	E	257	CYS	4.7
1	F	86	TRP	4.7
1	C	77	THR	4.7
2	M	480	ILE	4.7
1	B	302	GLY	4.7
1	C	188	TYR	4.7
1	E	153	LEU	4.7
1	E	239	SER	4.7
1	F	338	SER	4.7
2	N	455	ARG	4.7
1	C	174	ALA	4.7
1	A	259	GLU	4.7
1	C	315	LYS	4.6
1	D	206	ARG	4.6
1	E	74	GLY	4.6
1	A	143	TYR	4.6
1	F	294	TYR	4.6
1	C	181	ALA	4.6
1	F	31	PHE	4.6
1	A	111	ASN	4.6
1	F	162	ASN	4.6
1	A	121	GLN	4.6
1	A	136	ILE	4.6
2	N	458	ILE	4.6
1	B	191	LYS	4.6
1	D	303	THR	4.6
1	E	249	THR	4.6
1	E	324	THR	4.6
1	F	229	THR	4.6
1	C	256	ARG	4.6
1	F	320	LEU	4.6
1	A	201	VAL	4.6
1	D	11	ASP	4.6
1	F	19	ALA	4.6
1	D	82	MET	4.6
1	E	132	MET	4.6
2	M	479	ASN	4.6
1	A	258	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	237	GLU	4.6
1	D	353	GLN	4.6
1	B	28	ARG	4.6
1	E	320	LEU	4.6
1	F	193	LEU	4.6
1	A	209	VAL	4.6
1	B	29	ALA	4.6
1	C	133	TYR	4.6
1	A	325	MET	4.6
1	B	119	MET	4.6
1	B	253	GLU	4.6
1	B	328	LYS	4.6
1	B	254	ARG	4.6
1	B	140	LEU	4.6
1	B	278	THR	4.6
1	A	23	GLY	4.6
1	A	342	GLY	4.6
1	E	15	GLY	4.6
1	E	55	GLY	4.6
1	E	174	ALA	4.6
1	C	306	TYR	4.6
2	M	497	LYS	4.6
1	D	300	SER	4.6
1	D	344	SER	4.6
1	F	345	ILE	4.6
1	D	167	GLU	4.6
2	N	495	GLU	4.6
2	N	514	ARG	4.6
1	A	252	ASN	4.6
1	D	171	LEU	4.6
1	D	221	LEU	4.6
1	D	318	THR	4.6
1	B	138	ALA	4.6
1	E	58	ALA	4.6
1	E	266	PHE	4.6
1	F	173	HIS	4.6
1	B	279	TYR	4.5
1	C	198	TYR	4.5
2	N	480	ILE	4.5
1	A	125	GLU	4.5
1	A	226	GLU	4.5
1	E	316	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	340	TRP	4.5
1	F	152	VAL	4.5
1	A	89	THR	4.5
1	D	19	ALA	4.5
1	E	303	THR	4.5
1	D	269	MET	4.5
1	A	206	ARG	4.5
1	C	362	TYR	4.5
1	B	122	ILE	4.5
1	B	307	PRO	4.5
1	C	142	LEU	4.5
1	D	205	GLU	4.5
1	D	224	GLU	4.5
1	F	334	GLU	4.5
2	M	495	GLU	4.5
2	M	504	LEU	4.5
1	E	158	GLY	4.5
1	E	190	MET	4.5
1	E	143	TYR	4.5
1	C	16	LEU	4.5
1	E	236	LEU	4.5
1	E	286	ASP	4.5
1	B	213	LYS	4.5
1	C	225	ASN	4.5
1	C	297	ASN	4.5
2	M	493	LYS	4.5
1	C	7	ALA	4.5
1	E	331	ALA	4.5
1	A	116	ARG	4.5
1	A	290	ARG	4.5
1	E	248	ILE	4.5
1	E	369	ILE	4.5
1	E	242	LEU	4.5
1	D	117	GLU	4.5
1	C	265	SER	4.5
1	E	124	PHE	4.5
1	F	124	PHE	4.5
1	F	92	ASN	4.5
1	A	192	ILE	4.5
1	E	317	ILE	4.5
1	C	221	LEU	4.5
1	E	112	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	238	LYS	4.5
1	A	205	GLU	4.5
1	B	361	GLU	4.5
1	C	117	GLU	4.5
2	M	473	GLU	4.5
1	B	30	VAL	4.5
1	B	95	ARG	4.5
1	C	124	PHE	4.5
1	D	116	ARG	4.5
1	B	108	ALA	4.4
1	C	157	ASP	4.4
1	C	273	GLY	4.4
1	D	150	GLY	4.4
1	F	81	ASP	4.4
1	A	327	ILE	4.4
1	E	216	LEU	4.4
1	F	188	TYR	4.4
2	N	525	TYR	4.4
1	B	336	LYS	4.4
1	C	264	PRO	4.4
1	F	254	ARG	4.4
1	C	90	PHE	4.4
1	A	110	LEU	4.4
1	C	34	ILE	4.4
1	C	287	ILE	4.4
1	E	232	SER	4.4
1	E	348	SER	4.4
1	D	120	THR	4.4
1	F	315	LYS	4.4
1	D	262	PHE	4.4
1	F	57	GLU	4.4
1	B	220	ALA	4.4
1	E	245	GLY	4.4
1	A	122	ILE	4.4
1	B	285	CYS	4.4
1	C	349	LEU	4.4
1	E	261	LEU	4.4
1	A	77	THR	4.4
1	D	106	THR	4.4
1	E	333	PRO	4.4
1	B	255	PHE	4.4
1	C	262	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	123	MET	4.4
1	F	167	GLU	4.4
1	D	220	ALA	4.4
1	E	251	GLY	4.4
1	E	171	LEU	4.4
1	F	8	LEU	4.4
1	B	280	ASN	4.4
1	E	164	PRO	4.4
1	B	325	MET	4.4
1	A	22	ALA	4.4
1	A	220	ALA	4.4
1	E	208	ILE	4.4
1	F	64	ILE	4.4
1	F	256	ARG	4.4
1	A	14	SER	4.4
1	A	322	PRO	4.4
1	F	280	ASN	4.4
1	F	305	MET	4.3
1	B	171	LEU	4.3
1	D	330	ILE	4.3
1	E	373	LYS	4.3
1	F	236	LEU	4.3
1	E	314	GLN	4.3
1	D	210	ARG	4.3
1	A	371	HIS	4.3
1	B	304	THR	4.3
1	C	194	THR	4.3
1	E	278	THR	4.3
1	C	190	MET	4.3
1	D	259	GLU	4.3
1	E	57	GLU	4.3
1	F	62	ARG	4.3
1	F	139	VAL	4.3
1	F	209	VAL	4.3
1	C	249	THR	4.3
1	C	109	PRO	4.3
1	B	216	LEU	4.3
1	C	92	ASN	4.3
1	D	329	ILE	4.3
1	F	290	ARG	4.3
2	M	438	GLU	4.3
1	A	263	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	370	VAL	4.3
1	B	186	THR	4.3
1	F	216	LEU	4.3
1	C	211	ASP	4.3
1	A	245	GLY	4.3
1	C	177	ARG	4.3
1	C	308	GLY	4.3
1	D	301	GLY	4.3
1	A	224	GLU	4.3
2	M	477	GLN	4.3
1	A	339	VAL	4.3
1	F	238	LYS	4.3
1	A	82	MET	4.3
1	C	283	MET	4.3
1	E	313	MET	4.3
1	A	109	PRO	4.3
1	A	108	ALA	4.3
1	C	147	ARG	4.3
1	F	138	ALA	4.3
1	F	335	ARG	4.3
1	B	306	TYR	4.3
1	C	294	TYR	4.3
1	B	162	ASN	4.3
1	E	125	GLU	4.3
2	M	434	LYS	4.2
1	E	325	MET	4.2
1	F	227	MET	4.2
1	A	261	LEU	4.2
1	C	255	PHE	4.2
1	F	27	PRO	4.2
1	C	278	THR	4.2
1	F	272	ALA	4.2
1	E	282	ILE	4.2
1	F	289	ILE	4.2
1	C	166	TYR	4.2
2	M	459	GLY	4.2
1	B	276	GLU	4.2
1	E	259	GLU	4.2
1	C	152	VAL	4.2
1	B	299	MET	4.2
1	F	299	MET	4.2
1	A	131	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	341	ILE	4.2
1	F	175	ILE	4.2
1	E	146	GLY	4.2
1	F	205	GLU	4.2
1	A	162	ASN	4.2
1	F	311	ASP	4.2
1	C	300	SER	4.2
1	C	257	CYS	4.2
1	E	9	VAL	4.2
1	F	201	VAL	4.2
1	B	261	LEU	4.2
1	E	95	ARG	4.2
1	E	140	LEU	4.2
1	E	255	PHE	4.2
1	F	149	THR	4.2
1	C	279	TYR	4.2
1	F	133	TYR	4.2
2	M	450	GLU	4.2
1	D	219	VAL	4.2
1	B	177	ARG	4.2
1	C	246	GLN	4.2
1	E	285	CYS	4.2
1	E	360	GLN	4.2
1	A	340	TRP	4.2
1	D	20	GLY	4.2
1	D	55	GLY	4.2
1	E	194	THR	4.2
1	F	63	GLY	4.2
1	F	342	GLY	4.2
1	A	328	LYS	4.2
2	M	488	GLU	4.2
1	A	335	ARG	4.2
1	F	178	LEU	4.2
1	D	127	PHE	4.2
1	E	223	PHE	4.2
2	M	467	SER	4.2
1	C	85	ILE	4.2
1	C	208	ILE	4.2
1	C	356	TRP	4.2
2	M	454	LEU	4.1
1	C	222	ASP	4.1
1	A	272	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	271	SER	4.1
1	E	365	ALA	4.1
1	F	365	ALA	4.1
1	F	264	PRO	4.1
1	C	268	GLY	4.1
1	B	303	THR	4.1
2	M	516	ARG	4.1
1	B	247	VAL	4.1
1	C	104	LEU	4.1
1	A	276	GLU	4.1
1	A	176	MET	4.1
1	A	190	MET	4.1
1	A	227	MET	4.1
1	B	118	LYS	4.1
1	B	272	ALA	4.1
1	D	162	ASN	4.1
1	D	319	ALA	4.1
1	B	271	SER	4.1
1	E	363	ASP	4.1
1	C	98	PRO	4.1
1	D	164	PRO	4.1
1	D	281	SER	4.1
1	B	251	GLY	4.1
1	C	197	GLY	4.1
2	M	445	ARG	4.1
1	C	105	LEU	4.1
1	B	352	PHE	4.1
1	F	18	LYS	4.1
1	D	263	GLN	4.1
2	N	507	ARG	4.1
1	B	159	VAL	4.1
1	E	176	MET	4.1
1	B	226	GLU	4.1
1	B	373	LYS	4.1
1	E	64	ILE	4.1
1	F	319	ALA	4.1
1	D	121	GLN	4.1
1	D	332	PRO	4.1
2	M	505	SER	4.1
1	A	129	VAL	4.1
1	F	163	VAL	4.1
1	C	274	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	295	ALA	4.1
2	N	477	GLN	4.1
1	F	36	GLY	4.1
1	C	280	ASN	4.0
1	B	61	LYS	4.0
1	E	113	LYS	4.0
1	E	336	LYS	4.0
1	F	82	MET	4.0
1	F	359	LYS	4.0
1	A	10	CYS	4.0
1	B	267	ILE	4.0
1	F	282	ILE	4.0
1	A	347	ALA	4.0
1	E	22	ALA	4.0
1	F	210	ARG	4.0
1	C	243	PRO	4.0
1	A	74	GLY	4.0
1	F	105	LEU	4.0
1	F	301	GLY	4.0
1	C	161	HIS	4.0
1	D	118	LYS	4.0
1	C	305	MET	4.0
1	C	325	MET	4.0
1	E	227	MET	4.0
1	F	222	ASP	4.0
1	B	282	ILE	4.0
1	F	262	PHE	4.0
2	N	484	ARG	4.0
1	A	83	GLU	4.0
1	B	144	ALA	4.0
1	F	310	ALA	4.0
1	E	307	PRO	4.0
1	A	238	LYS	4.0
1	D	342	GLY	4.0
1	E	219	VAL	4.0
1	C	309	ILE	4.0
1	F	179	ASP	4.0
2	M	514	ARG	4.0
2	M	521	ARG	4.0
1	B	291	LYS	4.0
2	M	446	GLN	4.0
1	C	369	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	165	ILE	4.0
1	B	265	SER	4.0
1	C	106	THR	4.0
1	C	260	THR	4.0
1	E	228	ALA	4.0
1	E	304	THR	4.0
1	F	218	TYR	4.0
1	C	332	PRO	4.0
2	N	432	PRO	4.0
1	A	168	GLY	4.0
1	C	372	ARG	4.0
2	M	451	ARG	4.0
1	A	21	PHE	4.0
1	B	274	ILE	4.0
1	D	195	GLU	4.0
1	E	33	SER	4.0
2	M	437	LEU	4.0
1	B	20	GLY	3.9
1	F	257	CYS	3.9
1	A	329	ILE	3.9
1	B	287	ILE	3.9
1	B	315	LYS	3.9
1	C	68	LYS	3.9
1	D	18	LYS	3.9
1	C	125	GLU	3.9
1	C	303	THR	3.9
1	F	260	THR	3.9
1	C	154	ASP	3.9
1	F	10	CYS	3.9
1	F	266	PHE	3.9
1	A	331	ALA	3.9
1	C	331	ALA	3.9
1	F	213	LYS	3.9
1	D	226	GLU	3.9
1	F	111	ASN	3.9
1	F	125	GLU	3.9
2	M	453	GLU	3.9
1	E	96	VAL	3.9
2	M	478	ARG	3.9
2	M	498	ARG	3.9
1	D	227	MET	3.9
1	D	212	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	329	ILE	3.9
1	B	26	ALA	3.9
1	E	65	LEU	3.9
1	F	170	ALA	3.9
1	C	28	ARG	3.9
1	C	253	GLU	3.9
1	F	239	SER	3.9
1	F	309	ILE	3.9
1	F	330	ILE	3.9
1	E	315	LYS	3.9
1	F	255	PHE	3.9
1	A	349	LEU	3.9
1	A	191	LYS	3.9
1	A	153	LEU	3.9
1	A	138	ALA	3.9
1	B	214	GLU	3.8
1	C	313	MET	3.8
2	M	447	THR	3.8
1	C	336	LYS	3.8
1	F	61	LYS	3.8
1	F	251	GLY	3.8
1	A	145	SER	3.8
1	B	31	PHE	3.8
2	N	457	GLN	3.8
1	C	319	ALA	3.8
1	D	88	HIS	3.8
1	B	269	MET	3.8
1	D	343	GLY	3.8
1	C	140	LEU	3.8
1	C	153	LEU	3.8
1	A	281	SER	3.8
1	F	183	ARG	3.8
1	F	220	ALA	3.8
1	D	328	LYS	3.8
1	D	276	GLU	3.8
1	C	148	THR	3.8
1	B	139	VAL	3.8
2	M	440	LYS	3.8
1	D	305	MET	3.8
1	E	214	GLU	3.8
1	B	126	THR	3.8
1	B	148	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	335	ARG	3.8
2	M	452	LEU	3.8
2	M	441	ASN	3.8
1	C	271	SER	3.8
1	D	238	LYS	3.8
1	A	208	ILE	3.8
1	B	169	TYR	3.8
1	B	243	PRO	3.8
1	C	37	ARG	3.8
1	E	39	ARG	3.8
1	E	361	GLU	3.8
2	M	469	ARG	3.8
2	M	499	ARG	3.8
1	C	31	PHE	3.8
1	C	178	LEU	3.8
1	B	296	ASN	3.7
1	C	213	LYS	3.7
1	C	132	MET	3.7
1	B	109	PRO	3.7
1	D	153	LEU	3.7
2	M	503	LYS	3.7
1	E	299	MET	3.7
1	B	151	ILE	3.7
1	B	94	LEU	3.7
1	F	118	LYS	3.7
1	F	114	ALA	3.7
1	B	263	GLN	3.7
1	A	312	ARG	3.7
1	A	282	ILE	3.7
1	B	340	TRP	3.7
1	D	185	LEU	3.7
1	B	301	GLY	3.7
1	C	32	PRO	3.7
1	C	284	LYS	3.7
1	D	331	ALA	3.7
1	F	230	ALA	3.7
1	F	196	ARG	3.7
2	N	516	ARG	3.7
1	B	93	GLU	3.7
1	F	107	GLU	3.7
1	C	277	THR	3.7
1	F	129	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	180	LEU	3.7
1	A	158	GLY	3.7
2	M	439	GLU	3.6
2	M	448	ASP	3.6
1	B	149	THR	3.6
1	B	227	MET	3.6
1	C	176	MET	3.6
1	E	175	ILE	3.6
1	F	140	LEU	3.6
1	C	130	PRO	3.6
1	F	112	PRO	3.6
1	B	338	SER	3.6
1	F	361	GLU	3.6
1	E	337	TYR	3.6
1	B	346	LEU	3.6
1	E	349	LEU	3.6
1	F	250	ILE	3.6
1	E	328	LYS	3.6
1	D	296	ASN	3.6
1	C	220	ALA	3.6
1	E	319	ALA	3.6
1	F	270	GLU	3.6
2	N	488	GLU	3.6
1	C	299	MET	3.6
1	F	373	LYS	3.6
2	N	520	ILE	3.6
1	C	146	GLY	3.6
1	F	98	PRO	3.6
1	C	144	ALA	3.6
1	C	230	ALA	3.6
1	F	325	MET	3.6
1	A	180	LEU	3.6
2	M	443	LEU	3.6
1	F	275	HIS	3.6
1	D	9	VAL	3.6
1	E	35	VAL	3.6
1	E	201	VAL	3.6
1	E	191	LYS	3.6
1	E	213	LYS	3.6
1	C	101	HIS	3.5
1	D	62	ARG	3.5
1	A	160	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	266	PHE	3.5
1	C	156	GLY	3.5
1	B	298	VAL	3.5
1	C	29	ALA	3.5
1	D	213	LYS	3.5
1	F	328	LYS	3.5
1	E	264	PRO	3.5
2	N	513	LEU	3.5
1	E	7	ALA	3.5
1	C	102	PRO	3.5
1	B	76	ILE	3.5
1	F	233	SER	3.5
1	C	95	ARG	3.5
1	E	196	ARG	3.5
1	E	308	GLY	3.5
1	B	170	ALA	3.5
1	C	165	ILE	3.5
1	C	254	ARG	3.5
1	C	373	LYS	3.4
1	E	92	ASN	3.4
1	F	318	THR	3.4
2	N	462	LEU	3.4
1	C	258	PRO	3.4
1	E	116	ARG	3.4
1	C	107	GLU	3.4
1	F	20	GLY	3.4
1	C	116	ARG	3.4
1	C	27	PRO	3.4
1	B	257	CYS	3.4
1	E	67	LEU	3.4
1	B	197	GLY	3.4
1	E	301	GLY	3.4
1	F	116	ARG	3.4
1	A	313	MET	3.4
2	M	463	THR	3.4
1	E	300	SER	3.4
1	A	210	ARG	3.4
1	C	42	GLY	3.4
2	N	439	GLU	3.4
1	F	84	LYS	3.4
1	C	263	GLN	3.4
1	F	314	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	242	LEU	3.3
1	C	320	LEU	3.3
1	C	350	SER	3.3
1	E	217	CYS	3.3
1	C	250	ILE	3.3
1	F	71	ILE	3.3
1	A	332	PRO	3.3
1	D	302	GLY	3.3
1	F	121	GLN	3.3
2	M	444	PRO	3.3
1	C	304	THR	3.3
1	E	335	ARG	3.3
1	B	175	ILE	3.3
1	E	97	ALA	3.3
1	E	150	GLY	3.3
1	F	174	ALA	3.3
1	C	113	LYS	3.3
1	C	237	GLU	3.3
1	C	63	GLY	3.3
1	B	286	ASP	3.3
1	F	322	PRO	3.3
1	F	171	LEU	3.3
1	B	136	ILE	3.3
1	C	209	VAL	3.2
1	E	351	THR	3.2
1	B	305	MET	3.2
1	B	295	ALA	3.2
1	D	131	ALA	3.2
1	E	23	GLY	3.2
1	F	245	GLY	3.2
1	D	290	ARG	3.2
1	A	294	TYR	3.2
1	C	62	ARG	3.2
1	C	226	GLU	3.2
1	B	153	LEU	3.2
1	F	142	LEU	3.2
1	E	68	LYS	3.2
1	C	261	LEU	3.2
1	C	143	TYR	3.2
1	B	313	MET	3.2
1	B	147	ARG	3.2
1	C	318	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	11	ASP	3.2
1	F	312	ARG	3.2
2	M	466	LEU	3.2
1	A	309	ILE	3.2
1	C	357	ILE	3.2
1	B	342	GLY	3.1
1	F	217	CYS	3.1
1	A	256	ARG	3.1
1	A	137	GLN	3.1
1	C	353	GLN	3.1
1	B	284	LYS	3.1
1	E	62	ARG	3.1
1	B	27	PRO	3.1
1	B	106	THR	3.1
1	F	207	GLU	3.1
1	F	164	PRO	3.1
1	E	267	ILE	3.1
1	F	362	TYR	3.1
1	B	150	GLY	3.1
1	F	206	ARG	3.1
1	A	262	PHE	3.1
1	E	318	THR	3.0
1	D	23	GLY	3.0
1	B	174	ALA	3.0
1	C	196	ARG	3.0
1	C	18	LYS	3.0
2	M	427	LYS	3.0
1	C	163	VAL	3.0
1	C	223	PHE	3.0
1	A	277	THR	3.0
1	B	290	ARG	3.0
2	M	442	ILE	3.0
1	A	142	LEU	2.9
1	B	172	PRO	2.9
1	B	273	GLY	2.9
1	E	157	ASP	2.9
1	E	302	GLY	2.9
1	B	262	PHE	2.9
1	C	6	THR	2.9
1	D	304	THR	2.9
1	B	22	ALA	2.9
1	E	118	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	296	ASN	2.9
1	C	368	SER	2.9
1	B	161	HIS	2.9
1	B	312	ARG	2.9
2	N	469	ARG	2.9
1	A	299	MET	2.9
1	B	289	ILE	2.9
1	E	326	LYS	2.9
1	F	291	LYS	2.9
1	C	131	ALA	2.9
1	C	259	GLU	2.9
1	E	306	TYR	2.9
1	E	305	MET	2.9
1	D	359	LYS	2.8
1	E	263	GLN	2.8
1	F	83	GLU	2.8
1	A	284	LYS	2.8
1	E	156	GLY	2.8
1	E	275	HIS	2.8
2	M	432	PRO	2.8
1	E	262	PHE	2.8
1	C	317	ILE	2.8
1	B	154	ASP	2.7
1	B	245	GLY	2.7
1	B	18	LYS	2.7
1	D	186	THR	2.7
2	M	457	GLN	2.7
1	A	283	MET	2.7
1	C	93	GLU	2.7
1	D	189	LEU	2.7
1	A	188	TYR	2.7
1	B	330	ILE	2.7
1	F	150	GLY	2.7
1	F	134	VAL	2.6
1	A	215	LYS	2.6
1	E	204	ALA	2.6
1	F	186	THR	2.6
1	B	332	PRO	2.6
1	E	61	LYS	2.6
1	F	243	PRO	2.5
1	F	153	LEU	2.5
1	A	219	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	124	PHE	2.5
1	B	158	GLY	2.5
1	C	312	ARG	2.5
1	A	213	LYS	2.5
1	F	268	GLY	2.5
1	C	158	GLY	2.4
2	N	517	LYS	2.4
1	A	228	ALA	2.4
1	B	256	ARG	2.4
1	A	248	ILE	2.4
1	C	108	ALA	2.4
1	C	266	PHE	2.4
1	B	215	LYS	2.3
1	C	150	GLY	2.3
1	A	231	ALA	2.2
1	B	281	SER	2.2
1	A	254	ARG	2.2
1	C	316	GLU	2.1
1	B	264	PRO	2.1
1	F	168	GLY	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
5	GOL	E	1378	6/6	0.33	0.36	82,82,82,82	0
3	ATP	D	1376	31/31	0.40	0.41	131,131,131,131	0
5	GOL	N	1529	6/6	0.40	0.39	99,99,99,99	0

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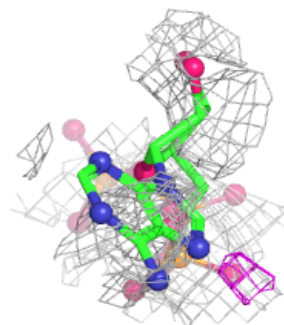
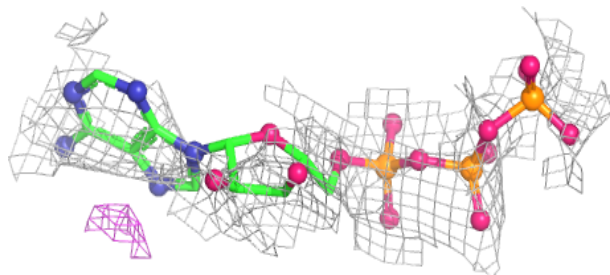
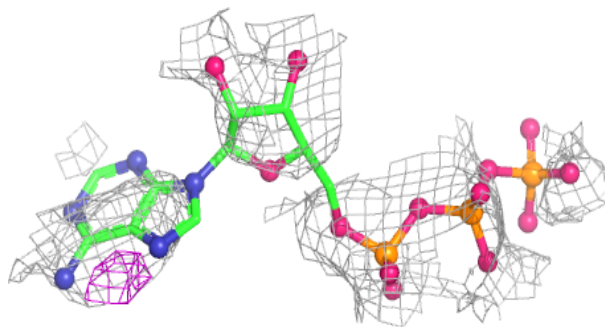
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	F	1376	31/31	0.42	0.37	91,91,91,91	0
3	ATP	A	1376	31/31	0.45	0.37	99,99,99,99	0
5	GOL	B	1378	6/6	0.47	0.64	89,89,89,89	0
4	MG	F	1377	1/1	0.48	0.31	53,53,53,53	0
3	ATP	E	1376	31/31	0.49	0.35	112,112,112,112	0
3	ATP	C	1376	31/31	0.49	0.33	84,84,84,84	0
3	ATP	B	1376	31/31	0.49	0.36	81,81,81,81	0
5	GOL	F	1378	6/6	0.53	0.38	64,64,64,64	0
5	GOL	A	1379	6/6	0.53	0.50	89,89,89,89	0
4	MG	E	1377	1/1	0.56	0.29	50,50,50,50	0
5	GOL	C	1379	6/6	0.59	0.46	80,80,80,80	0
5	GOL	A	1378	6/6	0.59	0.37	73,73,73,73	0
4	MG	B	1377	1/1	0.60	0.20	39,39,39,39	0
5	GOL	C	1378	6/6	0.61	0.36	68,68,68,68	0
4	MG	A	1377	1/1	0.68	0.28	42,42,42,42	0
4	MG	D	1377	1/1	0.81	0.23	56,56,56,56	0
4	MG	C	1377	1/1	0.83	0.13	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

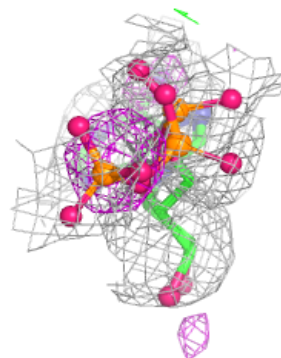
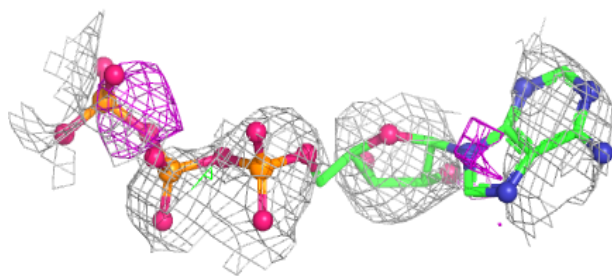
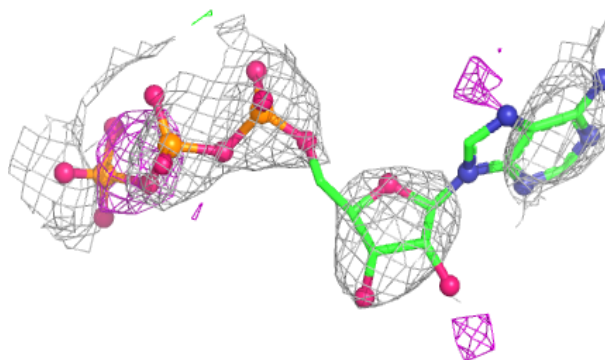
Electron density around ATP D 1376:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

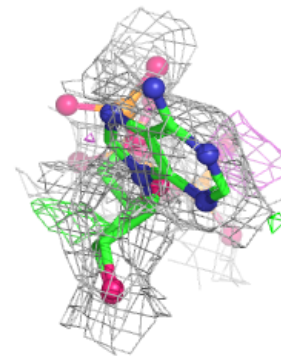
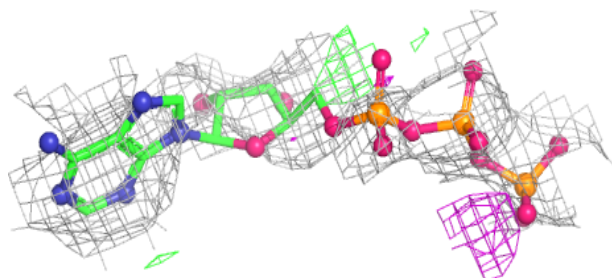
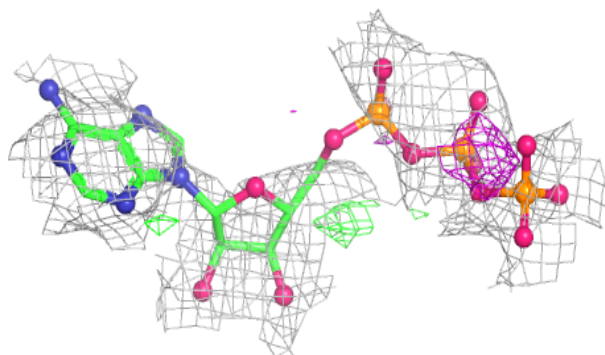


Electron density around ATP F 1376:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

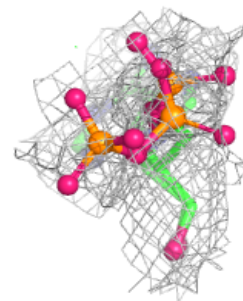
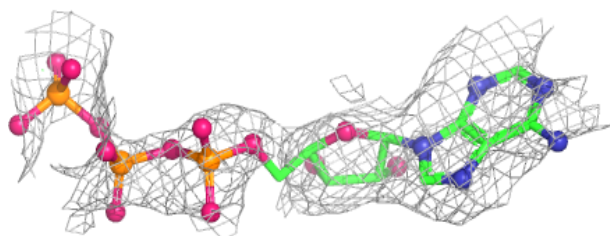
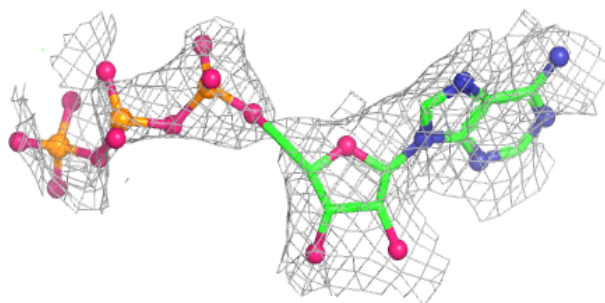
**Electron density around ATP A 1376:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

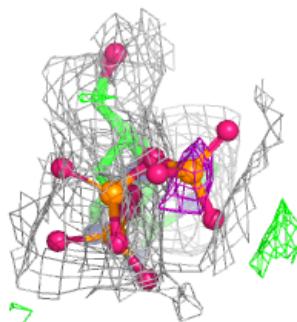
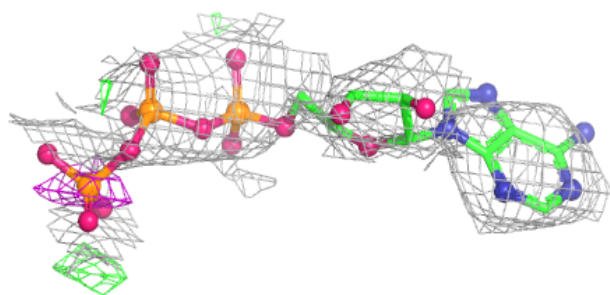
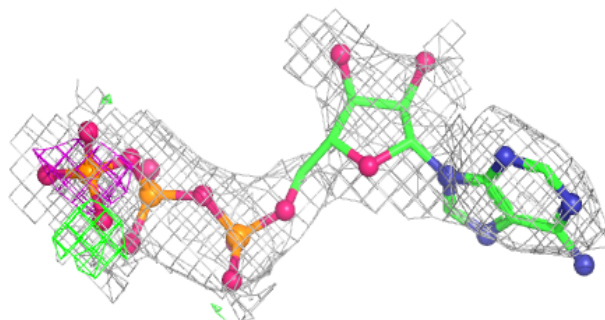


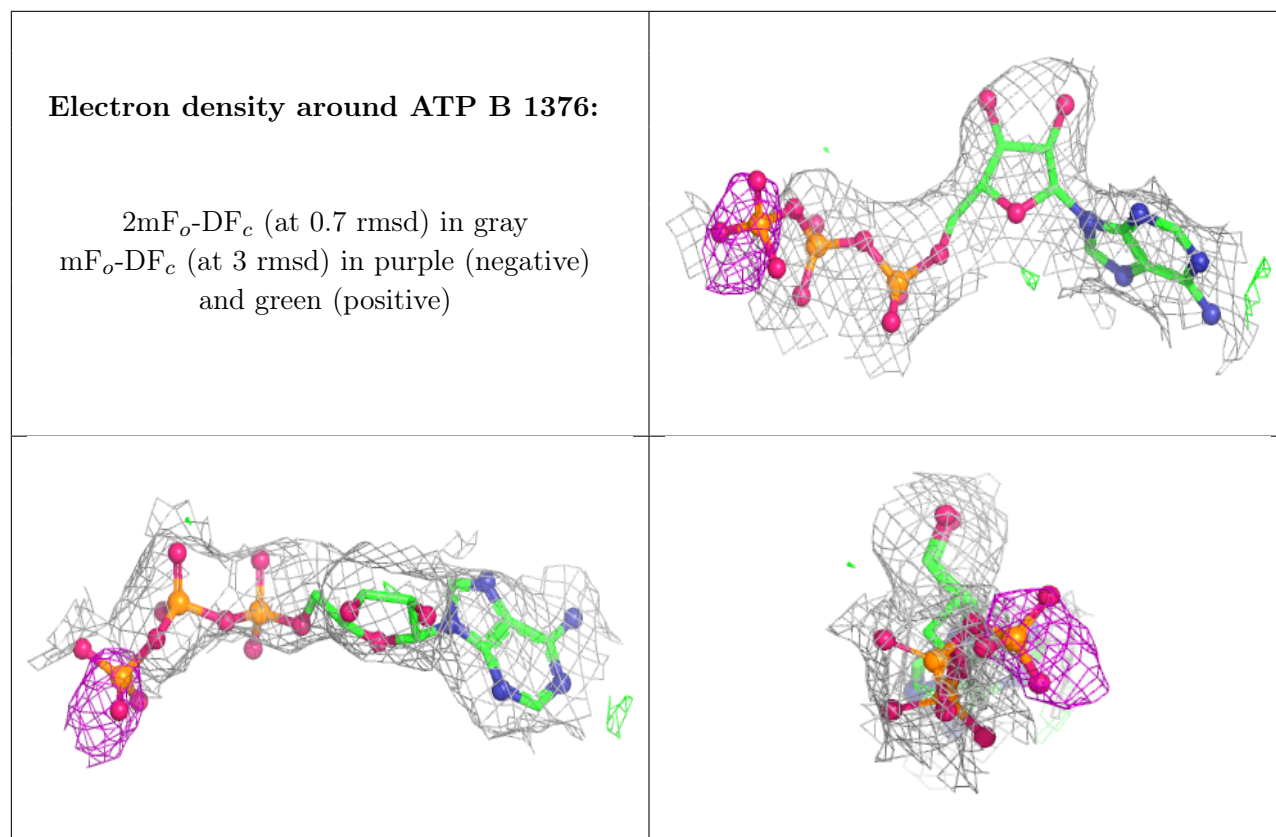
Electron density around ATP E 1376:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP C 1376:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.