



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 09:44 AM EDT

PDB ID : 5CBM / pdb_00005cbm
Title : Crystal structure of PfA-M17 with virtual ligand inhibitor
Authors : Ruggeri, C.; Drinkwater, N.; McGowan, S.
Deposited on : 2015-07-01
Resolution : 2.30 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

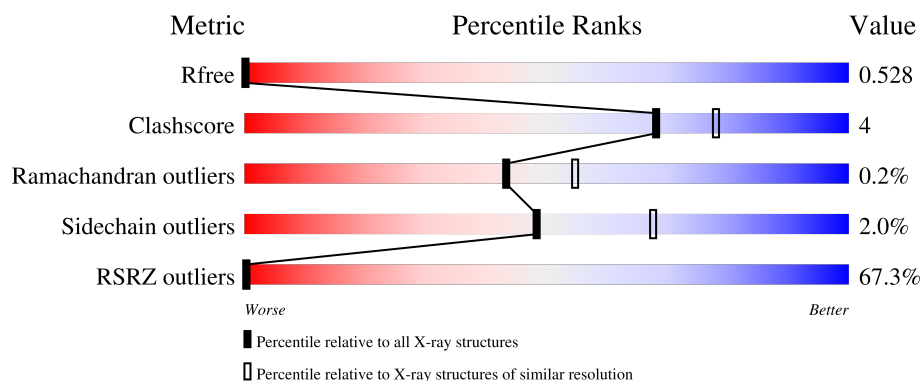
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	519	63% 91% 8%
1	B	519	74% 89% 10%
1	C	519	66% 90% 9%
1	D	519	59% 88% 10%
1	E	519	61% 89% 8%

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Mol	Chain	Length	Quality of chain
1	F	519	72% 90% 8% ..
1	G	519	63% 90% 9%
1	H	519	75% 89% 9% .
1	I	519	71% 92% 7%
1	J	519	65% 86% 12% ..
1	K	519	64% 91% 7% .
1	L	519	68% 89% 9% ..

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
7	SO4	A	712	-	-	X	X
7	SO4	C	709	-	-	-	X
7	SO4	C	710	-	-	-	X
7	SO4	C	711	-	-	-	X
7	SO4	E	709	-	-	-	X
7	SO4	F	707	-	-	-	X
7	SO4	G	711	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 50850 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 M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			3971	2547	639	766	19			
1	B	516	Total	C	N	O	S	0	0	0
			3902	2509	633	740	20			
1	C	517	Total	C	N	O	S	0	0	0
			3941	2532	637	753	19			
1	D	514	Total	C	N	O	S	0	0	0
			3920	2526	633	741	20			
1	E	509	Total	C	N	O	S	0	0	0
			3893	2509	624	741	19			
1	F	511	Total	C	N	O	S	0	0	0
			3851	2477	622	733	19			
1	G	519	Total	C	N	O	S	0	0	0
			3974	2554	640	760	20			
1	H	517	Total	C	N	O	S	1	0	0
			3902	2508	632	743	19			
1	I	517	Total	C	N	O	S	0	0	0
			3951	2540	637	754	20			
1	J	514	Total	C	N	O	S	0	0	0
			3926	2529	633	744	20			
1	K	509	Total	C	N	O	S	0	0	0
			3884	2504	623	738	19			
1	L	511	Total	C	N	O	S	0	0	0
			3848	2475	622	732	19			

There are 36 discrepancies between the modelled and reference sequences:

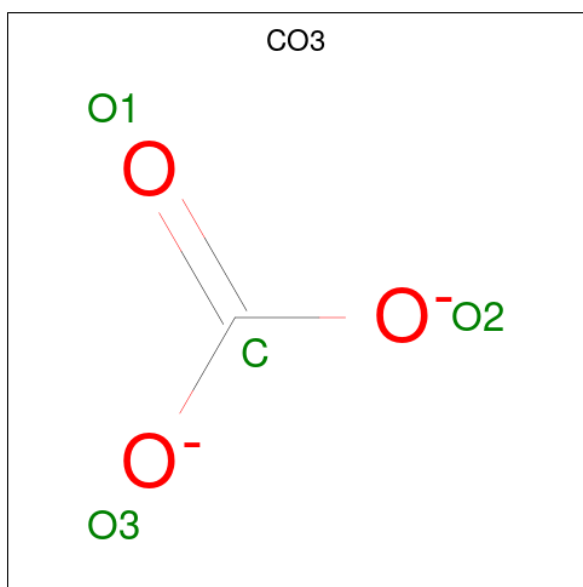
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	546	GLN	ASN	engineered mutation	UNP A0A024V0B1

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).

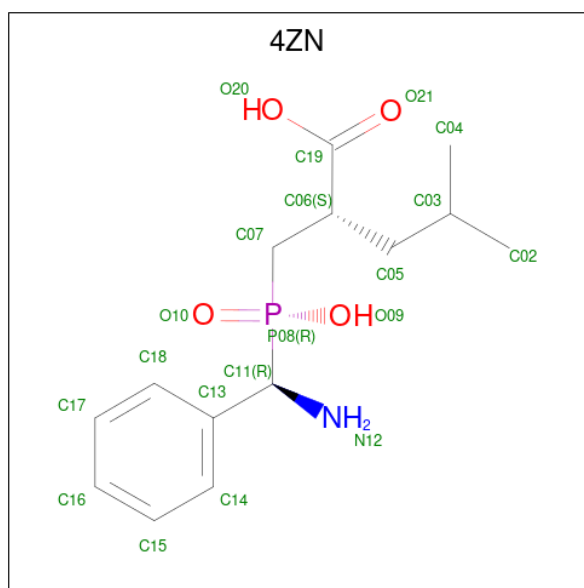


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		
2	G	1	Total	C	O	0	0
			4	1	3		
2	H	1	Total	C	O	0	0
			4	1	3		
2	I	1	Total	C	O	0	0
			4	1	3		
2	J	1	Total	C	O	0	0
			4	1	3		
2	K	1	Total	C	O	0	0
			4	1	3		
2	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

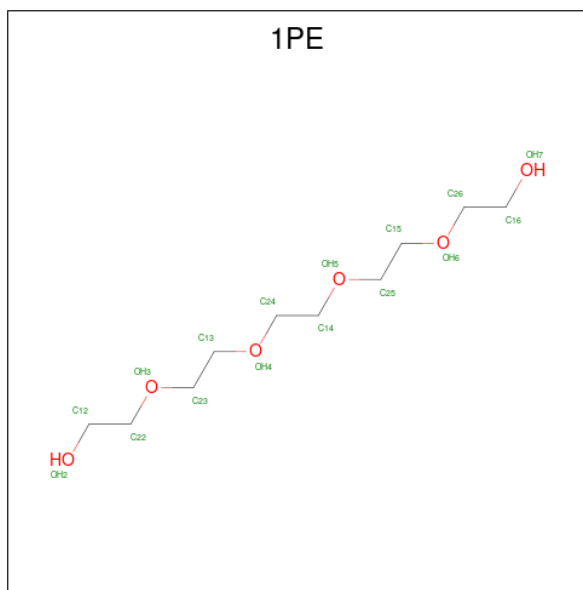
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total 2 Zn 2 2	0	0
3	B	2	Total 2 Zn 2 2	0	0
3	C	2	Total 2 Zn 2 2	0	0
3	D	2	Total 2 Zn 2 2	0	0
3	E	2	Total 2 Zn 2 2	0	0
3	F	2	Total 2 Zn 2 2	0	0
3	G	2	Total 2 Zn 2 2	0	0
3	H	2	Total 2 Zn 2 2	0	0
3	I	2	Total 2 Zn 2 2	0	0
3	J	2	Total 2 Zn 2 2	0	0
3	K	2	Total 2 Zn 2 2	0	0
3	L	2	Total 2 Zn 2 2	0	0

- Molecule 4 is (2S)-2-[[[(R)-[(R)-amino(phenyl)methyl](hydroxy)phosphoryl]methyl]-4-methylpentanoic acid (CCD ID: 4ZN) (formula: C₁₄H₂₂NO₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			20	14	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			20	14	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	I	1	Total	C	N	O	P	0	0
			12	8	1	2	1		
4	J	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			14	10	1	2	1		
4	L	1	Total	C	N	O	P	0	0
			16	10	1	4	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



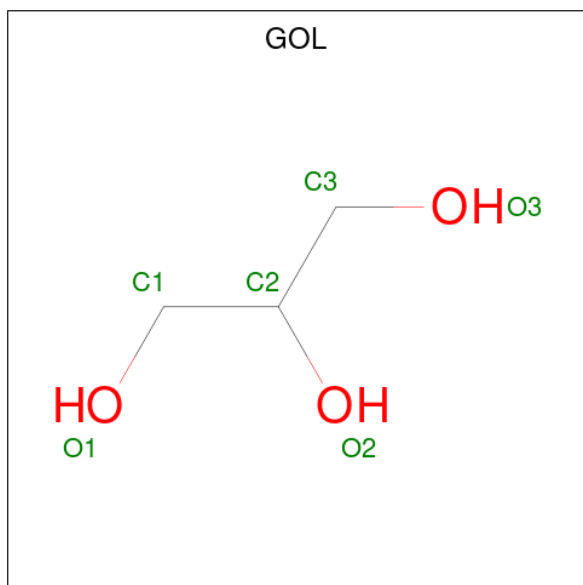
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 6 3	0	0
5	A	1	Total C O 12 8 4	0	0
5	B	1	Total C O 10 7 3	0	0
5	B	1	Total C O 10 7 3	0	0
5	C	1	Total C O 13 9 4	0	0
5	C	1	Total C O 9 6 3	0	0
5	D	1	Total C O 10 7 3	0	0
5	D	1	Total C O 10 7 3	0	0
5	E	1	Total C O 12 8 4	0	0
5	E	1	Total C O 12 8 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	G	1	Total C O 9 6 3	0	0
5	G	1	Total C O 6 4 2	0	0
5	G	1	Total C O 6 4 2	0	0
5	H	1	Total C O 10 7 3	0	0
5	H	1	Total C O 10 7 3	0	0
5	I	1	Total C O 12 8 4	0	0
5	I	1	Total C O 11 8 3	0	0
5	J	1	Total C O 11 7 4	0	0
5	J	1	Total C O 11 7 4	0	0
5	J	1	Total C O 10 6 4	0	0
5	K	1	Total C O 12 8 4	0	0

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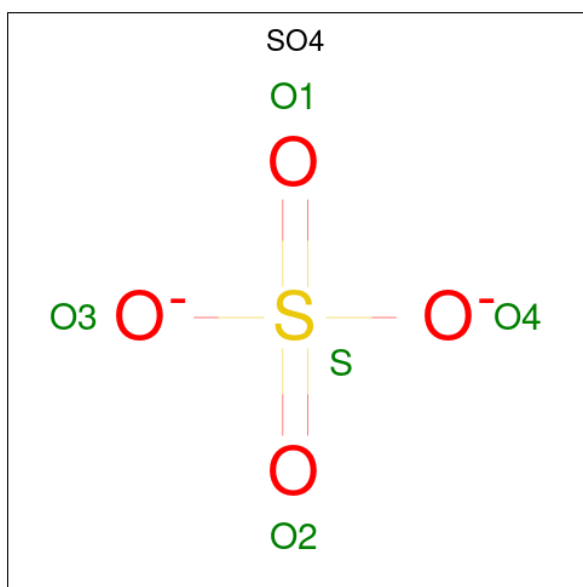
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			12	8	4		
5	L	1	Total	C	O	0	0
			7	4	3		
5	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	265	Total O 265 265	0	0
8	B	246	Total O 246 246	0	0
8	C	277	Total O 277 277	0	0
8	D	283	Total O 283 283	0	0
8	E	322	Total O 322 322	0	0

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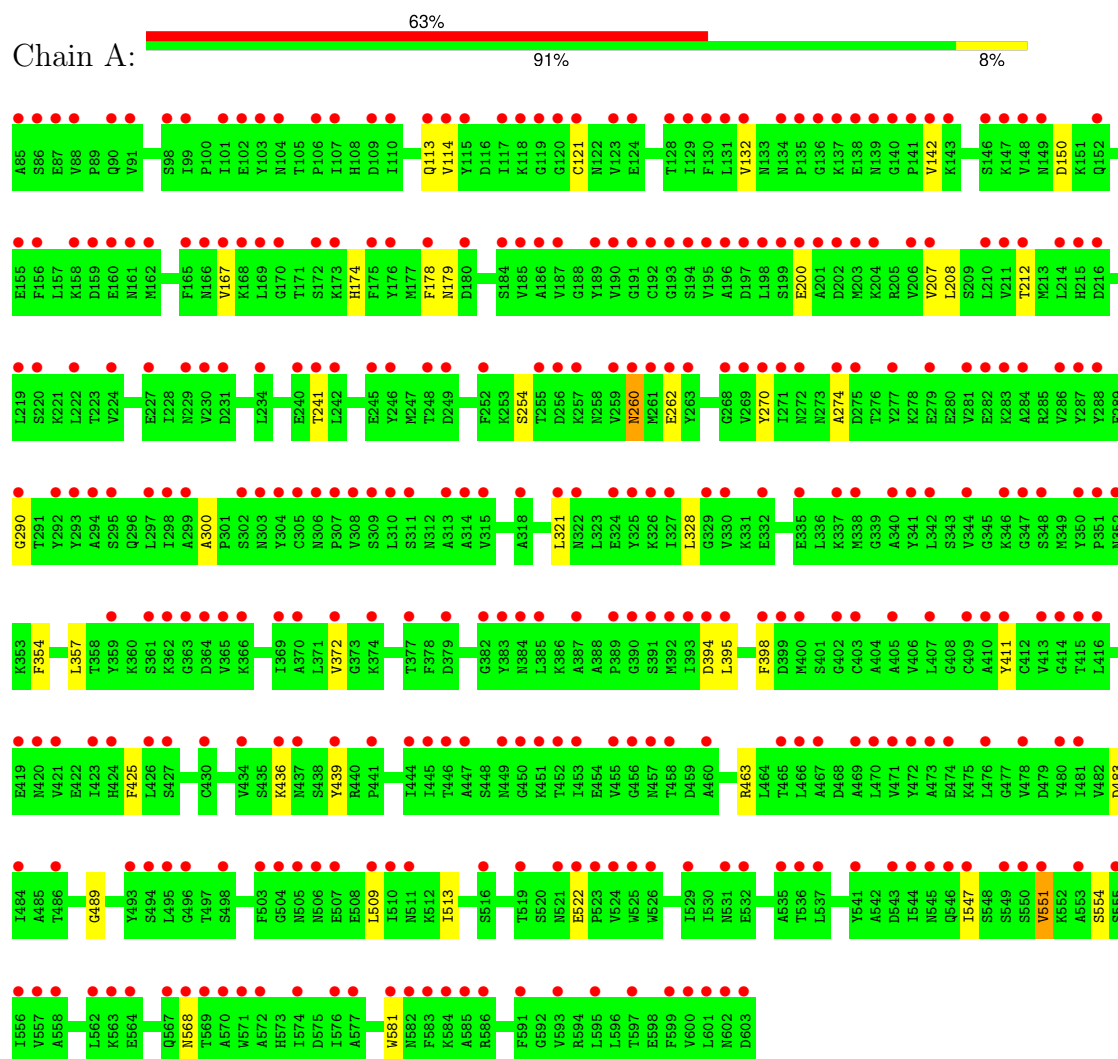
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	245	Total 245	O 245	0	0
8	G	281	Total 281	O 281	0	0
8	H	220	Total 220	O 220	0	0
8	I	272	Total 272	O 272	0	0
8	J	287	Total 287	O 287	0	0
8	K	283	Total 283	O 283	0	0
8	L	240	Total 240	O 240	0	0

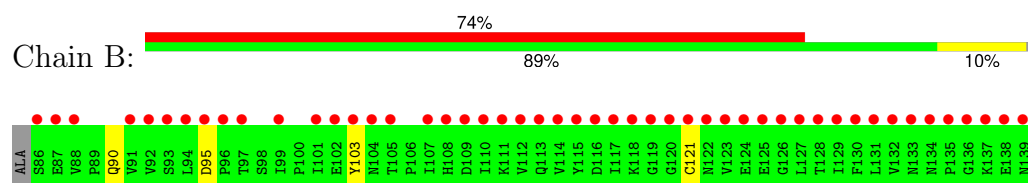
3 Residue-property plots

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.

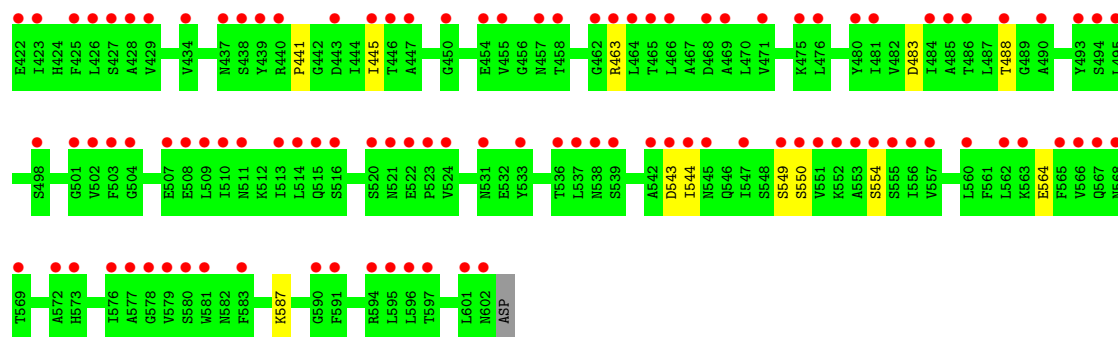
• Molecule 1: M17 family aminopeptidase



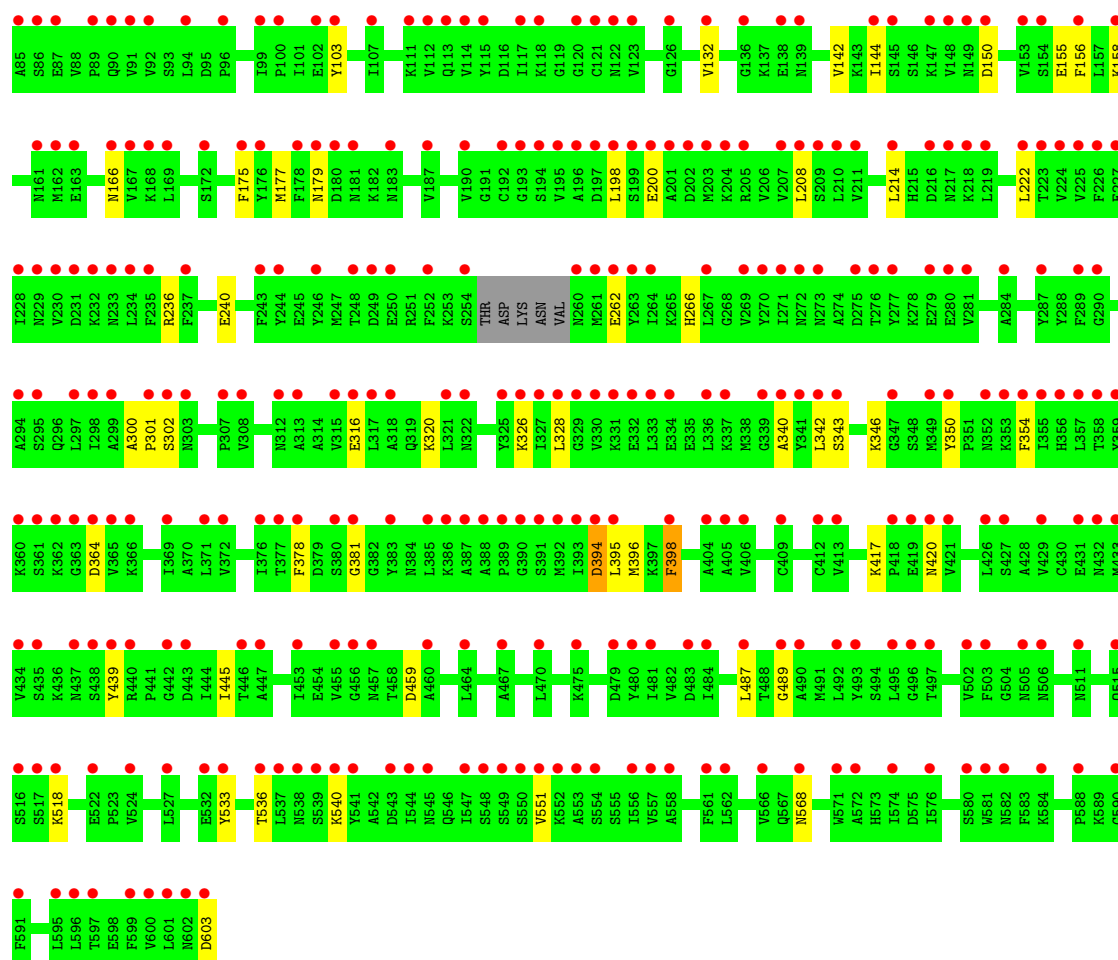
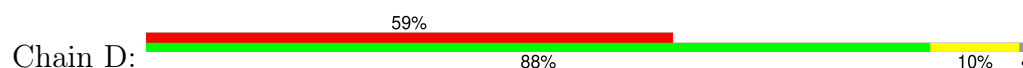
• Molecule 1: M17 family aminopeptidase



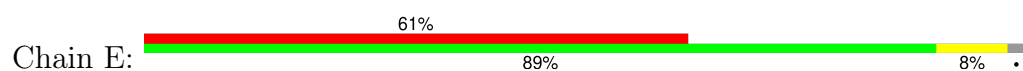


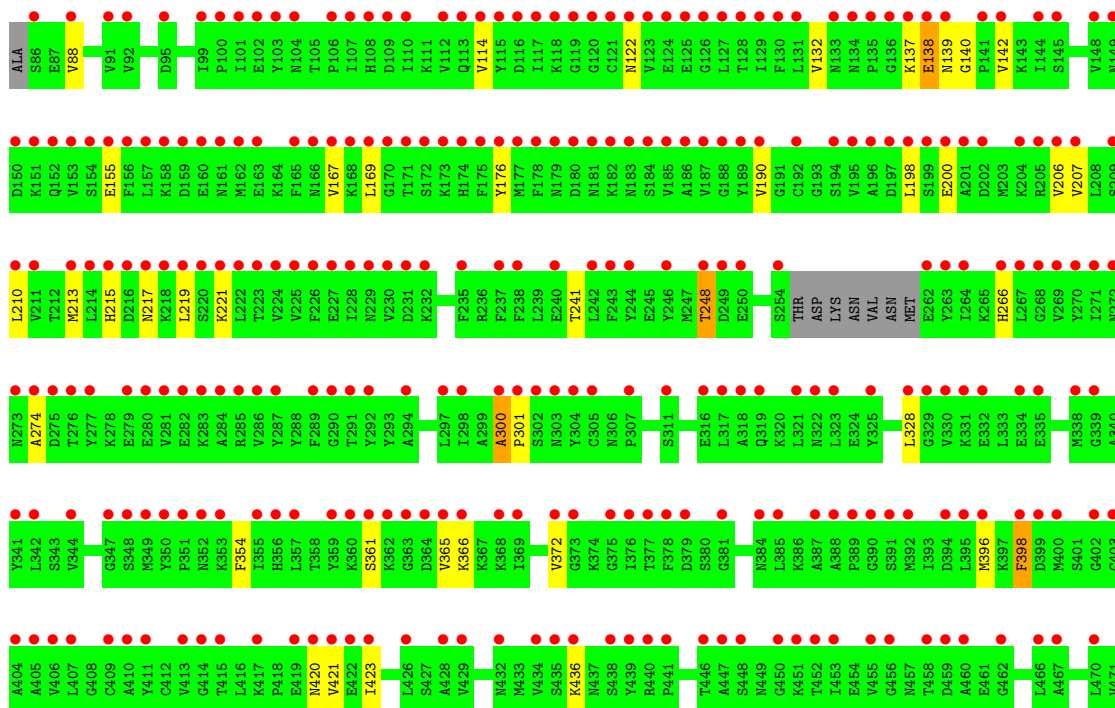


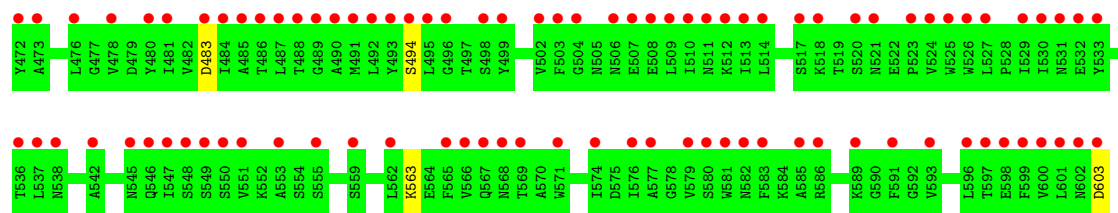
• Molecule 1: M17 family aminopeptidase



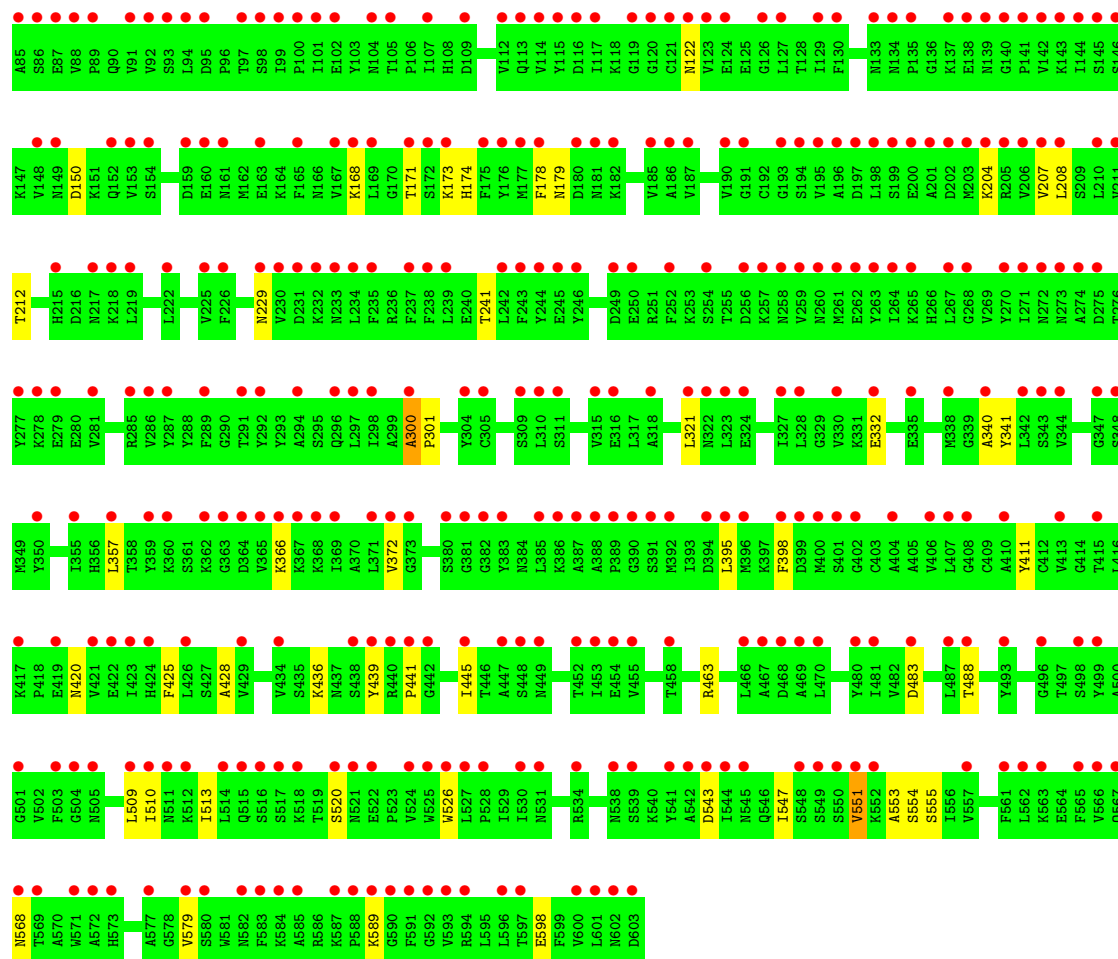
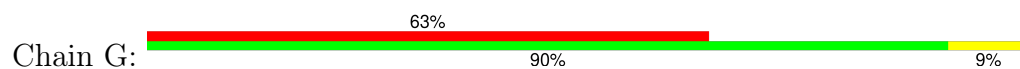
• Molecule 1: M17 family aminopeptidase



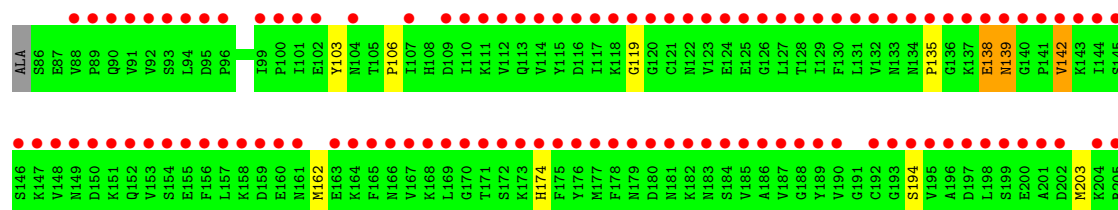
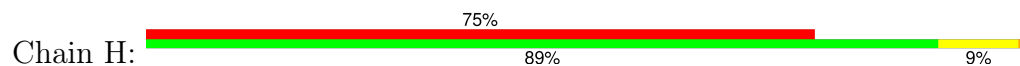


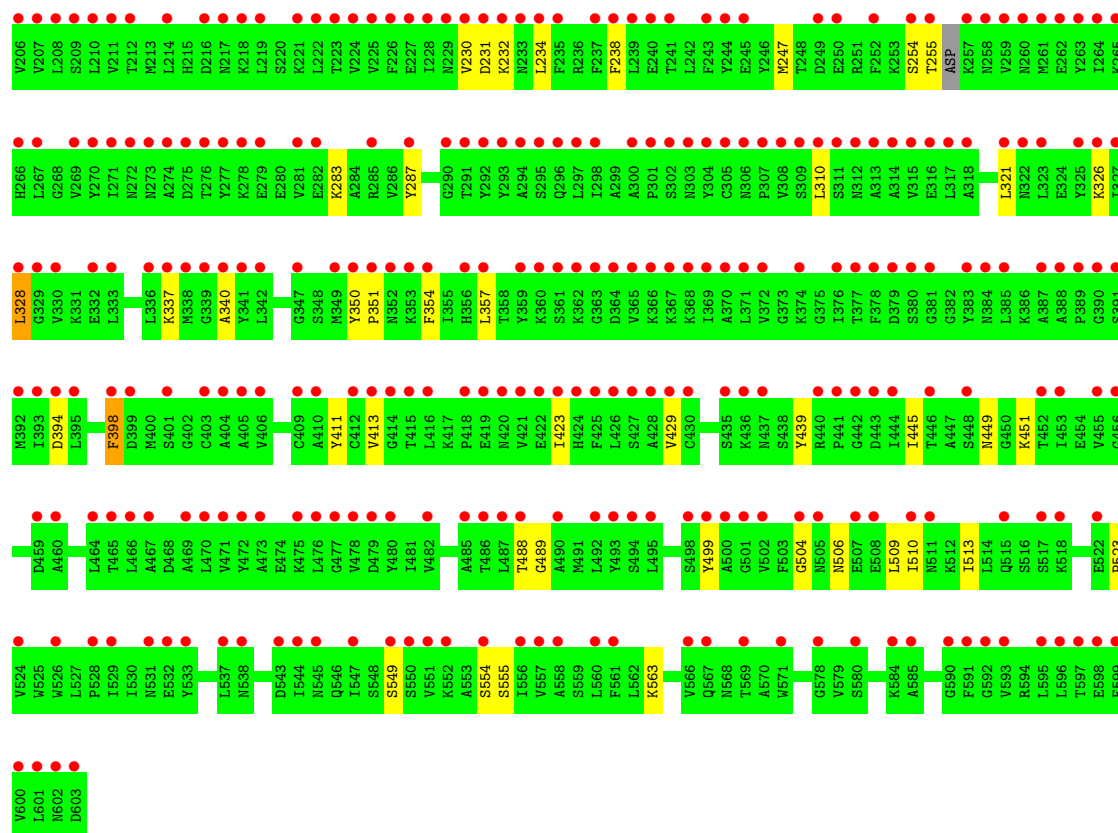


● Molecule 1: M17 family aminopeptidase

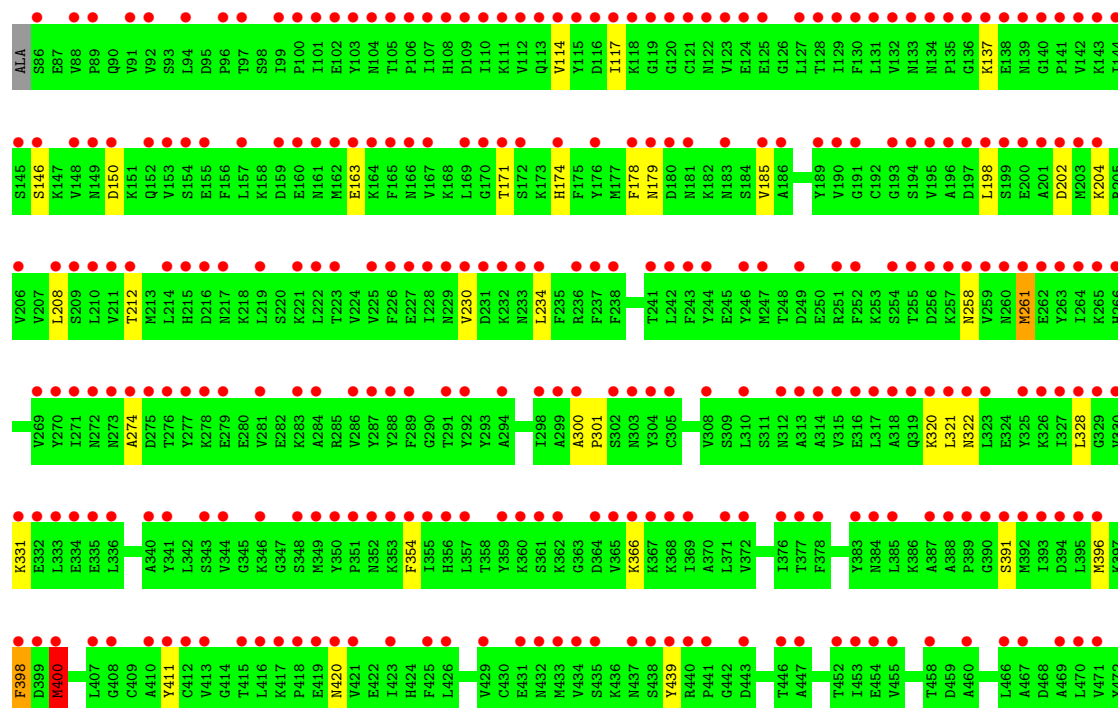
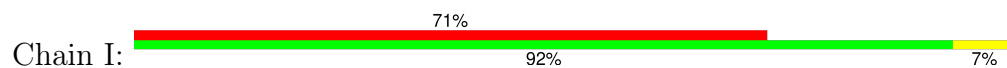


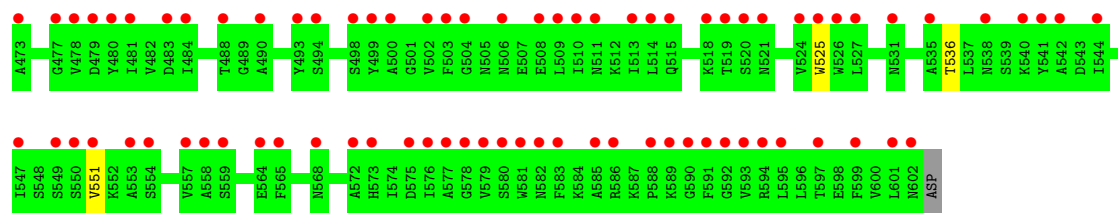
● Molecule 1: M17 family aminopeptidase



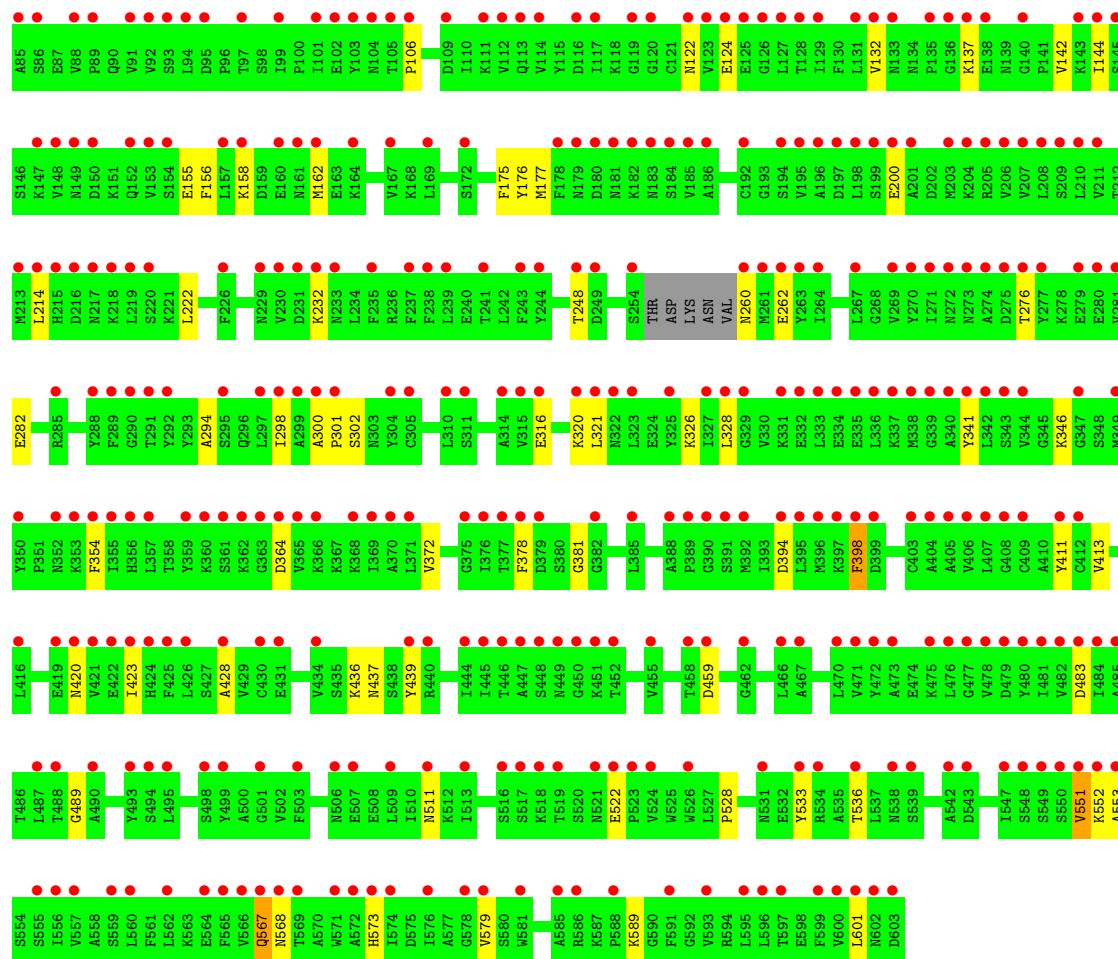
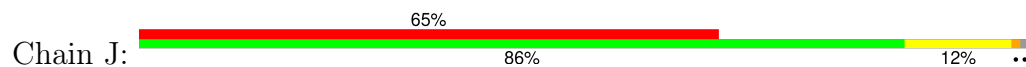


• Molecule 1: M17 family aminopeptidase

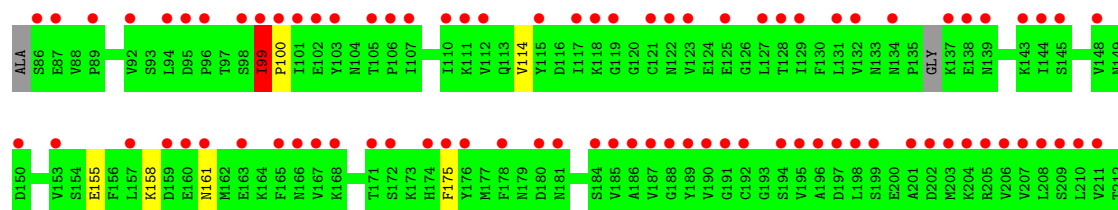


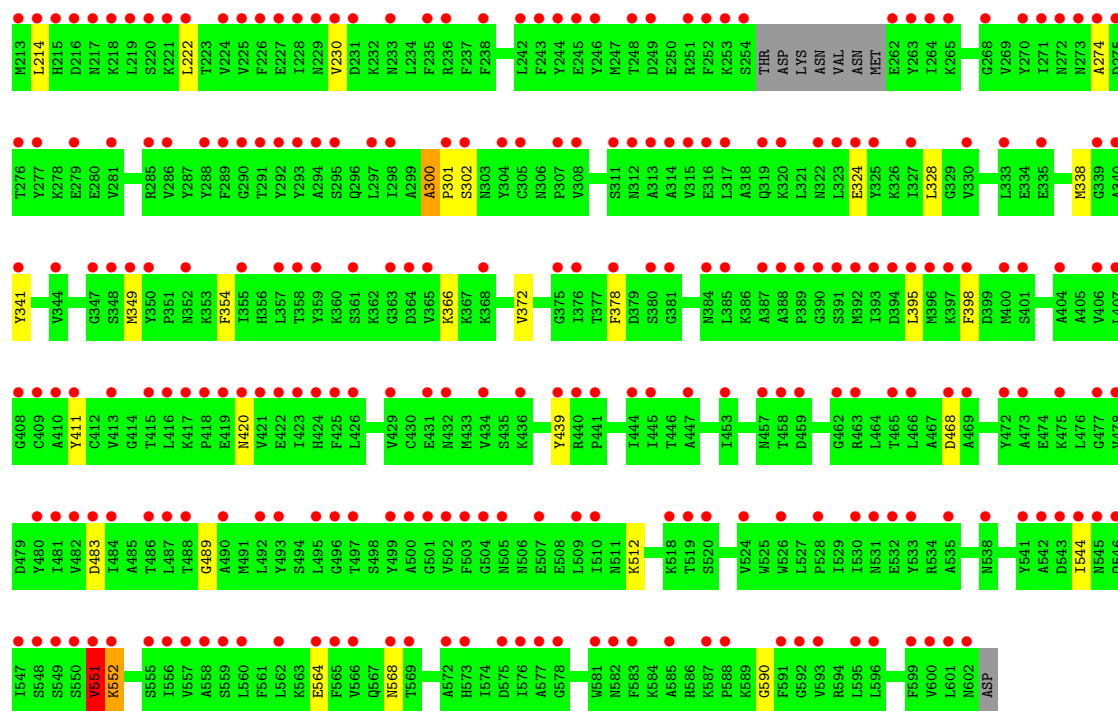


● Molecule 1: M17 family aminopeptidase

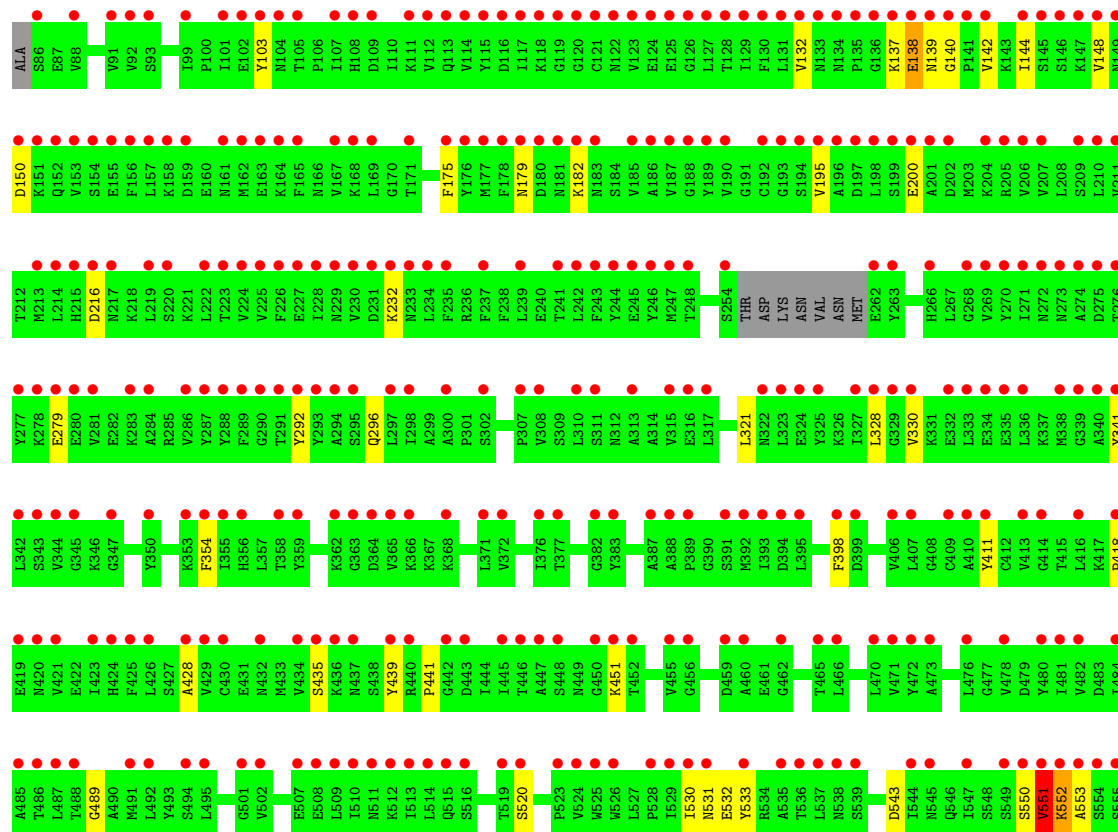
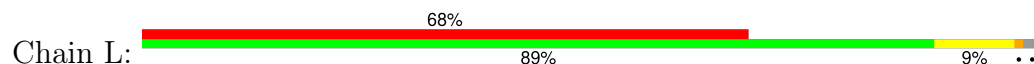


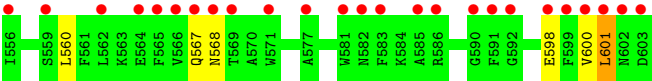
● Molecule 1: M17 family aminopeptidase





- Molecule 1: M17 family aminopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.09Å 177.73Å 230.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.30 48.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.98-2.30) 99.9 (48.98-2.30)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.182 , 0.235 0.515 , 0.528	Depositor DCC
R_{free} test set	15701 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	50850	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6001e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CO3, 1PE, ZN, SO4, 4ZN, GOL

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	0.53	0/4052	0.83	7/5502 (0.1%)
1	B	0.50	0/3979	0.80	0/5405
1	C	0.53	0/4019	0.80	2/5456 (0.0%)
1	D	0.52	0/3997	0.80	2/5422 (0.0%)
1	E	0.53	0/3969	0.81	3/5384 (0.1%)
1	F	0.51	0/3928	0.82	3/5342 (0.1%)
1	G	0.52	0/4052	0.83	3/5497 (0.1%)
1	H	0.48	0/3979	0.81	1/5407 (0.0%)
1	I	0.51	0/4029	0.80	1/5466 (0.0%)
1	J	0.52	0/4003	0.80	2/5430 (0.0%)
1	K	0.52	0/3960	0.86	9/5372 (0.2%)
1	L	0.51	0/3925	0.82	3/5338 (0.1%)
All	All	0.52	0/47892	0.81	36/65021 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	2
1	L	0	1
All	All	0	3

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	99	ILE	CA-C-N	13.36	136.54	119.84
1	K	99	ILE	C-N-CA	13.36	136.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	551	VAL	N-CA-C	9.33	120.14	110.62
1	A	522	GLU	CA-C-N	8.28	128.77	119.83
1	A	522	GLU	C-N-CA	8.28	128.77	119.83
1	K	99	ILE	C-N-CD	-8.16	91.55	125.00
1	L	138	GLU	N-CA-C	7.87	122.88	113.28
1	I	400	MET	CA-CB-CG	-6.89	100.31	114.10
1	F	138	GLU	N-CA-C	6.89	119.70	110.88
1	K	551	VAL	CA-C-N	6.51	133.42	121.70
1	K	551	VAL	C-N-CA	6.51	133.42	121.70
1	G	300	ALA	CA-C-N	6.40	127.84	119.84
1	G	300	ALA	C-N-CA	6.40	127.84	119.84
1	A	551	VAL	N-CA-C	6.19	122.22	109.34
1	A	300	ALA	CA-C-N	6.04	126.01	120.03
1	A	300	ALA	C-N-CA	6.04	126.01	120.03
1	L	551	VAL	CA-C-N	5.95	132.41	121.70
1	L	551	VAL	C-N-CA	5.95	132.41	121.70
1	J	522	GLU	CA-C-N	5.84	126.03	119.90
1	J	522	GLU	C-N-CA	5.84	126.03	119.90
1	K	590	GLY	N-CA-C	-5.73	106.26	115.08
1	H	119	GLY	N-CA-C	-5.67	106.70	114.64
1	E	400	MET	CA-CB-CG	-5.55	103.01	114.10
1	F	300	ALA	CA-C-N	5.50	125.80	119.92
1	F	300	ALA	C-N-CA	5.50	125.80	119.92
1	A	260	ASN	CB-CG-ND2	-5.46	108.21	116.40
1	D	350	TYR	CA-C-N	5.39	125.31	119.76
1	D	350	TYR	C-N-CA	5.39	125.31	119.76
1	C	400	MET	CA-CB-CG	-5.37	103.35	114.10
1	K	99	ILE	N-CA-C	5.34	120.41	108.88
1	A	290	GLY	N-CA-C	-5.34	106.18	112.64
1	E	99	ILE	CA-C-N	-5.24	114.52	119.76
1	E	99	ILE	C-N-CA	-5.24	114.52	119.76
1	C	274	ALA	N-CA-C	5.14	116.96	111.36
1	K	300	ALA	CA-C-N	5.07	125.34	119.92
1	K	300	ALA	C-N-CA	5.07	125.34	119.92

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	551	VAL	Peptide
1	K	99	ILE	Peptide
1	L	551	VAL	Peptide

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	3971	0	3875	26	0
1	B	3902	0	3787	31	0
1	C	3941	0	3855	28	0
1	D	3920	0	3851	31	0
1	E	3893	0	3820	26	0
1	F	3851	0	3726	21	0
1	G	3974	0	3899	31	0
1	H	3902	0	3774	34	0
1	I	3951	0	3877	22	0
1	J	3926	0	3854	48	0
1	K	3884	0	3805	21	0
1	L	3848	0	3716	32	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	16	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	9	2	0
4	C	16	0	9	1	0
4	D	20	0	20	3	0
4	E	20	0	19	2	0
4	F	16	0	9	0	0
4	G	16	0	9	0	0
4	H	16	0	9	1	0
4	I	12	0	7	0	0
4	J	16	0	9	2	0
4	K	14	0	9	1	0
4	L	16	0	9	1	0
5	A	21	0	22	0	0
5	B	20	0	20	2	0
5	C	22	0	24	1	0
5	D	20	0	20	2	0
5	E	24	0	28	2	0
5	F	10	0	13	0	0
5	G	21	0	20	4	0
5	H	20	0	20	1	0
5	I	23	0	26	2	0
5	J	32	0	39	12	0
5	K	24	0	28	2	0
5	L	17	0	21	6	0
6	A	6	0	8	0	0
7	A	25	0	0	2	0
7	B	5	0	0	0	0
7	C	25	0	0	2	0
7	D	5	0	0	1	0
7	E	15	0	0	1	0
7	F	10	0	0	0	0
7	G	20	0	0	2	0
7	I	10	0	0	0	0
7	J	10	0	0	0	0
7	K	10	0	0	0	0
7	L	5	0	0	0	0
8	A	265	0	0	3	0
8	B	246	0	0	3	0
8	C	277	0	0	3	0
8	D	283	0	0	5	0
8	E	322	0	0	5	0
8	F	245	0	0	4	0
8	G	281	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	220	0	0	3	0
8	I	272	0	0	3	0
8	J	287	0	0	5	0
8	K	283	0	0	1	0
8	L	240	0	0	4	0
All	All	50850	0	46255	339	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 4.

All (339) 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:J:320:LYS:HZ1	5:J:706:1PE:H151	1.30	0.96
1:J:489:GLY:N	4:J:704:4ZN:O20	2.06	0.88
1:L:532:GLU:HB2	5:L:705:1PE:H142	1.55	0.87
1:B:320:LYS:HZ1	5:B:706:1PE:H241	1.39	0.85
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.65	0.78
1:B:504:GLY:HA3	1:B:510:ILE:HD11	1.68	0.76
1:J:320:LYS:HZ1	5:J:706:1PE:H141	1.51	0.75
4:B:704:4ZN:H20	4:B:704:4ZN:H16	1.69	0.73
1:H:139:ASN:HD22	1:H:139:ASN:N	1.86	0.73
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.55	0.71
1:E:489:GLY:N	4:E:704:4ZN:O20	2.21	0.70
1:C:411:TYR:HE1	5:C:706:1PE:H232	1.58	0.69
1:K:338:MET:HE3	1:K:468:ASP:HB3	1.73	0.69
1:J:320:LYS:NZ	5:J:706:1PE:H151	2.07	0.69
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.74	0.68
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.76	0.68
1:C:587:LYS:NZ	8:C:802:HOH:O	2.24	0.67
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.74	0.67
1:A:260:ASN:O	8:A:801:HOH:O	2.12	0.67
1:B:332:GLU:OE2	8:B:801:HOH:O	2.13	0.66
1:E:262:GLU:N	8:E:805:HOH:O	2.27	0.66
5:J:705:1PE:H242	1:L:451:LYS:HE3	1.77	0.66
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.78	0.65
1:L:216:ASP:OD1	8:L:801:HOH:O	2.15	0.65
1:K:411:TYR:HE1	5:K:706:1PE:H241	1.62	0.65
1:E:230:VAL:HG22	1:E:234:LEU:HD23	1.79	0.64
1:A:113:GLN:NE2	8:A:805:HOH:O	2.31	0.64
1:D:603:ASP:O	8:D:802:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.79	0.64
1:G:122:ASN:HD22	5:G:706:1PE:H142	1.64	0.63
1:D:417:LYS:O	8:D:801:HOH:O	2.15	0.63
1:H:138:GLU:C	1:H:139:ASN:HD22	2.07	0.63
1:L:138:GLU:N	1:L:139:ASN:HA	2.13	0.63
4:D:704:4ZN:O20	8:D:803:HOH:O	2.16	0.62
1:I:366:LYS:HG3	1:I:420:ASN:HB3	1.80	0.62
1:A:463:ARG:NH1	7:A:712:SO4:O3	2.30	0.62
1:H:232:LYS:NZ	8:H:806:HOH:O	2.32	0.62
1:E:338:MET:HE3	1:E:468:ASP:HB3	1.82	0.61
1:F:190:VAL:HG11	1:F:206:VAL:HG13	1.83	0.61
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.81	0.61
1:J:282:GLU:OE1	8:J:801:HOH:O	2.16	0.61
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.82	0.61
1:J:122:ASN:OD1	1:J:124:GLU:HG2	2.01	0.60
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.83	0.60
1:B:248:THR:HG21	1:B:261:MET:HE1	1.83	0.60
1:F:603:ASP:O	8:F:801:HOH:O	2.17	0.60
1:L:182:LYS:O	8:L:802:HOH:O	2.16	0.59
1:E:164:LYS:NZ	8:E:810:HOH:O	2.35	0.59
1:K:338:MET:HE2	1:K:341:TYR:HD2	1.67	0.59
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.83	0.59
1:K:489:GLY:H	4:K:704:4ZN:C19	2.16	0.59
1:H:489:GLY:N	4:H:704:4ZN:O20	2.30	0.58
1:E:411:TYR:HE1	5:E:706:1PE:H241	1.68	0.58
1:F:137:LYS:CB	1:F:140:GLY:H	2.16	0.58
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.85	0.58
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.84	0.58
1:L:551:VAL:HA	1:L:552:LYS:CB	2.33	0.58
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.85	0.57
1:L:137:LYS:CB	1:L:140:GLY:H	2.18	0.57
1:G:208:LEU:O	1:G:212:THR:HG23	2.05	0.57
1:B:103:TYR:CD2	5:B:706:1PE:H132	2.40	0.57
1:D:533:TYR:O	1:D:536:THR:HG22	2.05	0.57
1:F:176:TYR:OH	1:F:217:ASN:OD1	2.13	0.57
1:E:483:ASP:OD1	1:E:573:HIS:ND1	2.35	0.57
1:H:504:GLY:HA3	1:H:510:ILE:HD11	1.87	0.57
1:J:156:PHE:O	1:J:162:MET:HE3	2.05	0.57
1:K:411:TYR:CE1	5:K:706:1PE:H241	2.40	0.57
1:D:487:LEU:O	4:D:704:4ZN:H17	2.04	0.57
1:J:436:LYS:HG3	1:K:349:MET:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.86	0.57
1:C:275:ASP:HA	1:C:278:LYS:HG3	1.86	0.57
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.70	0.56
1:L:530:ILE:HA	5:L:705:1PE:H152	1.86	0.56
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.88	0.56
1:G:207:VAL:HG11	1:G:241:THR:HG22	1.87	0.56
1:E:530:ILE:HD12	1:E:556:ILE:HD13	1.88	0.56
1:A:207:VAL:HG11	1:A:241:THR:HG22	1.87	0.56
1:L:232:LYS:NZ	1:L:279:GLU:OE2	2.31	0.56
1:B:207:VAL:HG11	1:B:241:THR:HG22	1.86	0.55
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.89	0.55
1:H:142:VAL:HG22	1:H:162:MET:HB3	1.89	0.55
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.89	0.55
1:K:114:VAL:HG12	1:K:274:ALA:HB1	1.88	0.55
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.72	0.55
5:J:705:1PE:H261	1:L:543:ASP:HB3	1.88	0.54
1:L:530:ILE:HG23	5:L:705:1PE:H141	1.89	0.54
1:C:90:GLN:HB3	1:C:95:ASP:HB2	1.90	0.54
1:I:391:SER:OG	8:I:801:HOH:O	2.17	0.54
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.90	0.54
1:A:489:GLY:N	4:A:704:4ZN:O21	2.35	0.54
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.89	0.54
1:H:174:HIS:HB3	1:L:175:PHE:CD2	2.43	0.53
1:J:533:TYR:O	1:J:536:THR:HG22	2.08	0.53
5:J:705:1PE:H262	1:L:451:LYS:HG2	1.89	0.53
1:G:411:TYR:HE1	5:G:705:1PE:H131	1.73	0.53
1:D:394:ASP:OD1	1:D:394:ASP:N	2.35	0.53
1:A:260:ASN:ND2	1:D:166:ASN:HB3	2.24	0.53
1:A:547:ILE:HA	7:A:712:SO4:O3	2.09	0.53
1:E:400:MET:HE2	1:E:404:ALA:HB2	1.90	0.53
1:J:579:VAL:O	1:J:589:LYS:HD2	2.09	0.53
1:H:103:TYR:CD2	5:H:705:1PE:H221	2.43	0.53
1:J:316:GLU:HG3	5:J:706:1PE:H262	1.89	0.53
1:B:528:PRO:HB3	1:E:525:TRP:CZ3	2.44	0.52
1:I:258:ASN:HB3	1:I:261:MET:HB2	1.91	0.52
1:H:139:ASN:N	1:H:139:ASN:ND2	2.57	0.52
1:B:506:ASN:O	1:B:510:ILE:HG12	2.09	0.52
1:F:563:LYS:NZ	8:F:802:HOH:O	2.19	0.52
1:D:540:LYS:NZ	8:D:811:HOH:O	2.43	0.52
1:I:174:HIS:NE2	8:I:810:HOH:O	2.32	0.52
1:E:86:SER:HB2	1:E:312:ASN:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:413:VAL:HG11	1:H:423:ILE:HD13	1.92	0.52
1:J:132:VAL:HG11	1:J:144:ILE:HD13	1.91	0.52
1:C:390:GLY:N	7:C:708:SO4:O2	2.43	0.51
1:J:260:ASN:N	8:J:808:HOH:O	2.42	0.51
1:A:395:LEU:HD11	1:A:581:TRP:CD1	2.45	0.51
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.92	0.51
1:L:567:GLN:HG3	8:L:986:HOH:O	2.10	0.51
1:A:208:LEU:O	1:A:212:THR:HG23	2.10	0.51
1:D:103:TYR:N	7:D:707:SO4:O3	2.30	0.51
1:I:198:LEU:HD22	1:I:202:ASP:HB3	1.92	0.51
1:K:338:MET:HE2	1:K:341:TYR:CD2	2.45	0.51
5:J:705:1PE:H262	1:L:451:LYS:HE2	1.93	0.51
1:F:122:ASN:HB3	8:F:966:HOH:O	2.11	0.50
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.46	0.50
1:E:346:LYS:NZ	8:E:808:HOH:O	2.33	0.50
1:G:122:ASN:ND2	5:G:706:1PE:H142	2.25	0.50
1:H:563:LYS:HE2	8:H:870:HOH:O	2.11	0.50
1:B:174:HIS:CE1	1:B:213:MET:HE2	2.46	0.50
1:D:302:SER:OG	1:D:378:PHE:HB2	2.12	0.50
1:G:551:VAL:HG12	1:G:553:ALA:H	1.76	0.50
1:F:221:LYS:HG3	1:F:266:HIS:HB2	1.93	0.49
1:J:326:LYS:NZ	8:J:810:HOH:O	2.45	0.49
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.94	0.49
1:B:520:SER:HB3	1:B:598:GLU:HG3	1.92	0.49
1:C:112:VAL:HG22	1:C:267:LEU:HB3	1.95	0.49
1:D:316:GLU:HG3	5:D:705:1PE:H221	1.95	0.49
1:L:139:ASN:N	8:L:810:HOH:O	2.43	0.49
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.48	0.49
1:A:150:ASP:OD2	1:A:179:ASN:HB2	2.12	0.49
1:G:463:ARG:NH1	7:G:711:SO4:O2	2.45	0.49
1:E:551:VAL:HG12	1:E:553:ALA:H	1.77	0.49
1:A:372:VAL:O	1:A:483:ASP:HA	2.13	0.49
1:L:489:GLY:N	4:L:704:4ZN:O21	2.25	0.49
1:B:90:GLN:HB3	1:B:95:ASP:HB2	1.95	0.49
1:C:117:ILE:HD13	1:C:270:TYR:HB3	1.95	0.48
1:F:138:GLU:N	1:F:139:ASN:HA	2.27	0.48
1:L:137:LYS:C	1:L:139:ASN:HA	2.38	0.48
1:A:254:SER:HB3	1:C:543:ASP:OD2	2.13	0.48
1:I:178:PHE:CZ	1:K:155:GLU:HG2	2.43	0.48
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.94	0.48
1:B:322:ASN:HB2	8:B:1011:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:520:SER:HB3	1:G:598:GLU:HG3	1.95	0.48
1:I:230:VAL:HG12	1:I:234:LEU:HD23	1.95	0.48
4:E:704:4ZN:H20	4:E:704:4ZN:H15	1.96	0.48
1:G:366:LYS:HG3	1:G:420:ASN:HB3	1.96	0.48
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.95	0.48
1:C:398:PHE:O	1:C:401:SER:OG	2.24	0.48
1:D:266:HIS:ND1	8:D:805:HOH:O	2.23	0.48
1:B:255:THR:HA	8:B:829:HOH:O	2.13	0.47
1:B:341:TYR:CE1	1:B:428:ALA:HB1	2.49	0.47
1:D:381:GLY:HA2	1:D:459:ASP:OD1	2.14	0.47
1:F:366:LYS:HG3	1:F:420:ASN:HB3	1.96	0.47
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.95	0.47
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.96	0.47
1:E:567:GLN:OE1	8:E:802:HOH:O	2.20	0.47
1:L:531:ASN:H	5:L:705:1PE:H152	1.78	0.47
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.96	0.47
1:D:155:GLU:O	1:D:158:LYS:HG2	2.14	0.47
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.97	0.47
1:K:214:LEU:HD11	1:K:222:LEU:HD22	1.97	0.47
4:B:704:4ZN:H20	4:B:704:4ZN:C07	2.43	0.47
1:J:156:PHE:CG	1:J:177:MET:HE1	2.50	0.47
1:J:411:TYR:HE1	5:J:707:1PE:H252	1.81	0.46
1:A:509:LEU:O	1:A:513:ILE:HG12	2.15	0.46
1:B:413:VAL:HG11	1:B:423:ILE:HD12	1.97	0.46
4:J:704:4ZN:H20	4:J:704:4ZN:O10	2.16	0.46
1:H:135:PRO:HA	1:H:194:SER:O	2.16	0.46
1:D:396:MET:SD	1:D:398:PHE:HE2	2.39	0.46
1:G:150:ASP:OD2	1:G:179:ASN:HB2	2.15	0.46
1:A:262:GLU:HA	8:A:835:HOH:O	2.16	0.46
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.51	0.46
1:J:568:ASN:O	1:J:568:ASN:ND2	2.49	0.46
1:B:460:ALA:HB3	1:B:546:GLN:NE2	2.31	0.45
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.98	0.45
1:L:341:TYR:CE1	1:L:428:ALA:HB1	2.51	0.45
1:G:300:ALA:HA	1:G:301:PRO:HD3	1.83	0.45
1:G:372:VAL:O	1:G:483:ASP:HA	2.16	0.45
1:B:168:LYS:O	1:B:171:THR:HG22	2.16	0.45
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.97	0.45
1:K:551:VAL:HA	1:K:552:LYS:CB	2.46	0.45
1:C:400:MET:HE2	1:C:400:MET:O	2.15	0.45
7:E:707:SO4:O4	1:F:436:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:396:MET:SD	1:I:398:PHE:HE2	2.40	0.45
1:H:142:VAL:CG2	1:H:162:MET:HB3	2.47	0.45
1:I:208:LEU:O	1:I:212:THR:HG23	2.16	0.45
1:C:216:ASP:HB3	8:E:916:HOH:O	2.17	0.45
1:G:341:TYR:CE1	1:G:428:ALA:HB1	2.51	0.45
1:I:525:TRP:CE2	1:J:528:PRO:HD3	2.51	0.45
1:J:411:TYR:CE1	5:J:707:1PE:H252	2.52	0.45
1:D:489:GLY:H	4:D:704:4ZN:H15	1.80	0.45
1:K:372:VAL:O	1:K:483:ASP:HA	2.17	0.45
1:G:543:ASP:CG	1:H:255:THR:H	2.25	0.44
5:J:706:1PE:H151	5:J:706:1PE:H141	1.67	0.44
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.99	0.44
1:D:343:SER:HA	1:D:346:LYS:HD3	1.98	0.44
1:H:283:LYS:HE2	1:H:287:TYR:CZ	2.52	0.44
1:H:506:ASN:O	1:H:510:ILE:HG12	2.18	0.44
1:L:551:VAL:HG12	1:L:553:ALA:H	1.82	0.44
1:B:175:PHE:N	1:B:187:VAL:O	2.41	0.44
1:D:156:PHE:CG	1:D:177:MET:HE1	2.52	0.44
1:F:248:THR:HG22	8:F:892:HOH:O	2.17	0.44
1:J:232:LYS:HD2	1:J:276:THR:HG22	1.99	0.44
1:A:395:LEU:HD11	1:A:581:TRP:CG	2.52	0.44
1:C:360:LYS:NZ	8:C:819:HOH:O	2.49	0.44
1:H:106:PRO:HD2	1:H:247:MET:SD	2.58	0.44
1:H:509:LEU:O	1:H:513:ILE:HG12	2.18	0.44
1:B:148:VAL:C	1:B:150:ASP:H	2.26	0.44
1:I:320:LYS:HE2	5:I:705:1PE:H131	1.99	0.44
1:C:463:ARG:NH1	7:C:711:SO4:O3	2.48	0.44
1:D:326:LYS:HG2	1:D:328:LEU:HD12	2.00	0.44
1:G:509:LEU:O	1:G:513:ILE:HG12	2.18	0.44
1:H:337:LYS:NZ	8:H:821:HOH:O	2.49	0.44
1:J:214:LEU:HD21	1:J:222:LEU:HD22	2.00	0.44
1:J:302:SER:OG	1:J:378:PHE:HB2	2.18	0.44
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.98	0.43
1:A:121:CYS:HA	1:A:270:TYR:CE2	2.53	0.43
1:F:114:VAL:HG12	1:F:274:ALA:HB1	2.00	0.43
1:G:436:LYS:HB3	1:G:436:LYS:HE2	1.81	0.43
1:I:204:LYS:HB2	1:I:204:LYS:HE2	1.83	0.43
1:E:340:ALA:HA	1:E:445:ILE:HD12	2.00	0.43
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.99	0.43
1:E:381:GLY:HA2	1:E:459:ASP:OD1	2.17	0.43
1:F:210:LEU:HA	1:F:213:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:579:VAL:O	1:G:589:LYS:HD2	2.18	0.43
1:L:533:TYR:HB2	1:L:560:LEU:HD11	1.99	0.43
5:L:705:1PE:H242	5:L:705:1PE:H252	1.83	0.43
1:B:398:PHE:CD2	1:B:398:PHE:C	2.97	0.43
1:E:338:MET:CE	1:E:468:ASP:HB3	2.45	0.43
1:K:512:LYS:NZ	8:K:814:HOH:O	2.51	0.43
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.99	0.43
1:A:489:GLY:H	4:A:704:4ZN:C19	2.29	0.43
1:C:230:VAL:HG12	1:C:234:LEU:HD23	2.01	0.43
1:G:168:LYS:HB3	1:G:171:THR:OG1	2.19	0.43
1:G:547:ILE:HB	7:G:711:SO4:O4	2.18	0.43
1:I:114:VAL:HG12	1:I:274:ALA:HB1	2.00	0.43
1:J:567:GLN:NE2	8:J:819:HOH:O	2.51	0.43
1:B:329:GLY:H	1:B:332:GLU:CD	2.27	0.43
1:D:236:ARG:O	1:D:240:GLU:HG3	2.18	0.43
1:G:204:LYS:HB2	1:G:204:LYS:HE3	1.78	0.43
1:G:441:PRO:HB2	1:H:394:ASP:HA	2.01	0.43
1:I:117:ILE:HD11	1:I:146:SER:OG	2.19	0.43
1:J:381:GLY:HA2	1:J:459:ASP:OD1	2.18	0.43
1:A:132:VAL:HG23	1:A:167:VAL:HG12	1.99	0.43
1:C:544:ILE:HD12	1:C:564:GLU:HG3	2.00	0.43
1:E:102:GLU:HG2	1:E:296:GLN:OE1	2.18	0.43
1:F:421:VAL:HG22	1:F:423:ILE:HG13	2.00	0.43
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.54	0.43
1:B:350:TYR:HA	1:B:351:PRO:HD3	1.89	0.43
1:D:150:ASP:OD2	1:D:179:ASN:HB2	2.19	0.43
1:D:320:LYS:HE2	5:D:705:1PE:H231	2.01	0.43
1:K:366:LYS:HG3	1:K:420:ASN:HB3	2.01	0.43
1:G:510:ILE:HD13	1:G:526:TRP:NE1	2.34	0.43
1:H:350:TYR:HA	1:H:351:PRO:HD3	1.89	0.43
1:H:310:LEU:HD23	1:H:429:VAL:HG11	2.01	0.42
1:H:326:LYS:HD2	1:H:328:LEU:HD11	2.00	0.42
1:C:153:VAL:O	1:C:157:LEU:HG	2.19	0.42
1:G:122:ASN:HD21	5:G:707:1PE:H251	1.84	0.42
1:G:488:THR:HG21	1:G:555:SER:HA	2.01	0.42
5:I:706:1PE:H242	8:I:924:HOH:O	2.19	0.42
1:J:155:GLU:O	1:J:158:LYS:HG2	2.19	0.42
1:L:103:TYR:HB3	5:L:706:1PE:H252	2.01	0.42
1:J:552:LYS:O	1:J:553:ALA:HB3	2.19	0.42
1:L:292:TYR:O	1:L:296:GLN:HG3	2.20	0.42
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:LEU:HD11	1:E:411:TYR:HA	2.01	0.42
1:K:300:ALA:HA	1:K:301:PRO:HD3	1.82	0.42
1:B:294:ALA:O	1:B:298:ILE:HG13	2.20	0.42
1:J:300:ALA:HA	1:J:301:PRO:HD3	1.92	0.42
1:J:364:ASP:O	1:J:420:ASN:HA	2.19	0.42
1:B:181:ASN:ND2	1:B:183:ASN:OD1	2.52	0.42
1:B:342:LEU:HD12	1:C:94:LEU:HD12	2.01	0.42
1:E:214:LEU:HD21	1:E:222:LEU:HD22	2.02	0.42
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.02	0.42
1:C:400:MET:HE2	1:C:404:ALA:HB2	2.01	0.42
1:F:207:VAL:HG11	1:F:241:THR:HG22	2.02	0.42
1:F:300:ALA:HA	1:F:301:PRO:HD3	1.86	0.42
1:C:126:GLY:O	1:C:221:LYS:O	2.37	0.42
1:G:173:LYS:HD2	1:J:176:TYR:HE1	1.84	0.42
1:G:340:ALA:HA	1:G:445:ILE:HD12	2.01	0.42
1:J:413:VAL:HG11	1:J:423:ILE:HD12	2.01	0.42
1:C:544:ILE:CD1	1:C:564:GLU:HG3	2.50	0.42
1:F:372:VAL:O	1:F:483:ASP:HA	2.20	0.42
1:H:231:ASP:OD1	1:H:231:ASP:N	2.49	0.42
1:I:150:ASP:OD2	1:I:179:ASN:HB2	2.20	0.42
1:J:483:ASP:OD1	1:J:573:HIS:ND1	2.37	0.42
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.55	0.41
1:J:398:PHE:CD2	1:J:398:PHE:C	2.97	0.41
1:K:544:ILE:HD12	1:K:564:GLU:HG3	2.01	0.41
1:C:135:PRO:HA	1:C:194:SER:O	2.19	0.41
1:J:551:VAL:HG12	1:J:552:LYS:O	2.20	0.41
1:K:158:LYS:HE2	1:K:161:ASN:ND2	2.34	0.41
1:L:150:ASP:OD2	1:L:179:ASN:HB2	2.20	0.41
1:H:488:THR:HG21	1:H:555:SER:HA	2.02	0.41
4:C:704:4ZN:O10	4:C:704:4ZN:H20	2.20	0.41
1:D:300:ALA:HA	1:D:301:PRO:HD3	1.92	0.41
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.89	0.41
1:E:150:ASP:OD2	1:E:179:ASN:HB2	2.21	0.41
1:L:418:PRO:HB3	1:L:601:LEU:HD12	2.03	0.41
1:B:287:TYR:CD2	1:B:594:ARG:HG2	2.56	0.41
1:B:372:VAL:O	1:B:483:ASP:HA	2.20	0.41
1:J:106:PRO:HD3	8:J:1001:HOH:O	2.20	0.41
1:J:294:ALA:O	1:J:298:ILE:HG13	2.20	0.41
1:C:488:THR:HG22	8:C:1002:HOH:O	2.21	0.41
1:J:214:LEU:HD11	1:J:222:LEU:HD22	2.02	0.41
1:J:346:LYS:HB3	1:J:437:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:MET:SD	1:F:398:PHE:HE2	2.44	0.41
1:H:138:GLU:O	1:H:194:SER:OG	2.39	0.41
1:H:398:PHE:CD2	1:H:398:PHE:C	2.99	0.41
1:B:383:TYR:HE1	1:B:438:SER:HB2	1.85	0.41
1:D:132:VAL:HG11	1:D:144:ILE:HD13	2.02	0.41
1:H:499:TYR:CD1	1:H:523:PRO:HB2	2.55	0.41
1:I:328:LEU:HB2	1:I:354:PHE:HB3	2.02	0.41
1:I:536:THR:HG21	1:I:551:VAL:HG23	2.03	0.41
1:J:320:LYS:HB3	5:J:707:1PE:H242	2.02	0.41
1:I:400:MET:H	1:I:400:MET:HG3	1.27	0.41
1:J:321:LEU:CD1	1:J:411:TYR:HA	2.51	0.41
1:K:302:SER:OG	1:K:378:PHE:HB2	2.21	0.41
1:J:372:VAL:O	1:J:483:ASP:HA	2.20	0.40
1:C:340:ALA:HA	1:C:445:ILE:HD12	2.02	0.40
1:F:436:LYS:HB3	1:F:436:LYS:HE2	1.98	0.40
1:H:449:ASN:HD21	1:H:451:LYS:HD2	1.86	0.40
1:J:341:TYR:CE1	1:J:428:ALA:HB1	2.56	0.40
1:L:138:GLU:N	1:L:139:ASN:CA	2.83	0.40
1:B:235:PHE:O	1:B:238:PHE:HB3	2.20	0.40
1:D:364:ASP:O	1:D:420:ASN:HA	2.21	0.40
1:E:103:TYR:CD2	5:E:705:1PE:H132	2.56	0.40
1:H:203:MET:SD	1:H:238:PHE:HD1	2.45	0.40
1:I:300:ALA:HA	1:I:301:PRO:HD3	1.86	0.40
1:C:300:ALA:HA	1:C:301:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

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	518/519 (100%)	501 (97%)	16 (3%)	1 (0%)	43 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	512/519 (99%)	495 (97%)	16 (3%)	1 (0%)	43	55
1	C	515/519 (99%)	499 (97%)	15 (3%)	1 (0%)	43	55
1	D	510/519 (98%)	496 (97%)	13 (2%)	1 (0%)	43	55
1	E	503/519 (97%)	493 (98%)	10 (2%)	0	100	100
1	F	507/519 (98%)	490 (97%)	17 (3%)	0	100	100
1	G	517/519 (100%)	503 (97%)	14 (3%)	0	100	100
1	H	513/519 (99%)	500 (98%)	11 (2%)	2 (0%)	30	38
1	I	515/519 (99%)	505 (98%)	8 (2%)	2 (0%)	30	38
1	J	510/519 (98%)	496 (97%)	12 (2%)	2 (0%)	30	38
1	K	503/519 (97%)	490 (97%)	10 (2%)	3 (1%)	21	27
1	L	507/519 (98%)	491 (97%)	14 (3%)	2 (0%)	30	38
All	All	6130/6228 (98%)	5959 (97%)	156 (2%)	15 (0%)	43	55

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	VAL
1	H	138	GLU
1	K	100	PRO
1	K	551	VAL
1	K	552	LYS
1	L	550	SER
1	J	551	VAL
1	L	552	LYS
1	C	126	GLY
1	B	149	ASN
1	J	137	LYS
1	H	254	SER
1	I	137	LYS
1	I	261	MET
1	D	551	VAL

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	423/447 (95%)	417 (99%)	6 (1%)	59	76
1	B	407/447 (91%)	402 (99%)	5 (1%)	63	79
1	C	418/447 (94%)	407 (97%)	11 (3%)	40	59
1	D	413/447 (92%)	403 (98%)	10 (2%)	43	62
1	E	413/447 (92%)	407 (98%)	6 (2%)	57	75
1	F	402/447 (90%)	389 (97%)	13 (3%)	34	51
1	G	422/447 (94%)	415 (98%)	7 (2%)	53	72
1	H	406/447 (91%)	398 (98%)	8 (2%)	48	67
1	I	420/447 (94%)	412 (98%)	8 (2%)	50	69
1	J	414/447 (93%)	406 (98%)	8 (2%)	50	69
1	K	410/447 (92%)	403 (98%)	7 (2%)	53	72
1	L	400/447 (90%)	388 (97%)	12 (3%)	36	53
All	All	4948/5364 (92%)	4847 (98%)	101 (2%)	48	67

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	GLU
1	A	398	PHE
1	A	436	LYS
1	A	439	TYR
1	A	554	SER
1	A	568	ASN
1	B	121	CYS
1	B	261	MET
1	B	398	PHE
1	B	549	SER
1	B	600	VAL
1	C	86	SER
1	C	185	VAL
1	C	276	THR
1	C	295	SER
1	C	366	LYS
1	C	398	PHE
1	C	400	MET
1	C	483	ASP

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Mol	Chain	Res	Type
1	C	549	SER
1	C	550	SER
1	C	554	SER
1	D	198	LEU
1	D	200	GLU
1	D	208	LEU
1	D	262	GLU
1	D	394	ASP
1	D	395	LEU
1	D	398	PHE
1	D	439	TYR
1	D	518	LYS
1	D	568	ASN
1	E	208	LEU
1	E	230	VAL
1	E	398	PHE
1	E	400	MET
1	E	547	ILE
1	E	601	LEU
1	F	88	VAL
1	F	155	GLU
1	F	167	VAL
1	F	169	LEU
1	F	198	LEU
1	F	200	GLU
1	F	215	HIS
1	F	219	LEU
1	F	248	THR
1	F	361	SER
1	F	365	VAL
1	F	398	PHE
1	F	494	SER
1	G	229	ASN
1	G	332	GLU
1	G	395	LEU
1	G	398	PHE
1	G	439	TYR
1	G	554	SER
1	G	568	ASN
1	H	139	ASN
1	H	142	VAL
1	H	328	LEU

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Mol	Chain	Res	Type
1	H	357	LEU
1	H	398	PHE
1	H	439	TYR
1	H	549	SER
1	H	554	SER
1	I	163	GLU
1	I	171	THR
1	I	185	VAL
1	I	322	ASN
1	I	331	LYS
1	I	398	PHE
1	I	400	MET
1	I	439	TYR
1	J	200	GLU
1	J	248	THR
1	J	262	GLU
1	J	398	PHE
1	J	439	TYR
1	J	511	ASN
1	J	567	GLN
1	J	601	LEU
1	K	99	ILE
1	K	230	VAL
1	K	324	GLU
1	K	395	LEU
1	K	398	PHE
1	K	439	TYR
1	K	568	ASN
1	L	144	ILE
1	L	148	VAL
1	L	195	VAL
1	L	200	GLU
1	L	330	VAL
1	L	398	PHE
1	L	435	SER
1	L	439	TYR
1	L	551	VAL
1	L	568	ASN
1	L	600	VAL
1	L	601	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	437	ASN
1	B	181	ASN
1	B	420	ASN
1	B	521	ASN
1	C	215	HIS
1	C	272	ASN
1	C	420	ASN
1	C	602	ASN
1	D	139	ASN
1	D	152	GLN
1	D	161	ASN
1	D	272	ASN
1	E	420	ASN
1	E	511	ASN
1	E	531	ASN
1	F	149	ASN
1	F	215	HIS
1	F	266	HIS
1	F	567	GLN
1	G	113	GLN
1	G	122	ASN
1	G	149	ASN
1	G	266	HIS
1	G	568	ASN
1	H	113	GLN
1	H	139	ASN
1	I	166	ASN
1	I	215	HIS
1	J	181	ASN
1	J	272	ASN
1	J	567	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 102 ligands modelled in this entry, 24 are monoatomic - leaving 78 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	$\# Z > 2$
7	SO4	A	712	-	4,4,4	0.30	0	6,6,6	0.60	0
5	1PE	K	705	-	11,11,15	0.72	0	10,10,14	0.24	0
5	1PE	A	706	-	11,11,15	0.79	0	10,10,14	0.35	0
7	SO4	L	707	-	4,4,4	0.25	0	6,6,6	0.19	0
7	SO4	C	709	-	4,4,4	0.37	0	6,6,6	0.36	0
4	4ZN	E	704	3	16,20,20	0.84	1 (6%)	19,28,28	2.09	4 (21%)
7	SO4	C	707	-	4,4,4	0.22	0	6,6,6	0.08	0
2	CO3	I	701	-	3,3,3	0.79	0	2,3,3	0.09	0
2	CO3	G	701	-	3,3,3	0.87	0	2,3,3	0.25	0
5	1PE	B	705	-	9,9,15	0.71	0	8,8,14	0.37	0
5	1PE	C	706	-	8,8,15	0.79	0	7,7,14	0.29	0
7	SO4	C	711	-	4,4,4	0.35	0	6,6,6	0.29	0
2	CO3	J	701	-	3,3,3	1.05	0	2,3,3	0.53	0
5	1PE	C	705	-	12,12,15	0.81	0	11,11,14	0.56	0
5	1PE	D	706	-	9,9,15	0.76	0	8,8,14	0.34	0
4	4ZN	C	704	3	13,16,20	1.44	1 (7%)	14,22,28	1.03	1 (7%)
7	SO4	I	708	-	4,4,4	0.25	0	6,6,6	0.12	0
7	SO4	E	709	-	4,4,4	0.34	0	6,6,6	0.12	0
4	4ZN	H	704	3	13,16,20	1.65	2 (15%)	14,22,28	0.91	1 (7%)
5	1PE	E	705	-	11,11,15	0.84	0	10,10,14	0.39	0
7	SO4	A	711	-	4,4,4	0.30	0	6,6,6	0.20	0
2	CO3	L	701	-	3,3,3	0.71	0	2,3,3	0.19	0
5	1PE	J	705	-	10,10,15	0.70	0	9,9,14	0.40	0
4	4ZN	J	704	3	13,16,20	1.45	1 (7%)	14,22,28	0.93	0
7	SO4	G	709	-	4,4,4	0.22	0	6,6,6	0.19	0
2	CO3	A	701	-	3,3,3	0.74	0	2,3,3	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	K	707	-	4,4,4	0.29	0	6,6,6	0.08	0
2	CO3	C	701	-	3,3,3	0.99	0	2,3,3	0.77	0
5	1PE	I	706	-	10,10,15	0.72	0	9,9,14	0.45	0
5	1PE	L	705	-	6,6,15	0.71	0	5,5,14	0.37	0
6	GOL	A	707	-	5,5,5	0.46	0	5,5,5	0.24	0
7	SO4	J	708	-	4,4,4	0.20	0	6,6,6	0.32	0
5	1PE	B	706	-	9,9,15	0.73	0	8,8,14	0.47	0
2	CO3	H	701	-	3,3,3	0.81	0	2,3,3	0.42	0
4	4ZN	D	704	3	16,20,20	1.43	2 (12%)	19,28,28	1.67	5 (26%)
7	SO4	J	709	-	4,4,4	0.25	0	6,6,6	0.16	0
7	SO4	E	708	-	4,4,4	0.25	0	6,6,6	0.22	0
2	CO3	E	701	-	3,3,3	0.88	0	2,3,3	0.45	0
7	SO4	A	710	-	4,4,4	0.30	0	6,6,6	0.37	0
5	1PE	I	705	-	11,11,15	0.76	0	10,10,14	0.40	0
7	SO4	G	708	-	4,4,4	0.29	0	6,6,6	0.17	0
7	SO4	B	707	-	4,4,4	0.23	0	6,6,6	0.25	0
7	SO4	A	708	-	4,4,4	0.27	0	6,6,6	0.24	0
5	1PE	K	706	-	11,11,15	0.75	0	10,10,14	0.44	0
5	1PE	H	705	-	9,9,15	0.76	0	8,8,14	0.27	0
4	4ZN	A	704	3	13,16,20	0.62	0	14,22,28	1.74	4 (28%)
7	SO4	F	707	-	4,4,4	0.33	0	6,6,6	0.13	0
5	1PE	D	705	-	9,9,15	0.83	0	8,8,14	0.49	0
4	4ZN	B	704	3	13,16,20	0.88	0	14,22,28	2.15	4 (28%)
4	4ZN	F	704	3	13,16,20	0.69	0	14,22,28	1.42	2 (14%)
7	SO4	D	707	-	4,4,4	0.32	0	6,6,6	0.21	0
7	SO4	G	710	-	4,4,4	0.31	0	6,6,6	0.19	0
5	1PE	E	706	-	11,11,15	0.71	0	10,10,14	0.31	0
7	SO4	C	708	-	4,4,4	0.28	0	6,6,6	0.24	0
5	1PE	A	705	-	8,8,15	0.75	0	7,7,14	0.33	0
5	1PE	G	706	-	5,5,15	0.61	0	4,4,14	0.57	0
2	CO3	K	701	-	3,3,3	0.77	0	2,3,3	0.14	0
7	SO4	F	706	-	4,4,4	0.31	0	6,6,6	0.19	0
7	SO4	A	709	-	4,4,4	0.30	0	6,6,6	0.15	0
7	SO4	G	711	-	4,4,4	0.20	0	6,6,6	0.51	0
4	4ZN	K	704	3	11,14,20	0.80	1 (9%)	12,19,28	1.40	2 (16%)
2	CO3	B	701	-	3,3,3	1.06	0	2,3,3	0.76	0
5	1PE	L	706	-	9,9,15	0.63	0	8,8,14	0.41	0
2	CO3	F	701	-	3,3,3	0.83	0	2,3,3	0.27	0
7	SO4	C	710	-	4,4,4	0.37	0	6,6,6	0.23	0
7	SO4	I	707	-	4,4,4	0.24	0	6,6,6	0.18	0
2	CO3	D	701	-	3,3,3	1.02	0	2,3,3	0.58	0
7	SO4	K	708	-	4,4,4	0.24	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1PE	H	706	-	9,9,15	0.75	0	8,8,14	0.20	0
4	4ZN	G	704	3	13,16,20	0.68	0	14,22,28	1.61	2 (14%)
5	1PE	G	707	-	5,5,15	0.69	0	4,4,14	0.42	0
4	4ZN	L	704	3	13,16,20	0.67	0	14,22,28	1.11	1 (7%)
4	4ZN	I	704	3	8,12,20	1.58	1 (12%)	11,17,28	1.69	1 (9%)
5	1PE	F	705	-	9,9,15	0.69	0	8,8,14	0.38	0
7	SO4	E	707	-	4,4,4	0.25	0	6,6,6	0.16	0
5	1PE	J	706	-	10,10,15	0.73	0	9,9,14	0.48	0
5	1PE	J	707	-	9,9,15	0.61	0	8,8,14	0.31	0
5	1PE	G	705	-	8,8,15	0.71	0	7,7,14	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	1PE	D	706	-	-	6/7/7/13	-
4	4ZN	D	704	3	-	5/18/23/23	0/1/1/1
4	4ZN	C	704	3	-	7/12/16/23	0/1/1/1
5	1PE	I	705	-	-	6/9/9/13	-
5	1PE	K	706	-	-	4/9/9/13	-
4	4ZN	K	704	3	-	6/10/14/23	0/1/1/1
5	1PE	H	705	-	-	4/7/7/13	-
5	1PE	K	705	-	-	3/9/9/13	-
5	1PE	A	706	-	-	3/9/9/13	-
4	4ZN	A	704	3	-	9/12/16/23	0/1/1/1
5	1PE	D	705	-	-	6/7/7/13	-
5	1PE	L	706	-	-	5/7/7/13	-
4	4ZN	H	704	3	-	9/12/16/23	0/1/1/1
5	1PE	E	705	-	-	3/9/9/13	-
4	4ZN	B	704	3	-	8/12/16/23	0/1/1/1
4	4ZN	F	704	3	-	6/12/16/23	0/1/1/1
5	1PE	J	705	-	-	4/8/8/13	-
4	4ZN	J	704	3	-	8/12/16/23	0/1/1/1
5	1PE	E	706	-	-	5/9/9/13	-
4	4ZN	E	704	3	-	10/18/23/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	H	706	-	-	4/7/7/13	-
5	1PE	A	705	-	-	3/6/6/13	-
4	4ZN	G	704	3	-	6/12/16/23	0/1/1/1
5	1PE	G	706	-	-	2/3/3/13	-
5	1PE	G	707	-	-	2/3/3/13	-
5	1PE	I	706	-	-	4/8/8/13	-
4	4ZN	L	704	3	-	7/12/16/23	0/1/1/1
4	4ZN	I	704	3	-	3/6/10/23	0/1/1/1
5	1PE	F	705	-	-	6/7/7/13	-
5	1PE	B	705	-	-	4/7/7/13	-
5	1PE	L	705	-	-	2/4/4/13	-
5	1PE	C	706	-	-	4/6/6/13	-
6	GOL	A	707	-	-	2/4/4/4	-
5	1PE	B	706	-	-	6/7/7/13	-
5	1PE	J	706	-	-	5/8/8/13	-
5	1PE	J	707	-	-	4/7/7/13	-
5	1PE	G	705	-	-	4/6/6/13	-
5	1PE	C	705	-	-	4/10/10/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	704	4ZN	P08-O10	4.82	1.58	1.49
4	J	704	4ZN	P08-O10	4.59	1.58	1.49
4	C	704	4ZN	P08-O10	4.43	1.58	1.49
4	D	704	4ZN	P08-O10	4.30	1.57	1.49
4	I	704	4ZN	P08-O10	4.07	1.57	1.49
4	D	704	4ZN	P08-C07	2.82	1.82	1.79
4	H	704	4ZN	P08-C07	2.58	1.82	1.79
4	K	704	4ZN	P08-C07	2.19	1.81	1.79
4	E	704	4ZN	P08-C07	2.12	1.81	1.79

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	4ZN	C07-C06-C19	5.59	122.13	113.38
4	I	704	4ZN	O09-P08-O10	-5.14	107.35	114.23
4	E	704	4ZN	C05-C06-C07	4.72	118.47	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	704	4ZN	C06-C05-C03	4.70	125.35	115.60
4	A	704	4ZN	C07-C06-C19	-4.12	106.93	113.38
4	B	704	4ZN	O10-P08-C11	-3.75	104.65	111.51
4	D	704	4ZN	C06-C05-C03	3.44	122.74	115.60
4	G	704	4ZN	C07-C06-C19	-3.39	108.08	113.38
4	E	704	4ZN	O10-P08-C11	-3.35	105.38	111.51
4	G	704	4ZN	O10-P08-C11	-3.27	105.52	111.51
4	F	704	4ZN	C07-C06-C19	-3.23	108.32	113.38
4	E	704	4ZN	C05-C06-C19	2.95	115.94	109.89
4	A	704	4ZN	O10-P08-C11	-2.94	106.12	111.51
4	K	704	4ZN	O10-P08-C11	-2.67	106.62	111.51
4	A	704	4ZN	O09-P08-C11	2.65	112.80	106.77
4	D	704	4ZN	O20-C19-C06	2.62	120.95	114.16
4	D	704	4ZN	C18-C13-C11	-2.58	117.83	120.76
4	B	704	4ZN	C18-C13-C11	-2.50	117.92	120.76
4	D	704	4ZN	O20-C19-O21	-2.46	118.49	124.08
4	K	704	4ZN	O09-P08-C11	2.39	112.21	106.77
4	L	704	4ZN	O20-C19-C06	2.31	121.30	114.00
4	F	704	4ZN	O20-C19-C06	2.27	121.17	114.00
4	B	704	4ZN	O20-C19-C06	2.24	121.08	114.00
4	D	704	4ZN	C05-C06-C19	2.19	114.39	109.89
4	H	704	4ZN	C07-C06-C19	-2.16	109.99	113.38
4	C	704	4ZN	O20-C19-C06	2.09	120.61	114.00
4	A	704	4ZN	O20-C19-C06	2.01	120.35	114.00

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	4ZN	C19-C06-C07-P08
4	A	704	4ZN	C06-C07-P08-O09
4	A	704	4ZN	C06-C07-P08-O10
4	A	704	4ZN	C06-C07-P08-C11
4	B	704	4ZN	C06-C07-P08-O09
4	B	704	4ZN	C06-C07-P08-O10
4	B	704	4ZN	C06-C07-P08-C11
4	C	704	4ZN	C19-C06-C07-P08
4	C	704	4ZN	C06-C07-P08-O09
4	C	704	4ZN	C06-C07-P08-O10
4	D	704	4ZN	C03-C05-C06-C19
4	E	704	4ZN	C19-C06-C07-P08
4	E	704	4ZN	C07-C06-C19-O20

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Mol	Chain	Res	Type	Atoms
4	E	704	4ZN	C07-C06-C19-O21
4	E	704	4ZN	C06-C07-P08-O10
4	F	704	4ZN	C19-C06-C07-P08
4	F	704	4ZN	C06-C07-P08-O09
4	F	704	4ZN	C06-C07-P08-O10
4	F	704	4ZN	C06-C07-P08-C11
4	G	704	4ZN	C19-C06-C07-P08
4	G	704	4ZN	C06-C07-P08-O09
4	G	704	4ZN	C06-C07-P08-O10
4	G	704	4ZN	C06-C07-P08-C11
4	H	704	4ZN	C19-C06-C07-P08
4	H	704	4ZN	C06-C07-P08-O09
4	H	704	4ZN	C06-C07-P08-O10
4	H	704	4ZN	C06-C07-P08-C11
4	J	704	4ZN	C19-C06-C07-P08
4	J	704	4ZN	C06-C07-P08-O09
4	J	704	4ZN	C06-C07-P08-O10
4	J	704	4ZN	C06-C07-P08-C11
4	K	704	4ZN	C19-C06-C07-P08
4	K	704	4ZN	C06-C07-P08-O09
4	K	704	4ZN	C06-C07-P08-O10
4	K	704	4ZN	C06-C07-P08-C11
4	L	704	4ZN	C19-C06-C07-P08
4	L	704	4ZN	C06-C07-P08-O09
4	L	704	4ZN	C06-C07-P08-O10
4	L	704	4ZN	C06-C07-P08-C11
6	A	707	GOL	C1-C2-C3-O3
5	J	706	1PE	C15-C25-OH5-C14
5	I	705	1PE	OH5-C14-C24-OH4
4	D	704	4ZN	P08-C11-C13-C14
4	D	704	4ZN	P08-C11-C13-C18
4	E	704	4ZN	P08-C11-C13-C14
4	E	704	4ZN	P08-C11-C13-C18
4	J	704	4ZN	P08-C11-C13-C14
4	L	704	4ZN	P08-C11-C13-C14
4	L	704	4ZN	P08-C11-C13-C18
5	J	705	1PE	OH5-C14-C24-OH4
5	J	707	1PE	OH6-C15-C25-OH5
5	K	705	1PE	OH4-C13-C23-OH3
5	E	706	1PE	OH6-C15-C25-OH5
5	D	706	1PE	OH5-C14-C24-OH4
5	F	705	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
5	K	706	1PE	OH4-C13-C23-OH3
5	A	705	1PE	OH4-C13-C23-OH3
5	B	706	1PE	OH4-C13-C23-OH3
5	H	706	1PE	OH5-C14-C24-OH4
5	B	706	1PE	C23-C13-OH4-C24
6	A	707	GOL	O2-C2-C3-O3
5	E	706	1PE	OH5-C14-C24-OH4
5	H	706	1PE	OH4-C13-C23-OH3
5	F	705	1PE	OH7-C16-C26-OH6
5	G	707	1PE	OH6-C15-C25-OH5
5	D	706	1PE	OH4-C13-C23-OH3
5	G	705	1PE	OH4-C13-C23-OH3
5	K	706	1PE	OH5-C14-C24-OH4
5	L	705	1PE	C24-C14-OH5-C25
5	L	706	1PE	OH6-C15-C25-OH5
4	B	704	4ZN	P08-C11-C13-C14
4	B	704	4ZN	P08-C11-C13-C18
4	F	704	4ZN	P08-C11-C13-C14
4	F	704	4ZN	P08-C11-C13-C18
4	G	704	4ZN	P08-C11-C13-C14
4	I	704	4ZN	P08-C11-C13-C14
4	I	704	4ZN	P08-C11-C13-C18
4	J	704	4ZN	P08-C11-C13-C18
5	F	705	1PE	OH5-C14-C24-OH4
5	J	707	1PE	OH7-C16-C26-OH6
5	B	706	1PE	OH5-C14-C24-OH4
5	C	706	1PE	OH4-C13-C23-OH3
5	I	705	1PE	C12-C22-OH3-C23
5	A	705	1PE	OH5-C14-C24-OH4
5	A	706	1PE	OH4-C13-C23-OH3
5	D	705	1PE	OH4-C13-C23-OH3
5	D	706	1PE	C12-C22-OH3-C23
4	A	704	4ZN	P08-C11-C13-C14
4	A	704	4ZN	P08-C11-C13-C18
4	C	704	4ZN	P08-C11-C13-C14
4	C	704	4ZN	P08-C11-C13-C18
4	G	704	4ZN	P08-C11-C13-C18
4	H	704	4ZN	P08-C11-C13-C14
4	H	704	4ZN	P08-C11-C13-C18
4	K	704	4ZN	P08-C11-C13-C14
4	K	704	4ZN	P08-C11-C13-C18
5	J	707	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
5	L	706	1PE	OH7-C16-C26-OH6
5	I	706	1PE	OH4-C13-C23-OH3
5	C	706	1PE	OH5-C14-C24-OH4
5	G	706	1PE	OH6-C15-C25-OH5
5	D	705	1PE	OH5-C14-C24-OH4
5	E	705	1PE	OH5-C14-C24-OH4
5	B	705	1PE	OH4-C13-C23-OH3
4	J	704	4ZN	C07-C06-C19-O20
5	G	707	1PE	C24-C14-OH5-C25
5	A	705	1PE	C12-C22-OH3-C23
4	D	704	4ZN	C02-C03-C05-C06
5	D	705	1PE	C12-C22-OH3-C23
5	D	706	1PE	C13-C23-OH3-C22
5	H	706	1PE	C13-C23-OH3-C22
4	H	704	4ZN	C07-C06-C19-O21
5	E	706	1PE	C24-C14-OH5-C25
5	G	705	1PE	C14-C24-OH4-C13
5	A	706	1PE	C13-C23-OH3-C22
5	L	706	1PE	C25-C15-OH6-C26
5	E	705	1PE	C13-C23-OH3-C22
5	B	705	1PE	C13-C23-OH3-C22
5	I	705	1PE	C13-C23-OH3-C22
5	J	707	1PE	C25-C15-OH6-C26
5	E	706	1PE	C23-C13-OH4-C24
5	H	705	1PE	C14-C24-OH4-C13
5	D	706	1PE	C23-C13-OH4-C24
5	I	705	1PE	C14-C24-OH4-C13
5	J	705	1PE	OH6-C15-C25-OH5
5	H	705	1PE	C13-C23-OH3-C22
5	L	706	1PE	C24-C14-OH5-C25
5	B	705	1PE	C24-C14-OH5-C25
5	K	705	1PE	C13-C23-OH3-C22
5	C	705	1PE	C24-C14-OH5-C25
5	I	706	1PE	OH5-C14-C24-OH4
5	D	705	1PE	C24-C14-OH5-C25
5	F	705	1PE	C25-C15-OH6-C26
5	E	705	1PE	OH6-C15-C25-OH5
5	I	705	1PE	OH6-C15-C25-OH5
5	B	706	1PE	C14-C24-OH4-C13
5	L	705	1PE	OH6-C15-C25-OH5
5	G	706	1PE	C15-C25-OH5-C14
5	D	705	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
5	H	705	1PE	C24-C14-OH5-C25
5	H	706	1PE	C14-C24-OH4-C13
4	C	704	4ZN	C07-C06-C19-O20
4	J	704	4ZN	C07-C06-C19-O21
4	E	704	4ZN	C06-C07-P08-O09
5	J	706	1PE	OH6-C15-C25-OH5
5	L	706	1PE	C16-C26-OH6-C15
5	J	706	1PE	OH5-C14-C24-OH4
5	B	706	1PE	C24-C14-OH5-C25
5	H	705	1PE	OH5-C14-C24-OH4
5	C	705	1PE	C23-C13-OH4-C24
5	K	706	1PE	C24-C14-OH5-C25
5	K	705	1PE	OH6-C15-C25-OH5
5	I	705	1PE	OH4-C13-C23-OH3
5	D	706	1PE	C24-C14-OH5-C25
5	C	706	1PE	C14-C24-OH4-C13
5	F	705	1PE	C24-C14-OH5-C25
4	B	704	4ZN	C07-C06-C19-O20
4	B	704	4ZN	C07-C06-C19-O21
4	C	704	4ZN	C07-C06-C19-O21
4	H	704	4ZN	C07-C06-C19-O20
5	K	706	1PE	C23-C13-OH4-C24
5	G	705	1PE	C13-C23-OH3-C22
4	D	704	4ZN	C03-C05-C06-C07
5	G	705	1PE	C24-C14-OH5-C25
5	D	705	1PE	C13-C23-OH3-C22
5	J	706	1PE	C25-C15-OH6-C26
5	C	706	1PE	C12-C22-OH3-C23
5	J	705	1PE	C16-C26-OH6-C15
5	J	706	1PE	OH7-C16-C26-OH6
4	E	704	4ZN	C04-C03-C05-C06
4	A	704	4ZN	C07-C06-C19-O20
5	I	706	1PE	C23-C13-OH4-C24
5	B	706	1PE	C12-C22-OH3-C23
5	C	705	1PE	C12-C22-OH3-C23
5	J	705	1PE	OH7-C16-C26-OH6
5	A	706	1PE	OH6-C15-C25-OH5
5	F	705	1PE	C15-C25-OH5-C14
5	E	706	1PE	OH4-C13-C23-OH3
5	I	706	1PE	C12-C22-OH3-C23
4	A	704	4ZN	N12-C11-C13-C14
4	A	704	4ZN	N12-C11-C13-C18

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Mol	Chain	Res	Type	Atoms
4	B	704	4ZN	N12-C11-C13-C14
4	E	704	4ZN	N12-C11-C13-C14
4	H	704	4ZN	N12-C11-C13-C18
4	I	704	4ZN	N12-C11-C13-C18
4	L	704	4ZN	N12-C11-C13-C14
5	C	705	1PE	OH4-C13-C23-OH3
5	B	705	1PE	OH5-C14-C24-OH4
4	E	704	4ZN	C05-C06-C07-P08

There are no ring outliers.

32 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	712	SO4	2	0
4	E	704	4ZN	2	0
5	C	706	1PE	1	0
7	C	711	SO4	1	0
4	C	704	4ZN	1	0
4	H	704	4ZN	1	0
5	E	705	1PE	1	0
5	J	705	1PE	4	0
4	J	704	4ZN	2	0
5	I	706	1PE	1	0
5	L	705	1PE	5	0
5	B	706	1PE	2	0
4	D	704	4ZN	3	0
5	I	705	1PE	1	0
5	K	706	1PE	2	0
5	H	705	1PE	1	0
4	A	704	4ZN	2	0
5	D	705	1PE	2	0
4	B	704	4ZN	2	0
7	D	707	SO4	1	0
5	E	706	1PE	1	0
7	C	708	SO4	1	0
5	G	706	1PE	2	0
7	G	711	SO4	2	0
4	K	704	4ZN	1	0
5	L	706	1PE	1	0
5	G	707	1PE	1	0
4	L	704	4ZN	1	0
7	E	707	SO4	1	0

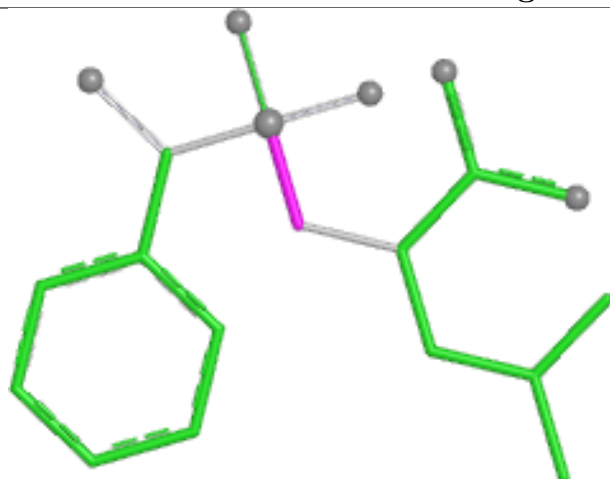
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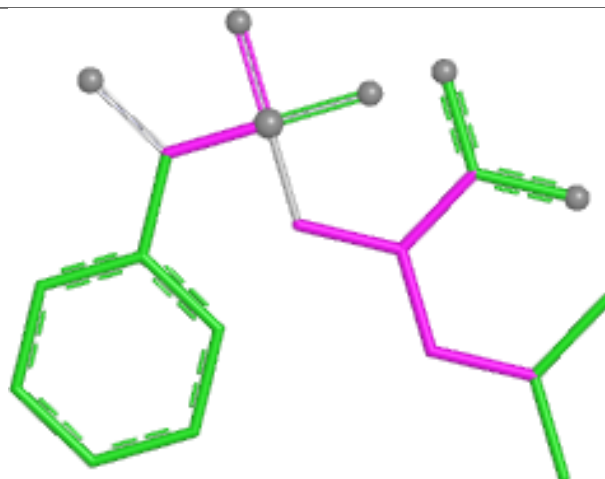
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	706	1PE	5	0
5	J	707	1PE	3	0
5	G	705	1PE	1	0

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.

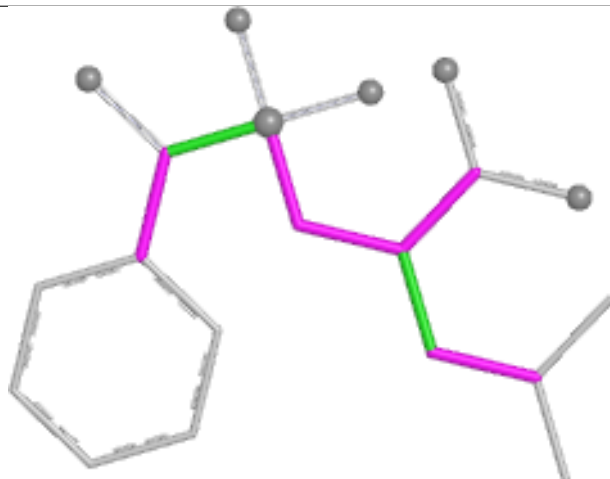
Ligand 4ZN E 704



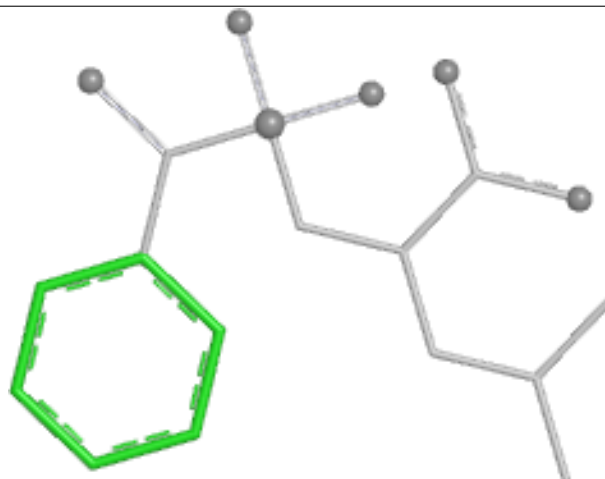
Bond lengths



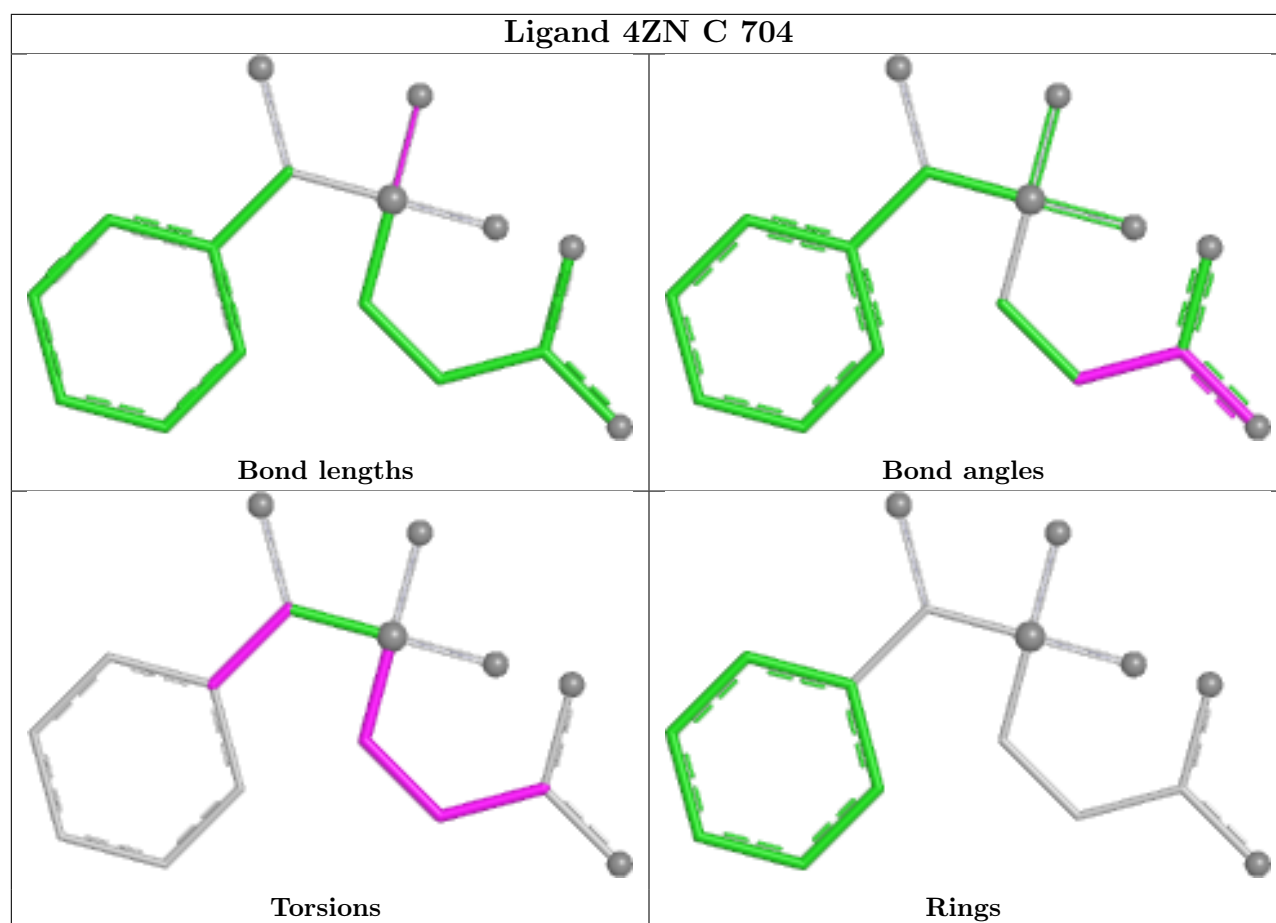
Bond angles

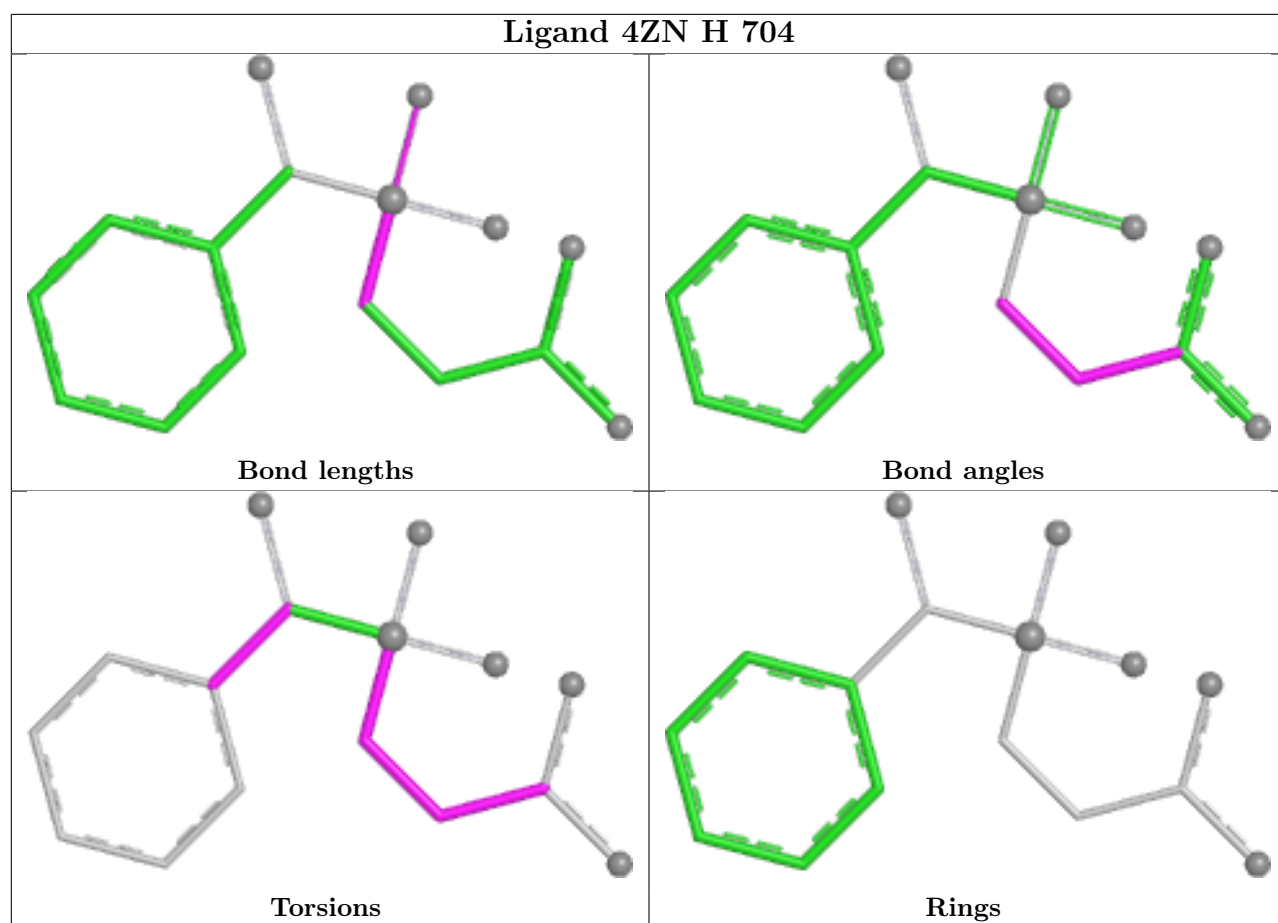


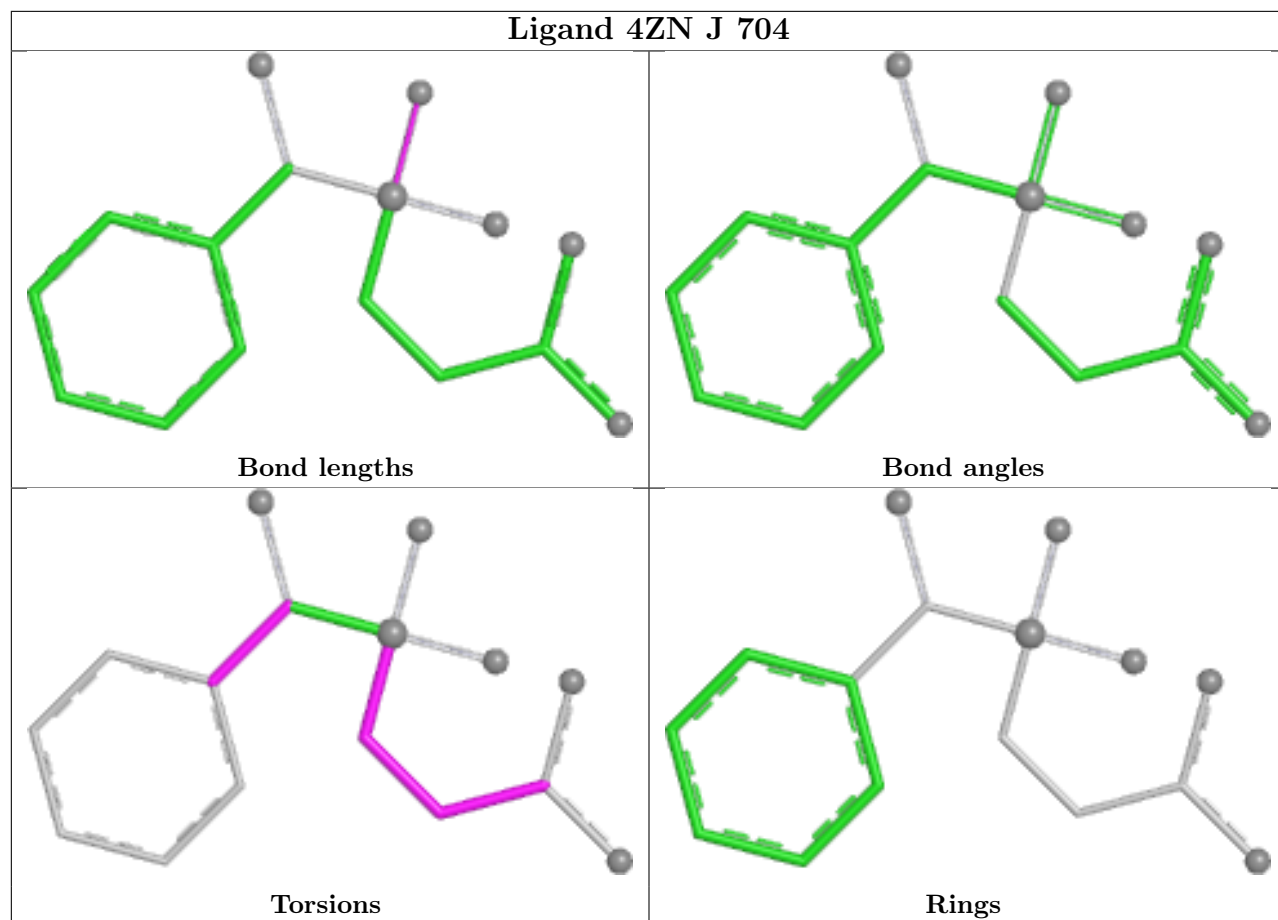
Torsions



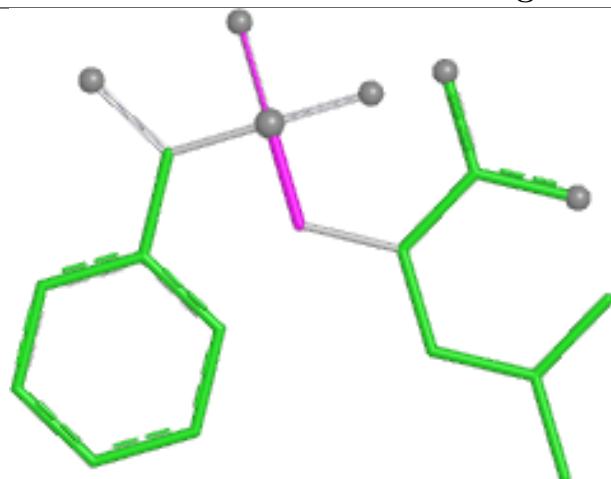
Rings



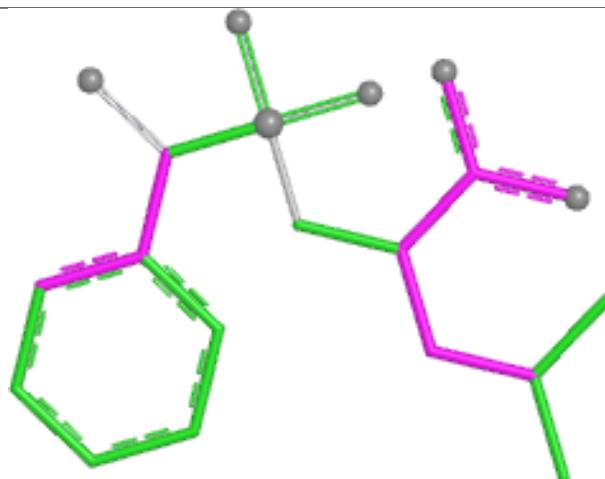




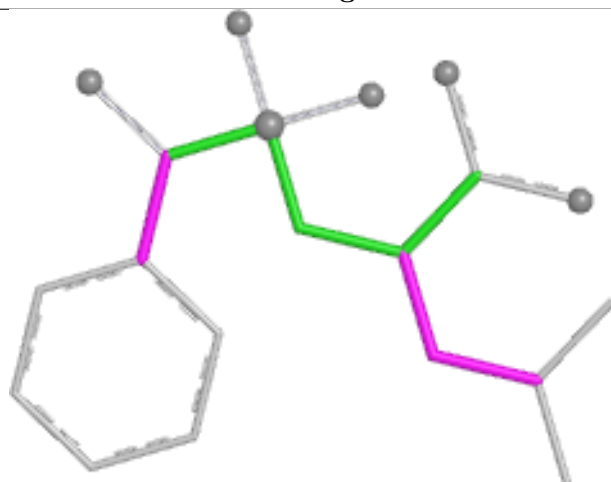
Ligand 4ZN D 704



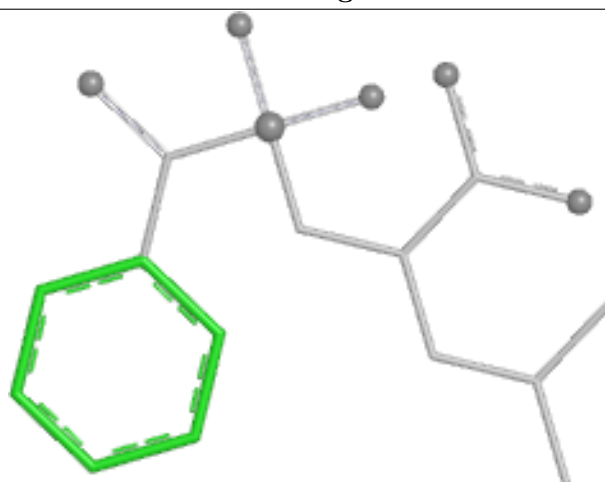
Bond lengths



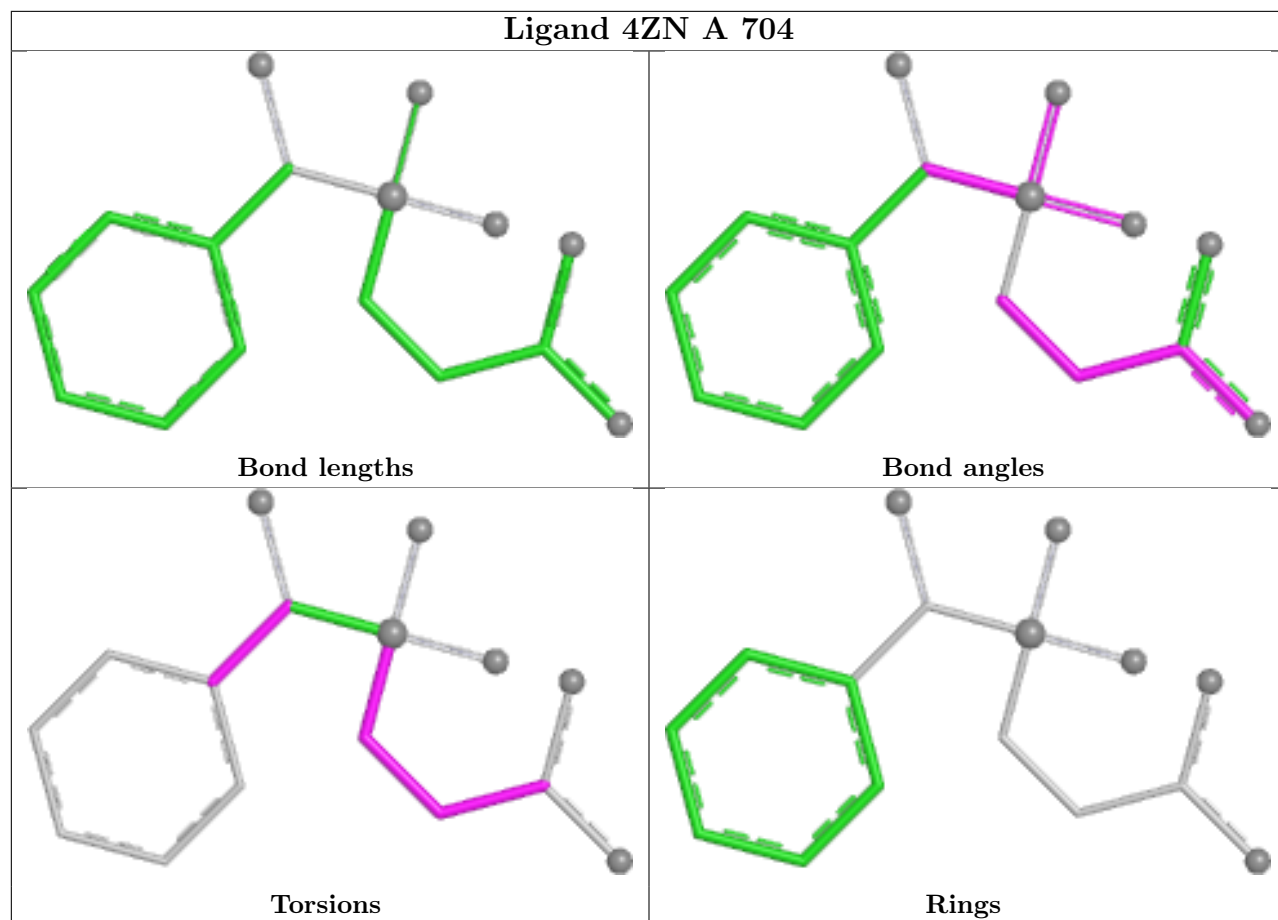
Bond angles

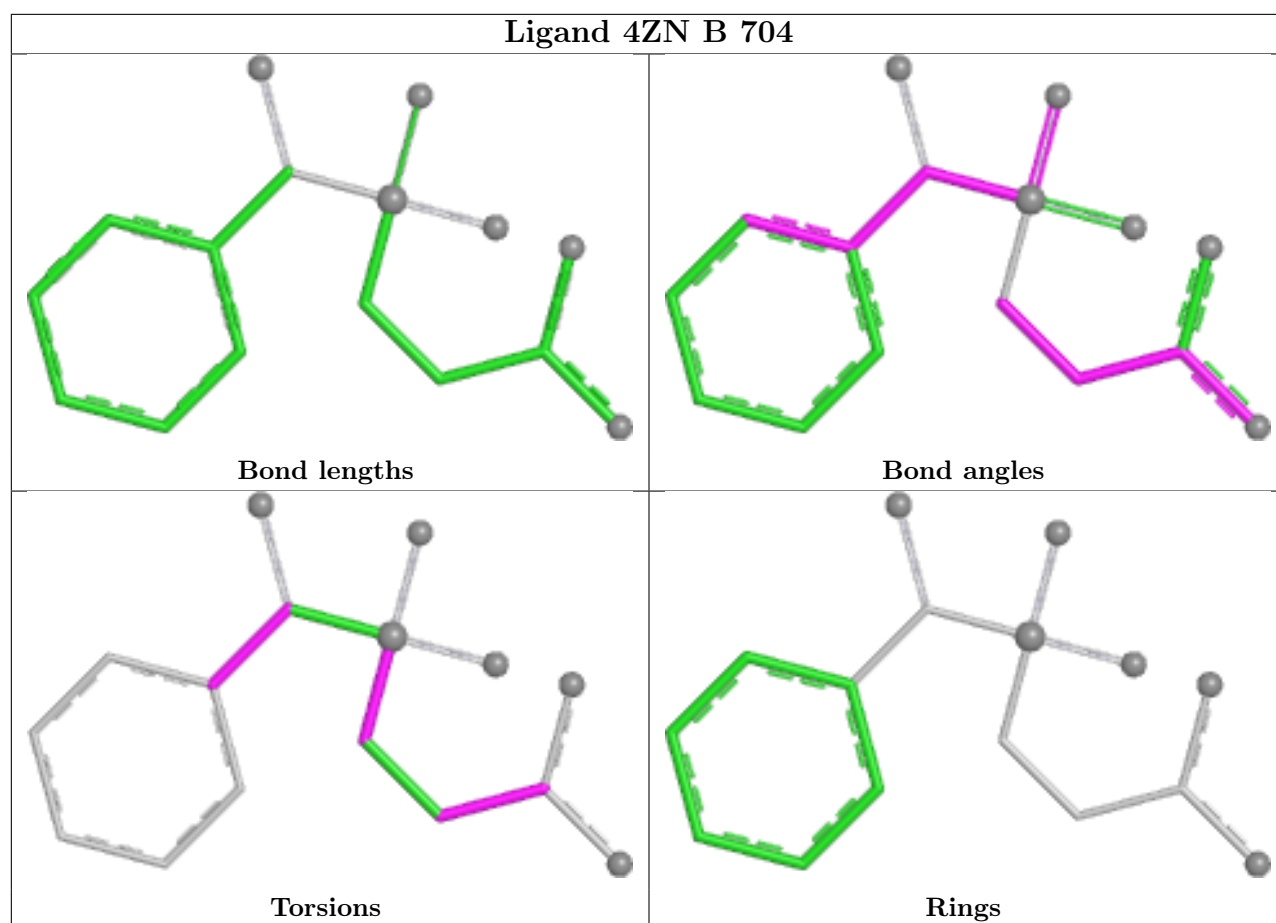


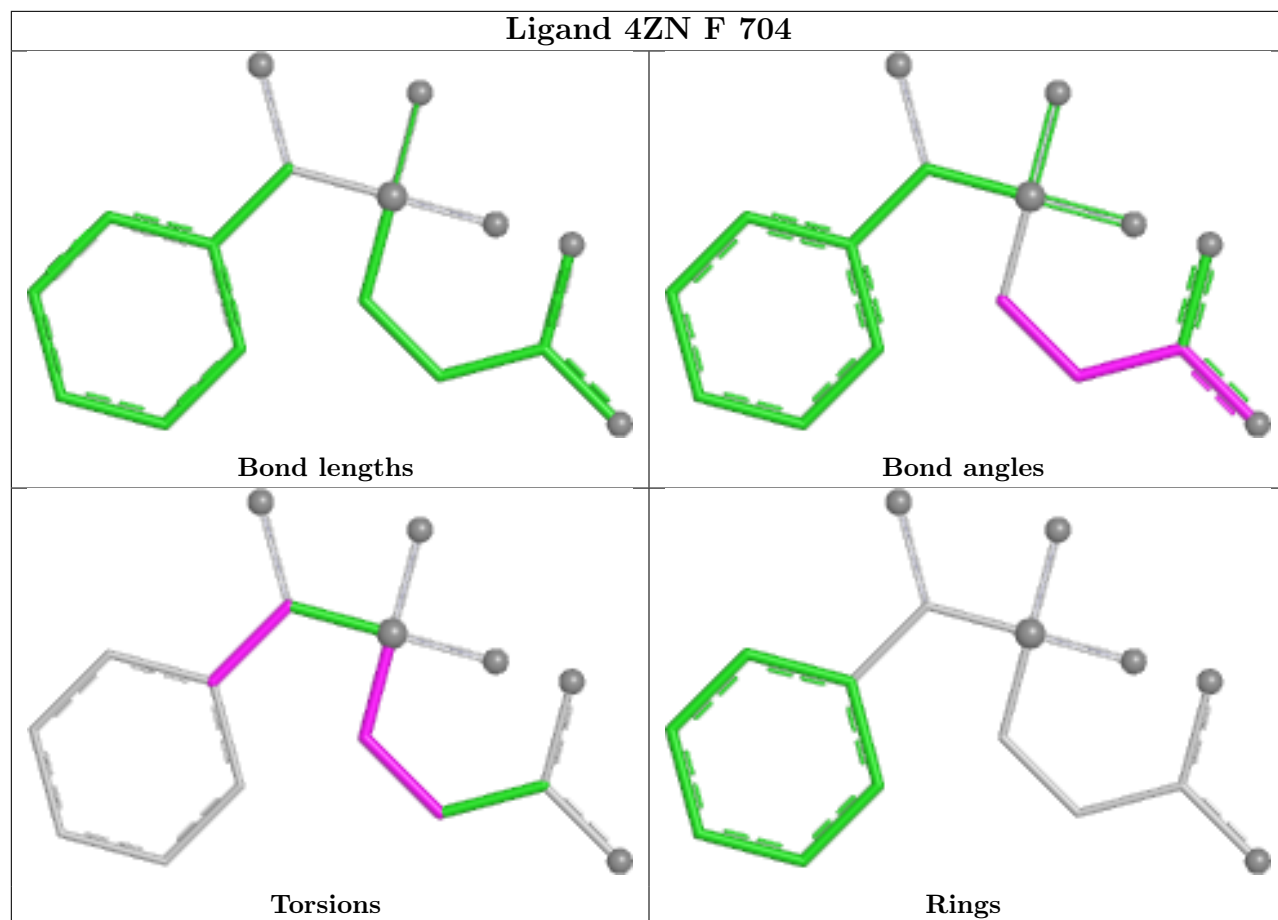
Torsions



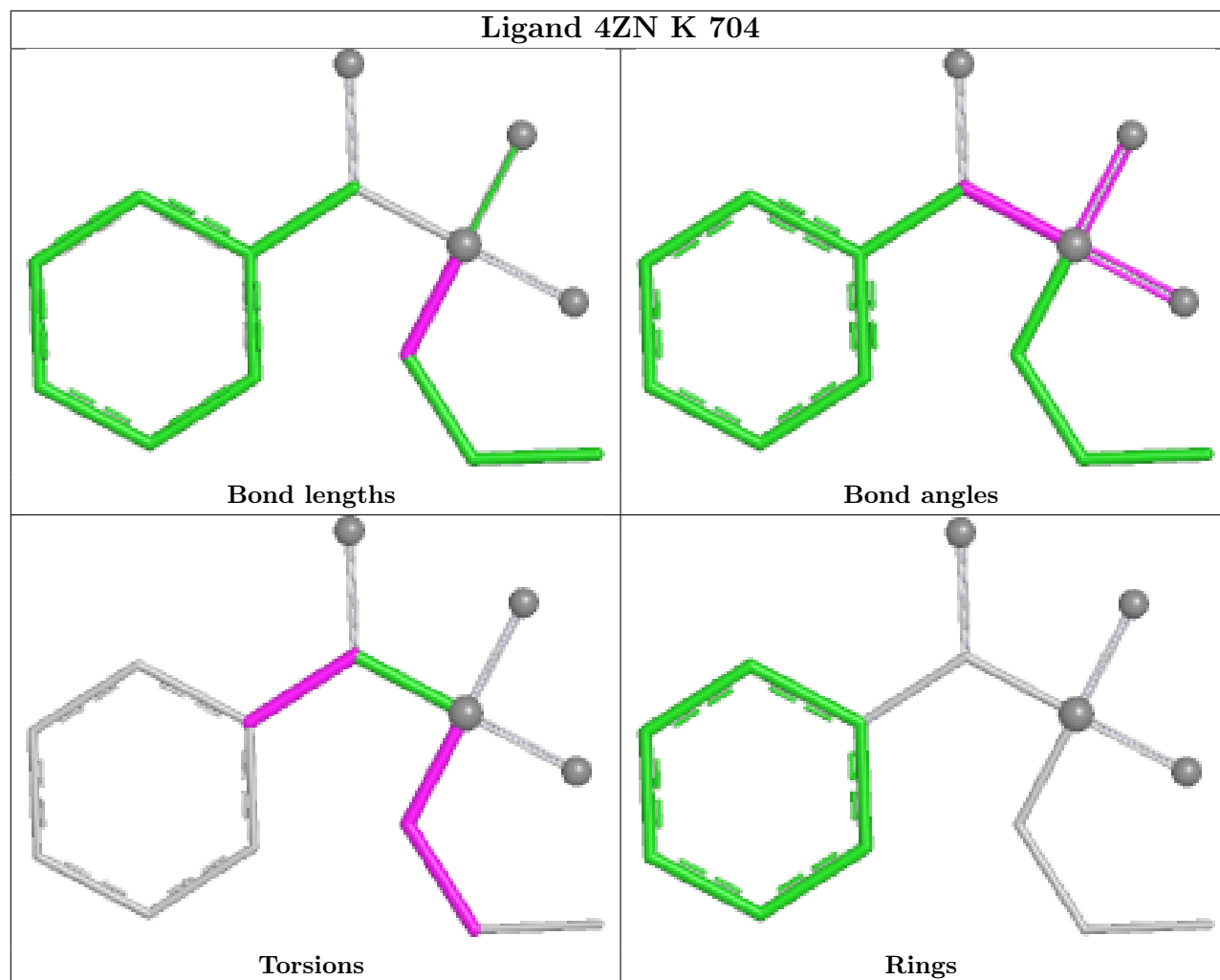
Rings

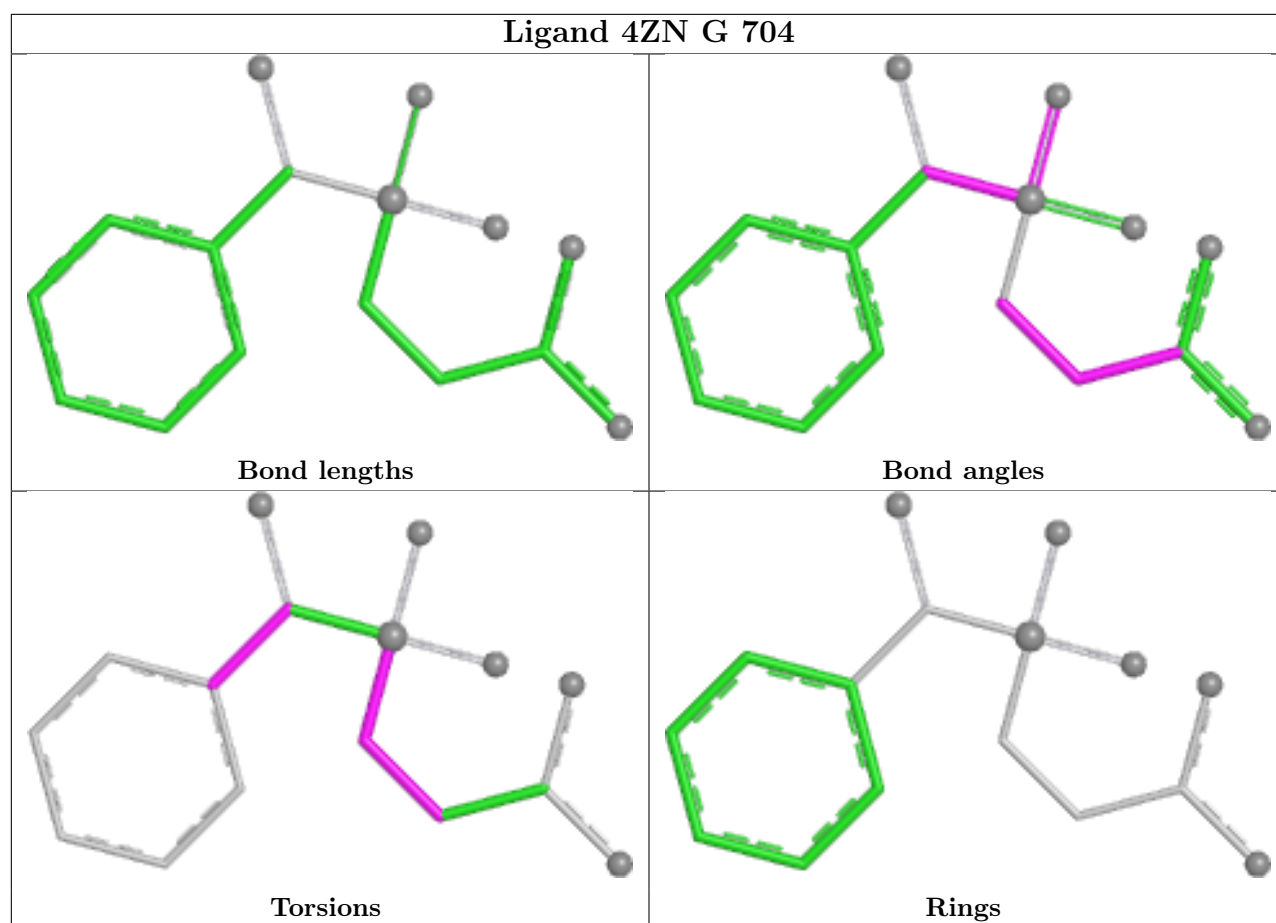




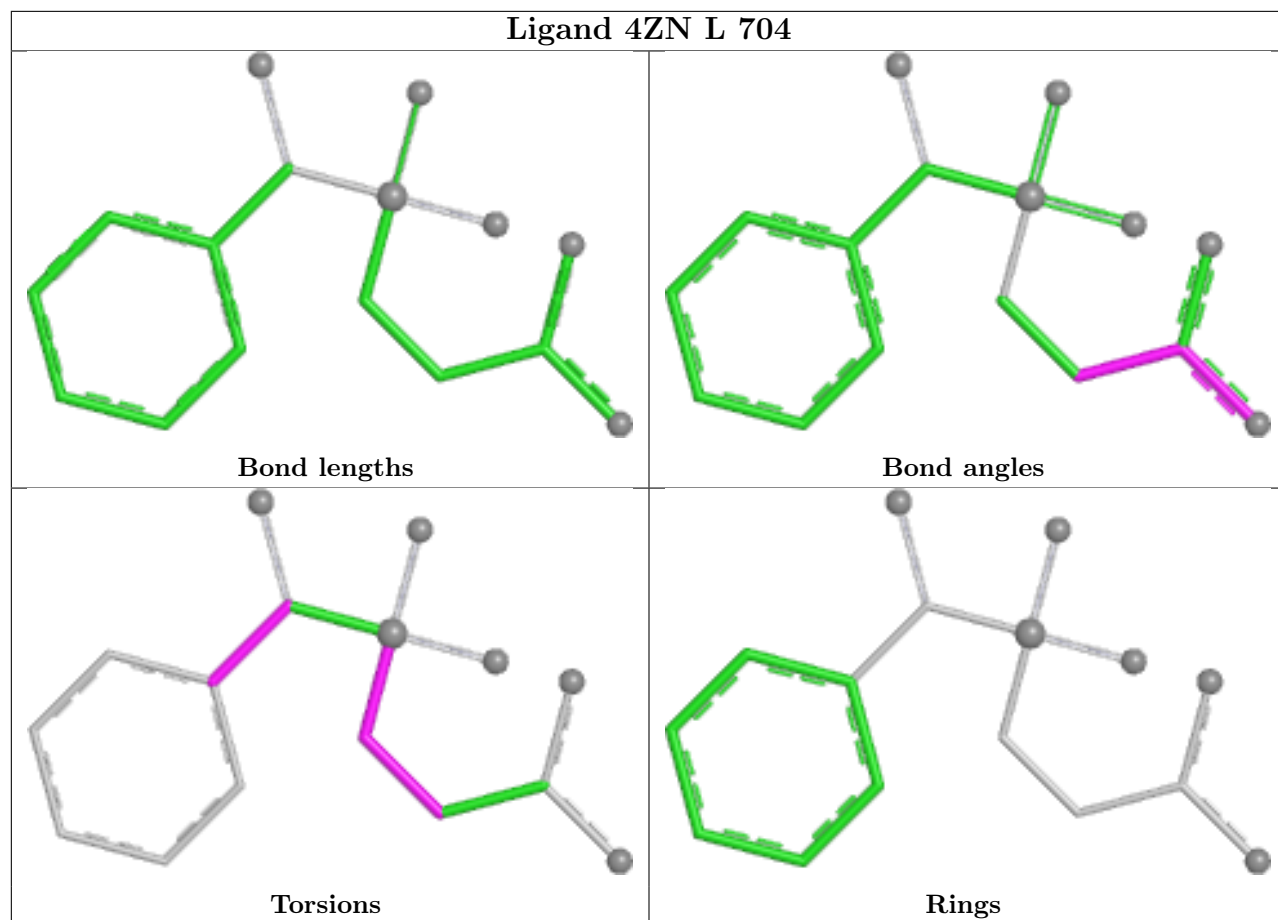


Ligand 4ZN K 704

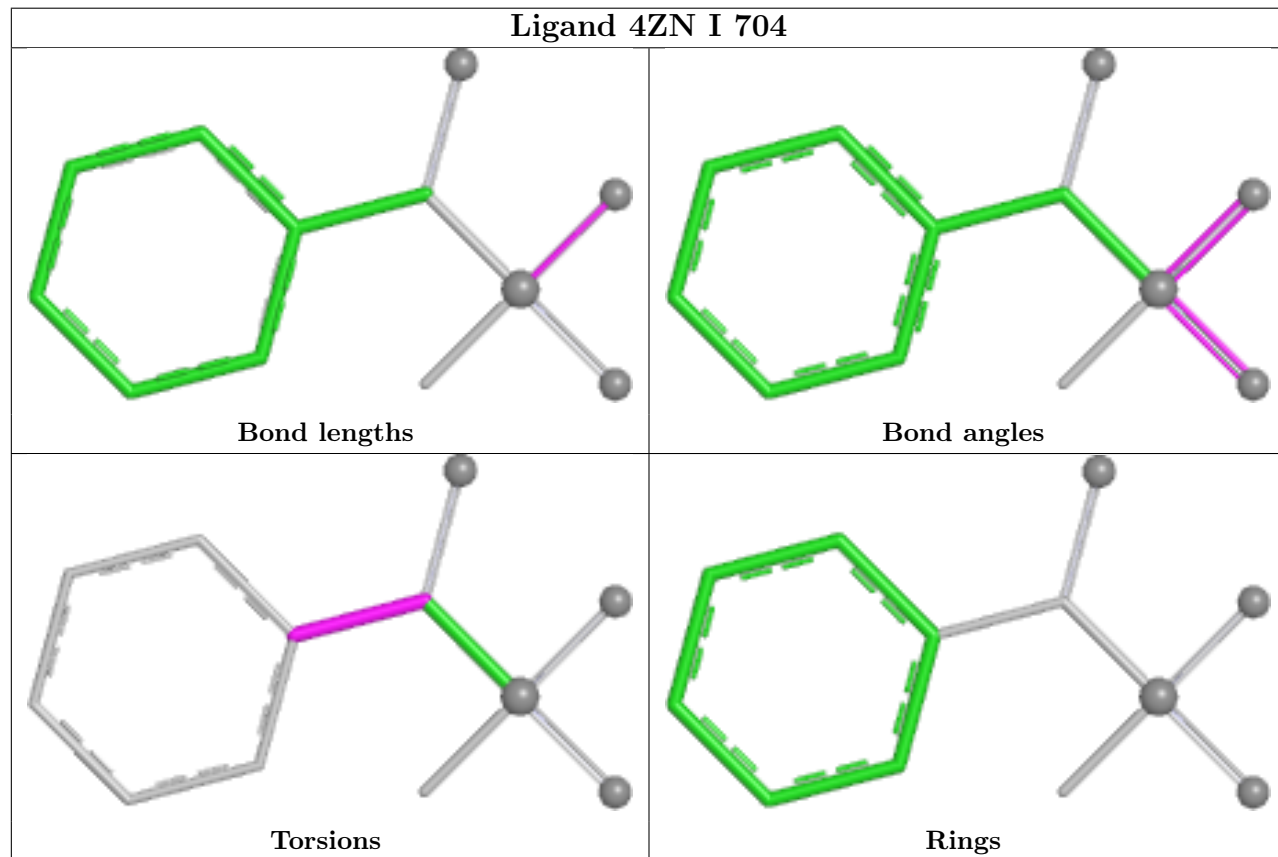




Ligand 4ZN L 704



Ligand 4ZN I 704



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	519/519 (100%)	2.42	327 (63%) 0 0	14, 23, 41, 61	4 (0%)
1	B	516/519 (99%)	2.74	382 (74%) 0 0	13, 25, 56, 73	5 (0%)
1	C	517/519 (99%)	2.44	341 (65%) 0 0	13, 23, 43, 60	3 (0%)
1	D	514/519 (99%)	2.27	304 (59%) 0 0	14, 23, 38, 58	1 (0%)
1	E	509/519 (98%)	2.36	318 (62%) 0 0	13, 22, 35, 48	2 (0%)
1	F	511/519 (98%)	2.69	374 (73%) 0 0	16, 26, 54, 71	9 (1%)
1	G	519/519 (100%)	2.37	327 (63%) 0 0	14, 23, 40, 55	5 (0%)
1	H	517/519 (99%)	2.87	390 (75%) 0 0	14, 26, 58, 73	5 (0%)
1	I	517/519 (99%)	2.56	368 (71%) 0 0	13, 25, 46, 63	5 (0%)
1	J	514/519 (99%)	2.42	336 (65%) 0 0	13, 23, 39, 55	6 (1%)
1	K	509/519 (98%)	2.45	334 (65%) 0 0	15, 23, 37, 62	3 (0%)
1	L	511/519 (98%)	2.61	351 (68%) 0 0	15, 25, 52, 62	6 (1%)
All	All	6173/6228 (99%)	2.52	4152 (67%) 0 0	13, 24, 48, 73	54 (0%)

All (4152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	121	CYS	7.6
1	D	603	ASP	7.5
1	J	603	ASP	7.4
1	I	121	CYS	7.2
1	F	138	GLU	7.1
1	A	363	GLY	7.0
1	L	136	GLY	6.8
1	B	193	GLY	6.8
1	H	165	PHE	6.7
1	I	200	GLU	6.7
1	G	363	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
1	H	119	GLY	6.5
1	L	550	SER	6.5
1	D	85	ALA	6.5
1	B	136	GLY	6.5
1	K	99	ILE	6.4
1	G	551	VAL	6.4
1	H	197	ASP	6.4
1	H	234	LEU	6.4
1	B	159	ASP	6.4
1	H	202	ASP	6.4
1	H	178	PHE	6.3
1	B	255	THR	6.3
1	H	159	ASP	6.2
1	B	197	ASP	6.2
1	H	135	PRO	6.2
1	H	255	THR	6.2
1	C	602	ASN	6.2
1	K	551	VAL	6.2
1	H	390	GLY	6.1
1	B	258	ASN	6.0
1	B	271	ILE	6.0
1	F	549	SER	6.0
1	F	123	VAL	6.0
1	K	188	GLY	5.9
1	I	230	VAL	5.9
1	A	603	ASP	5.9
1	F	364	ASP	5.9
1	L	138	GLU	5.9
1	G	120	GLY	5.8
1	L	144	ILE	5.8
1	J	136	GLY	5.8
1	F	178	PHE	5.8
1	L	511	ASN	5.7
1	F	185	VAL	5.7
1	J	178	PHE	5.7
1	F	603	ASP	5.7
1	B	261	MET	5.7
1	H	603	ASP	5.7
1	I	260	ASN	5.7
1	L	139	ASN	5.7
1	H	522	GLU	5.7
1	B	272	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	H	477	GLY	5.6
1	H	144	ILE	5.6
1	B	548	SER	5.6
1	I	344	VAL	5.6
1	C	134	ASN	5.6
1	L	544	ILE	5.5
1	D	229	ASN	5.5
1	G	268	GLY	5.5
1	F	478	VAL	5.5
1	A	395	LEU	5.5
1	B	273	ASN	5.4
1	H	155	GLU	5.4
1	L	421	VAL	5.4
1	H	254	SER	5.3
1	H	201	ALA	5.3
1	B	315	VAL	5.3
1	I	114	VAL	5.3
1	B	149	ASN	5.3
1	L	603	ASP	5.3
1	C	194	SER	5.3
1	C	393	ILE	5.3
1	J	572	ALA	5.3
1	B	123	VAL	5.3
1	F	157	LEU	5.3
1	B	165	PHE	5.3
1	B	171	THR	5.3
1	H	602	ASN	5.3
1	H	261	MET	5.3
1	J	550	SER	5.3
1	F	579	VAL	5.2
1	C	121	CYS	5.2
1	G	104	ASN	5.2
1	L	161	ASN	5.2
1	L	364	ASP	5.2
1	A	427	SER	5.2
1	F	110	ILE	5.2
1	K	592	GLY	5.2
1	H	275	ASP	5.2
1	J	104	ASN	5.2
1	H	257	LYS	5.2
1	I	602	ASN	5.2
1	A	193	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	263	TYR	5.1
1	L	176	TYR	5.1
1	A	85	ALA	5.1
1	B	198	LEU	5.1
1	I	300	ALA	5.1
1	A	362	LYS	5.1
1	A	259	VAL	5.1
1	B	259	VAL	5.1
1	L	494	SER	5.1
1	G	389	PRO	5.1
1	L	198	LEU	5.1
1	A	260	ASN	5.1
1	L	134	ASN	5.1
1	L	197	ASP	5.1
1	F	195	VAL	5.1
1	J	600	VAL	5.1
1	G	549	SER	5.1
1	F	347	GLY	5.1
1	J	196	ALA	5.1
1	A	104[A]	ASN	5.1
1	F	216	ASP	5.1
1	C	365	VAL	5.1
1	F	114	VAL	5.1
1	K	550	SER	5.1
1	H	392	MET	5.1
1	C	127	LEU	5.1
1	J	260	ASN	5.1
1	A	600	VAL	5.1
1	H	169	LEU	5.0
1	H	219	LEU	5.0
1	F	139	ASN	5.0
1	B	118	LYS	5.0
1	I	365	VAL	5.0
1	L	395	LEU	5.0
1	K	518	LYS	5.0
1	G	171	THR	5.0
1	G	85	ALA	5.0
1	H	410	ALA	5.0
1	B	167	VAL	5.0
1	G	261	MET	5.0
1	B	143	LYS	5.0
1	B	234	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	149	ASN	5.0
1	I	196	ALA	5.0
1	J	194	SER	4.9
1	F	155	GLU	4.9
1	H	273	ASN	4.9
1	K	490	ALA	4.9
1	L	410	ALA	4.9
1	H	259	VAL	4.9
1	H	421	VAL	4.9
1	J	551	VAL	4.9
1	L	195	VAL	4.9
1	H	271	ILE	4.9
1	L	216	ASP	4.9
1	E	549	SER	4.9
1	H	145	SER	4.9
1	H	189	TYR	4.9
1	A	531	ASN	4.9
1	C	524	VAL	4.9
1	H	383	TYR	4.9
1	I	178	PHE	4.9
1	H	217	ASN	4.9
1	A	305	CYS	4.8
1	H	486	THR	4.8
1	H	122	ASN	4.8
1	E	507	GLU	4.8
1	D	549	SER	4.8
1	L	119	GLY	4.8
1	B	121	CYS	4.8
1	I	195	VAL	4.8
1	L	276	THR	4.8
1	C	260	ASN	4.8
1	E	196	ALA	4.8
1	C	86	SER	4.8
1	C	136	GLY	4.8
1	I	580	SER	4.8
1	H	365	VAL	4.8
1	F	144	ILE	4.8
1	H	117	ILE	4.8
1	G	178	PHE	4.8
1	L	157	LEU	4.8
1	K	305	CYS	4.8
1	K	190	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	L	600	VAL	4.8
1	A	544	ILE	4.7
1	H	310	LEU	4.7
1	D	196	ALA	4.7
1	H	196	ALA	4.7
1	C	88	VAL	4.7
1	D	390	GLY	4.7
1	J	85	ALA	4.7
1	F	184	SER	4.7
1	B	316	GLU	4.7
1	E	422	GLU	4.7
1	E	372	VAL	4.7
1	G	121	CYS	4.7
1	C	423	ILE	4.7
1	H	156	PHE	4.7
1	H	143	LYS	4.7
1	G	480	TYR	4.7
1	A	340	ALA	4.7
1	B	274	ALA	4.7
1	E	442	GLY	4.7
1	D	391	SER	4.7
1	C	180	ASP	4.7
1	J	123	VAL	4.7
1	L	183	ASN	4.7
1	L	470	LEU	4.7
1	E	268	GLY	4.7
1	I	247	MET	4.7
1	F	183	ASN	4.6
1	F	187	VAL	4.6
1	J	183	ASN	4.6
1	L	568	ASN	4.6
1	F	129	ILE	4.6
1	K	110	ILE	4.6
1	D	194	SER	4.6
1	F	186	ALA	4.6
1	J	137	LYS	4.6
1	B	216	ASP	4.6
1	B	229	ASN	4.6
1	E	272	ASN	4.6
1	H	538	ASN	4.6
1	B	195	VAL	4.6
1	H	276	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	323	LEU	4.6
1	C	200	GLU	4.6
1	B	135	PRO	4.6
1	H	549	SER	4.6
1	L	480	TYR	4.6
1	B	181	ASN	4.6
1	B	202	ASP	4.6
1	B	262	GLU	4.6
1	J	262	GLU	4.6
1	L	117	ILE	4.6
1	A	550	SER	4.6
1	F	86	SER	4.6
1	E	273	ASN	4.6
1	K	150	ASP	4.6
1	I	259	VAL	4.6
1	L	323	LEU	4.6
1	L	228	ILE	4.6
1	B	226	PHE	4.5
1	C	178	PHE	4.5
1	C	381	GLY	4.5
1	E	592	GLY	4.5
1	F	300	ALA	4.5
1	J	553	ALA	4.5
1	D	138	GLU	4.5
1	E	229	ASN	4.5
1	L	229	ASN	4.5
1	D	601	LEU	4.5
1	G	259	VAL	4.5
1	H	198	LEU	4.5
1	K	365	VAL	4.5
1	F	311	SER	4.5
1	H	302	SER	4.5
1	A	526	TRP	4.5
1	B	405	ALA	4.5
1	C	262	GLU	4.5
1	B	176	TYR	4.5
1	G	603	ASP	4.5
1	L	602	ASN	4.5
1	E	466	LEU	4.5
1	H	132	VAL	4.5
1	H	142	VAL	4.5
1	E	490	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	J	405	ALA	4.5
1	L	147	LYS	4.5
1	L	567	GLN	4.5
1	B	185	VAL	4.5
1	H	167	VAL	4.5
1	L	135	PRO	4.5
1	H	136	GLY	4.5
1	K	578	GLY	4.5
1	C	580	SER	4.5
1	I	316	GLU	4.5
1	H	493	TYR	4.4
1	E	106	PRO	4.4
1	D	576	ILE	4.4
1	E	148	VAL	4.4
1	L	123	VAL	4.4
1	L	142	VAL	4.4
1	L	363	GLY	4.4
1	L	145	SER	4.4
1	K	398	PHE	4.4
1	I	118	LYS	4.4
1	J	300	ALA	4.4
1	H	139	ASN	4.4
1	K	122	ASN	4.4
1	D	219	LEU	4.4
1	K	395	LEU	4.4
1	B	270	TYR	4.4
1	L	528	PRO	4.4
1	B	225	VAL	4.4
1	C	144	ILE	4.4
1	F	225	VAL	4.4
1	H	376	ILE	4.4
1	K	315	VAL	4.4
1	L	132	VAL	4.4
1	C	578	GLY	4.4
1	H	193	GLY	4.4
1	F	177	MET	4.4
1	H	258	ASN	4.4
1	C	198	LEU	4.4
1	H	241	THR	4.4
1	J	135	PRO	4.4
1	I	138	GLU	4.4
1	H	123	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	J	375	GLY	4.4
1	D	147	LYS	4.4
1	H	436	LYS	4.4
1	A	602	ASN	4.4
1	B	294	ALA	4.4
1	B	318	ALA	4.4
1	F	133	ASN	4.4
1	H	313	ALA	4.4
1	I	202	ASP	4.4
1	J	149	ASN	4.4
1	J	124	GLU	4.4
1	B	257	LYS	4.4
1	B	153	VAL	4.4
1	B	277	TYR	4.4
1	C	117	ILE	4.4
1	I	117	ILE	4.4
1	K	339	GLY	4.4
1	L	478	VAL	4.4
1	L	592	GLY	4.4
1	J	361	SER	4.4
1	B	183	ASN	4.4
1	F	217	ASN	4.4
1	H	233	ASN	4.4
1	I	161	ASN	4.4
1	I	229	ASN	4.4
1	I	565	PHE	4.4
1	J	428	ALA	4.3
1	I	262	GLU	4.3
1	K	419	GLU	4.3
1	J	395	LEU	4.3
1	A	195	VAL	4.3
1	H	176	TYR	4.3
1	H	480	TYR	4.3
1	K	185	VAL	4.3
1	B	139	ASN	4.3
1	F	197	ASP	4.3
1	G	483	ASP	4.3
1	F	274	ALA	4.3
1	K	175	PHE	4.3
1	B	140	GLY	4.3
1	E	117	ILE	4.3
1	I	136	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	185	VAL	4.3
1	E	480	TYR	4.3
1	A	295	SER	4.3
1	B	194	SER	4.3
1	E	602	ASN	4.3
1	H	181	ASN	4.3
1	H	322	ASN	4.3
1	J	197	ASP	4.3
1	J	394	ASP	4.3
1	B	156	PHE	4.3
1	F	414	GLY	4.3
1	B	142	VAL	4.3
1	B	207	VAL	4.3
1	F	148	VAL	4.3
1	B	146	SER	4.3
1	F	550	SER	4.3
1	D	443	ASP	4.3
1	F	602	ASN	4.3
1	I	163	GLU	4.3
1	L	217	ASN	4.3
1	D	490	ALA	4.3
1	H	328	LEU	4.3
1	F	567	GLN	4.3
1	K	376	ILE	4.3
1	H	429	VAL	4.2
1	F	507	GLU	4.2
1	H	508	GLU	4.2
1	B	364	ASP	4.2
1	G	277	TYR	4.2
1	B	201	ALA	4.2
1	A	119	GLY	4.2
1	A	290	GLY	4.2
1	B	409	CYS	4.2
1	F	362	LYS	4.2
1	B	200	GLU	4.2
1	K	163	GLU	4.2
1	F	254	SER	4.2
1	H	249	ASP	4.2
1	H	272	ASN	4.2
1	K	558	ALA	4.2
1	F	395	LEU	4.2
1	I	328	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	223	THR	4.2
1	K	191	GLY	4.2
1	K	375	GLY	4.2
1	F	334	GLU	4.2
1	F	117	ILE	4.2
1	C	132	VAL	4.2
1	C	195	VAL	4.2
1	F	142	VAL	4.2
1	B	394	ASP	4.2
1	J	217	ASN	4.2
1	C	493	TYR	4.2
1	E	541	TYR	4.2
1	H	325	TYR	4.2
1	I	287	TYR	4.2
1	F	141	PRO	4.2
1	J	389	PRO	4.2
1	B	321	LEU	4.2
1	F	276	THR	4.2
1	G	362	LYS	4.2
1	F	161	ASN	4.2
1	H	225	VAL	4.2
1	H	455	VAL	4.2
1	I	194	SER	4.2
1	J	229	ASN	4.2
1	I	204	LYS	4.2
1	G	165	PHE	4.2
1	I	321	LEU	4.2
1	K	509	LEU	4.2
1	L	526	TRP	4.2
1	B	138	GLU	4.2
1	D	279	GLU	4.2
1	H	316	GLU	4.2
1	A	268	GLY	4.1
1	K	117	ILE	4.1
1	C	275	ASP	4.1
1	F	180	ASP	4.1
1	J	114	VAL	4.1
1	J	145	SER	4.1
1	J	220	SER	4.1
1	L	272	ASN	4.1
1	L	330	VAL	4.1
1	H	152	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	472	TYR	4.1
1	G	404	ALA	4.1
1	I	542	ALA	4.1
1	B	416	LEU	4.1
1	F	377	THR	4.1
1	I	377	THR	4.1
1	B	119	GLY	4.1
1	E	119	GLY	4.1
1	J	347	GLY	4.1
1	A	86	SER	4.1
1	C	139	ASN	4.1
1	L	146	SER	4.1
1	L	194	SER	4.1
1	A	269	VAL	4.1
1	G	593	VAL	4.1
1	K	195	VAL	4.1
1	L	281	VAL	4.1
1	E	143	LYS	4.1
1	J	218	LYS	4.1
1	D	102	GLU	4.1
1	H	200	GLU	4.1
1	G	487	LEU	4.1
1	I	466	LEU	4.1
1	I	499	TYR	4.1
1	B	398	PHE	4.1
1	H	597	THR	4.1
1	L	165	PHE	4.1
1	B	184	SER	4.1
1	B	275	ASP	4.1
1	B	515	GLN	4.1
1	C	261	MET	4.1
1	F	122	ASN	4.1
1	K	216	ASP	4.1
1	D	395	LEU	4.1
1	A	156	PHE	4.1
1	A	170	GLY	4.1
1	I	193	GLY	4.1
1	B	221	LYS	4.1
1	G	571	TRP	4.1
1	A	271	ILE	4.1
1	B	133	ASN	4.1
1	G	117	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	272	ASN	4.1
1	H	443	ASP	4.1
1	J	117	ILE	4.1
1	B	230	VAL	4.1
1	E	429	VAL	4.1
1	G	528	PRO	4.1
1	I	135	PRO	4.1
1	A	460	ALA	4.0
1	L	196	ALA	4.0
1	F	219	LEU	4.0
1	J	565	PHE	4.0
1	K	504	GLY	4.0
1	B	122	ASN	4.0
1	G	543	ASP	4.0
1	H	423	ILE	4.0
1	I	144	ILE	4.0
1	E	121	CYS	4.0
1	L	121	CYS	4.0
1	B	278	LYS	4.0
1	I	387	ALA	4.0
1	J	94	LEU	4.0
1	A	569	THR	4.0
1	B	363	GLY	4.0
1	F	104	ASN	4.0
1	I	394	ASP	4.0
1	L	508	GLU	4.0
1	L	538	ASN	4.0
1	A	393	ILE	4.0
1	F	194	SER	4.0
1	E	418	PRO	4.0
1	F	167	VAL	4.0
1	L	141	PRO	4.0
1	D	362	LYS	4.0
1	H	430	CYS	4.0
1	C	208	LEU	4.0
1	E	395	LEU	4.0
1	F	267	LEU	4.0
1	H	131	LEU	4.0
1	I	329	GLY	4.0
1	L	177	MET	4.0
1	E	237	PHE	4.0
1	H	238	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	304	TYR	4.0
1	H	270	TYR	4.0
1	J	493	TYR	4.0
1	E	551	VAL	4.0
1	H	195	VAL	4.0
1	L	551	VAL	4.0
1	F	490	ALA	4.0
1	H	409	CYS	4.0
1	K	385	LEU	4.0
1	A	390	GLY	4.0
1	G	289	PHE	4.0
1	D	122	ASN	4.0
1	D	150	ASP	4.0
1	E	420	ASN	4.0
1	H	352	ASN	4.0
1	F	270	TYR	4.0
1	G	176	TYR	4.0
1	H	472	TYR	4.0
1	H	129	ILE	4.0
1	H	232	LYS	3.9
1	F	135	PRO	3.9
1	A	297	LEU	3.9
1	B	162	MET	3.9
1	C	296	GLN	3.9
1	F	321	LEU	3.9
1	I	198	LEU	3.9
1	C	590	GLY	3.9
1	D	405	ALA	3.9
1	H	485	ALA	3.9
1	I	469	ALA	3.9
1	K	196	ALA	3.9
1	E	532	GLU	3.9
1	K	364	ASP	3.9
1	D	438	SER	3.9
1	F	277	TYR	3.9
1	H	99	ILE	3.9
1	K	510	ILE	3.9
1	B	421	VAL	3.9
1	C	259	VAL	3.9
1	E	308	VAL	3.9
1	E	455	VAL	3.9
1	B	395	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	317	LEU	3.9
1	H	507	GLU	3.9
1	J	279	GLU	3.9
1	J	335	GLU	3.9
1	K	262	GLU	3.9
1	H	274	ALA	3.9
1	F	128	THR	3.9
1	D	260	ASN	3.9
1	C	550	SER	3.9
1	H	199	SER	3.9
1	K	220	SER	3.9
1	A	117	ILE	3.9
1	D	480	TYR	3.9
1	A	224	VAL	3.9
1	D	167	VAL	3.9
1	K	392	MET	3.9
1	L	91	VAL	3.9
1	B	227	GLU	3.9
1	D	94	LEU	3.9
1	L	219	LEU	3.9
1	A	382	GLY	3.9
1	E	128	THR	3.9
1	F	196	ALA	3.9
1	G	186	ALA	3.9
1	L	577	ALA	3.9
1	F	221	LYS	3.9
1	G	531	ASN	3.9
1	H	260	ASN	3.9
1	J	521	ASN	3.9
1	B	178	PHE	3.9
1	H	425	PHE	3.9
1	G	550	SER	3.9
1	B	301	PRO	3.9
1	C	481	ILE	3.9
1	I	101	ILE	3.9
1	I	107	ILE	3.9
1	J	439	TYR	3.9
1	B	392	MET	3.9
1	F	211	VAL	3.9
1	H	114	VAL	3.9
1	C	210	LEU	3.9
1	H	157	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	126	GLY	3.9
1	H	170	GLY	3.9
1	K	363	GLY	3.9
1	D	201	ALA	3.9
1	G	542	ALA	3.9
1	L	192	CYS	3.8
1	A	599	PHE	3.8
1	B	175	PHE	3.8
1	K	100	PRO	3.8
1	B	102	GLU	3.8
1	B	177	MET	3.8
1	I	227	GLU	3.8
1	K	493	TYR	3.8
1	C	114	VAL	3.8
1	E	365	VAL	3.8
1	G	195	VAL	3.8
1	L	286	VAL	3.8
1	L	344	VAL	3.8
1	E	385	LEU	3.8
1	H	239	LEU	3.8
1	H	416	LEU	3.8
1	K	408	GLY	3.8
1	C	196	ALA	3.8
1	C	255	THR	3.8
1	I	388	ALA	3.8
1	C	394	ASP	3.8
1	F	149	ASN	3.8
1	F	249	ASP	3.8
1	L	181	ASN	3.8
1	B	93	SER	3.8
1	I	113	GLN	3.8
1	I	145	SER	3.8
1	K	311	SER	3.8
1	K	431	GLU	3.8
1	K	441	PRO	3.8
1	B	413	VAL	3.8
1	G	112	VAL	3.8
1	H	406	VAL	3.8
1	I	153	VAL	3.8
1	I	308	VAL	3.8
1	A	426	LEU	3.8
1	G	119	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	402	GLY	3.8
1	H	347	GLY	3.8
1	I	170	GLY	3.8
1	J	219	LEU	3.8
1	J	601	LEU	3.8
1	K	495	LEU	3.8
1	B	404	ALA	3.8
1	C	276	THR	3.8
1	H	128	THR	3.8
1	B	116	ASP	3.8
1	H	109	ASP	3.8
1	I	109	ASP	3.8
1	I	364	ASP	3.8
1	D	192	CYS	3.8
1	F	226	PHE	3.8
1	F	237	PHE	3.8
1	F	491	MET	3.8
1	H	138	GLU	3.8
1	H	262	GLU	3.8
1	K	400	MET	3.8
1	A	434	VAL	3.8
1	D	136	GLY	3.8
1	F	596	LEU	3.8
1	H	342	LEU	3.8
1	J	359	TYR	3.8
1	J	406	VAL	3.8
1	L	126	GLY	3.8
1	E	300	ALA	3.8
1	F	223	THR	3.8
1	A	149	ASN	3.8
1	C	256	ASP	3.8
1	G	602	ASN	3.8
1	H	150	ASP	3.8
1	H	364	ASP	3.8
1	H	405	ALA	3.8
1	J	161	ASN	3.8
1	J	388	ALA	3.8
1	K	602	ASN	3.8
1	L	274	ALA	3.8
1	A	137	LYS	3.8
1	A	549	SER	3.8
1	H	351	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	L	178	PHE	3.8
1	B	112	VAL	3.8
1	B	381	GLY	3.8
1	B	593	VAL	3.8
1	C	123	VAL	3.8
1	D	321	LEU	3.8
1	E	350	TYR	3.7
1	F	600	VAL	3.8
1	B	486	THR	3.7
1	A	196	ALA	3.7
1	B	260	ASN	3.7
1	D	457	ASN	3.7
1	E	322	ASN	3.7
1	F	272	ASN	3.7
1	H	186	ALA	3.7
1	J	483	ASP	3.7
1	A	200	GLU	3.7
1	D	419	GLU	3.7
1	F	366	LYS	3.7
1	G	552	LYS	3.7
1	J	138	GLU	3.7
1	A	523	PRO	3.7
1	C	555	SER	3.7
1	H	391	SER	3.7
1	H	130	PHE	3.7
1	H	192	CYS	3.7
1	B	131	LEU	3.7
1	F	339	GLY	3.7
1	L	169	LEU	3.7
1	L	487	LEU	3.7
1	H	269	VAL	3.7
1	I	132	VAL	3.7
1	I	225	VAL	3.7
1	L	566	VAL	3.7
1	C	366	LYS	3.7
1	D	200	GLU	3.7
1	I	103	TYR	3.7
1	L	115	TYR	3.7
1	B	217	ASN	3.7
1	F	181	ASN	3.7
1	H	133	ASN	3.7
1	C	274	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	349	MET	3.7
1	H	318	ALA	3.7
1	I	100	PRO	3.7
1	B	361	SER	3.7
1	B	401	SER	3.7
1	B	549	SER	3.7
1	F	361	SER	3.7
1	B	407	LEU	3.7
1	C	290	GLY	3.7
1	E	390	GLY	3.7
1	F	381	GLY	3.7
1	L	182	LYS	3.7
1	C	308	VAL	3.7
1	C	551	VAL	3.7
1	F	92	VAL	3.7
1	H	478	VAL	3.7
1	J	455	VAL	3.7
1	L	153	VAL	3.7
1	C	364	ASP	3.7
1	D	352	ASN	3.7
1	F	179	ASN	3.7
1	I	272	ASN	3.7
1	K	189	TYR	3.7
1	L	452	THR	3.7
1	A	294	ALA	3.7
1	C	542	ALA	3.7
1	E	460	ALA	3.7
1	F	585	ALA	3.7
1	I	209	SER	3.7
1	J	549	SER	3.7
1	B	232	LYS	3.7
1	B	403	CYS	3.7
1	I	526	TRP	3.7
1	K	192	CYS	3.7
1	L	409	CYS	3.7
1	C	422	GLU	3.7
1	B	219	LEU	3.7
1	F	210	LEU	3.7
1	F	342	LEU	3.7
1	F	402	GLY	3.7
1	F	462	GLY	3.7
1	K	268	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	317	LEU	3.7
1	L	342	LEU	3.7
1	C	538	ASN	3.7
1	D	233	ASN	3.7
1	E	505	ASN	3.7
1	F	344	VAL	3.7
1	F	399	ASP	3.7
1	H	161	ASN	3.7
1	G	135	PRO	3.7
1	B	254	SER	3.7
1	I	254	SER	3.7
1	L	311	SER	3.7
1	C	143	LYS	3.7
1	D	337	LYS	3.7
1	E	376	ILE	3.6
1	K	289	PHE	3.6
1	L	130	PHE	3.6
1	A	160	GLU	3.6
1	E	138	GLU	3.6
1	H	163	GLU	3.6
1	H	329	GLY	3.6
1	I	590	GLY	3.6
1	I	242	LEU	3.6
1	I	601	LEU	3.6
1	L	426	LEU	3.6
1	B	161	ASN	3.6
1	B	166	ASN	3.6
1	B	420	ASN	3.6
1	C	181	ASN	3.6
1	C	202	ASP	3.6
1	C	434	VAL	3.6
1	C	568	ASN	3.6
1	D	568	ASN	3.6
1	F	566	VAL	3.6
1	G	413	VAL	3.6
1	K	230	VAL	3.6
1	D	248	THR	3.6
1	L	428	ALA	3.6
1	L	270	TYR	3.6
1	J	555	SER	3.6
1	K	552	LYS	3.6
1	L	232	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	316	GLU	3.6
1	C	510	ILE	3.6
1	D	271	ILE	3.6
1	F	99	ILE	3.6
1	I	140	GLY	3.6
1	K	381	GLY	3.6
1	G	94	LEU	3.6
1	K	94	LEU	3.6
1	E	538	ASN	3.6
1	H	116	ASP	3.6
1	C	142	VAL	3.6
1	C	148	VAL	3.6
1	C	344	VAL	3.6
1	E	421	VAL	3.6
1	A	447	ALA	3.6
1	G	588	PRO	3.6
1	C	554	SER	3.6
1	D	548	SER	3.6
1	L	516	SER	3.6
1	A	392	MET	3.6
1	H	101	ILE	3.6
1	I	576	ILE	3.6
1	K	393	ILE	3.6
1	L	99	ILE	3.6
1	D	126	GLY	3.6
1	D	590	GLY	3.6
1	G	357	LEU	3.6
1	A	511	ASN	3.6
1	B	399	ASP	3.6
1	G	159	ASP	3.6
1	H	216	ASP	3.6
1	A	91	VAL	3.6
1	A	344	VAL	3.6
1	A	365	VAL	3.6
1	B	600	VAL	3.6
1	E	212	THR	3.6
1	G	187	VAL	3.6
1	I	97	THR	3.6
1	K	143	LYS	3.6
1	K	153	VAL	3.6
1	L	114	VAL	3.6
1	D	294	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	284	ALA	3.6
1	B	539	SER	3.6
1	D	550	SER	3.6
1	E	102	GLU	3.6
1	E	324	GLU	3.6
1	K	115	TYR	3.6
1	F	355	ILE	3.6
1	F	529	ILE	3.6
1	L	271	ILE	3.6
1	E	504	GLY	3.6
1	G	238	PHE	3.6
1	L	347	GLY	3.6
1	A	210	LEU	3.6
1	H	214	LEU	3.6
1	H	492	LEU	3.6
1	K	323	LEU	3.6
1	L	239	LEU	3.6
1	B	538	ASN	3.6
1	F	275	ASP	3.6
1	G	182	LYS	3.6
1	G	197	ASP	3.6
1	H	111	LYS	3.6
1	I	531	ASN	3.6
1	A	192	CYS	3.6
1	I	171	THR	3.6
1	I	167	VAL	3.6
1	L	148	VAL	3.6
1	D	250	GLU	3.6
1	F	473	ALA	3.6
1	B	302	SER	3.5
1	B	516	SER	3.5
1	C	343	SER	3.5
1	H	361	SER	3.5
1	A	480	TYR	3.5
1	A	423	ILE	3.5
1	L	393	ILE	3.5
1	A	436	LYS	3.5
1	B	267	LEU	3.5
1	E	475	LYS	3.5
1	G	137	LYS	3.5
1	H	173	LYS	3.5
1	H	362	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	511	ASN	3.5
1	I	255	THR	3.5
1	A	87	GLU	3.5
1	B	187	VAL	3.5
1	F	200	GLU	3.5
1	L	455	VAL	3.5
1	H	387	ALA	3.5
1	D	435	SER	3.5
1	F	220	SER	3.5
1	H	550	SER	3.5
1	F	213	MET	3.5
1	B	362	LYS	3.5
1	G	173	LYS	3.5
1	J	451	LYS	3.5
1	D	547	ILE	3.5
1	E	290	GLY	3.5
1	F	228	ILE	3.5
1	H	544	ILE	3.5
1	L	101	ILE	3.5
1	C	165	PHE	3.5
1	C	222	LEU	3.5
1	K	127	LEU	3.5
1	L	156	PHE	3.5
1	L	492	LEU	3.5
1	E	139	ASN	3.5
1	F	432	ASN	3.5
1	I	133	ASN	3.5
1	I	166	ASN	3.5
1	J	273	ASN	3.5
1	J	275	ASP	3.5
1	L	180	ASP	3.5
1	D	532	GLU	3.5
1	I	454	GLU	3.5
1	K	458	THR	3.5
1	D	230	VAL	3.5
1	F	365	VAL	3.5
1	K	524	VAL	3.5
1	G	585	ALA	3.5
1	K	387	ALA	3.5
1	K	500	ALA	3.5
1	H	184	SER	3.5
1	J	391	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	549	SER	3.5
1	A	493	TYR	3.5
1	I	292	TYR	3.5
1	F	271	ILE	3.5
1	A	109	ASP	3.5
1	B	322	ASN	3.5
1	B	352	ASN	3.5
1	C	565	PHE	3.5
1	F	175	PHE	3.5
1	G	161	ASN	3.5
1	H	175	PHE	3.5
1	I	104	ASN	3.5
1	I	214	LEU	3.5
1	K	226	PHE	3.5
1	L	175	PHE	3.5
1	L	398	PHE	3.5
1	A	335	GLU	3.5
1	G	163	GLU	3.5
1	L	155	GLU	3.5
1	F	113	GLN	3.5
1	J	523	PRO	3.5
1	J	597	THR	3.5
1	K	301	PRO	3.5
1	D	600	VAL	3.5
1	H	187	VAL	3.5
1	H	315	VAL	3.5
1	J	566	VAL	3.5
1	K	421	VAL	3.5
1	L	112	VAL	3.5
1	B	313	ALA	3.5
1	C	412	CYS	3.5
1	I	490	ALA	3.5
1	D	539	SER	3.5
1	F	172	SER	3.5
1	G	143	LYS	3.5
1	G	257	LYS	3.5
1	I	360	LYS	3.5
1	C	126	GLY	3.5
1	D	193	GLY	3.5
1	A	110	ILE	3.5
1	D	484	ILE	3.5
1	E	287	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	277	TYR	3.5
1	K	573	HIS	3.5
1	L	129	ILE	3.5
1	L	423	ILE	3.5
1	B	222	LEU	3.5
1	B	324	GLU	3.5
1	H	357	LEU	3.5
1	K	222	LEU	3.5
1	H	205	ARG	3.5
1	I	594	ARG	3.5
1	J	243	PHE	3.5
1	A	557	VAL	3.4
1	C	281	VAL	3.4
1	E	478	VAL	3.4
1	F	230	VAL	3.4
1	K	137	LYS	3.4
1	D	387	ALA	3.4
1	A	121	CYS	3.4
1	E	309	SER	3.4
1	E	311	SER	3.4
1	G	391	SER	3.4
1	F	119	GLY	3.4
1	F	581	TRP	3.4
1	G	382	GLY	3.4
1	A	176	TYR	3.4
1	A	420	ASN	3.4
1	B	95	ASP	3.4
1	B	127	LEU	3.4
1	B	157	LEU	3.4
1	B	208	LEU	3.4
1	B	479	ASP	3.4
1	C	159	ASP	3.4
1	D	495	LEU	3.4
1	D	506	ASN	3.4
1	F	394	ASP	3.4
1	F	533	TYR	3.4
1	H	149	ASN	3.4
1	H	437	ASN	3.4
1	I	150	ASP	3.4
1	I	197	ASP	3.4
1	I	231	ASP	3.4
1	K	229	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	468	ASP	3.4
1	L	122	ASN	3.4
1	J	378	PHE	3.4
1	F	232	LYS	3.4
1	I	283	LYS	3.4
1	I	433	MET	3.4
1	A	524	VAL	3.4
1	D	148	VAL	3.4
1	H	551	VAL	3.4
1	I	286	VAL	3.4
1	K	281	VAL	3.4
1	A	370	ALA	3.4
1	A	391	SER	3.4
1	C	145	SER	3.4
1	C	201	ALA	3.4
1	E	361	SER	3.4
1	G	343	SER	3.4
1	I	294	ALA	3.4
1	B	419	GLU	3.4
1	I	124	GLU	3.4
1	B	408	GLY	3.4
1	D	381	GLY	3.4
1	L	120	GLY	3.4
1	B	144	ILE	3.4
1	B	233	ASN	3.4
1	E	216	ASP	3.4
1	E	323	LEU	3.4
1	F	492	LEU	3.4
1	I	181	ASN	3.4
1	K	562	LEU	3.4
1	L	545	ASN	3.4
1	L	562	LEU	3.4
1	C	257	LYS	3.4
1	C	383	TYR	3.4
1	D	111	LYS	3.4
1	H	137	LYS	3.4
1	H	265	LYS	3.4
1	G	398	PHE	3.4
1	I	243	PHE	3.4
1	I	591	PHE	3.4
1	G	392	MET	3.4
1	A	519	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	291	THR	3.4
1	L	377	THR	3.4
1	C	579	VAL	3.4
1	F	88	VAL	3.4
1	H	593	VAL	3.4
1	I	281	VAL	3.4
1	L	185	VAL	3.4
1	B	485	ALA	3.4
1	E	194	SER	3.4
1	I	391	SER	3.4
1	J	254	SER	3.4
1	K	86	SER	3.4
1	L	473	ALA	3.4
1	E	424	HIS	3.4
1	F	250	GLU	3.4
1	G	332	GLU	3.4
1	L	102	GLU	3.4
1	L	262	GLU	3.4
1	H	121	CYS	3.4
1	A	120	GLY	3.4
1	A	113	GLN	3.4
1	A	166	ASN	3.4
1	A	563	LYS	3.4
1	B	323	LEU	3.4
1	C	231	ASP	3.4
1	G	139	ASN	3.4
1	G	204	LYS	3.4
1	I	149	ASN	3.4
1	I	352	ASN	3.4
1	J	323	LEU	3.4
1	L	537	LEU	3.4
1	E	571	TRP	3.4
1	F	176	TYR	3.4
1	G	115	TYR	3.4
1	K	304	TYR	3.4
1	L	277	TYR	3.4
1	L	287	TYR	3.4
1	L	341	TYR	3.4
1	I	276	THR	3.4
1	L	569	THR	3.4
1	B	269	VAL	3.4
1	C	146	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	167	VAL	3.4
1	D	114	VAL	3.4
1	D	190	VAL	3.4
1	F	207	VAL	3.4
1	F	286	VAL	3.4
1	C	163	GLU	3.4
1	E	334	GLU	3.4
1	E	558	ALA	3.4
1	H	300	ALA	3.4
1	J	516	SER	3.4
1	K	138	GLU	3.4
1	C	363	GLY	3.4
1	C	417	LYS	3.4
1	C	515	GLN	3.4
1	F	158	LYS	3.4
1	F	268	GLY	3.4
1	G	296	GLN	3.4
1	H	168	LYS	3.4
1	A	229	ASN	3.4
1	A	521	ASN	3.4
1	C	352	ASN	3.4
1	E	545	ASN	3.4
1	F	116	ASP	3.4
1	F	231	ASP	3.4
1	G	258	ASN	3.4
1	H	134	ASN	3.4
1	H	183	ASN	3.4
1	J	133	ASN	3.4
1	J	231	ASP	3.4
1	K	420	ASN	3.4
1	L	109	ASP	3.4
1	L	394	ASP	3.4
1	B	371	LEU	3.3
1	E	576	ILE	3.3
1	G	342	LEU	3.3
1	H	267	LEU	3.3
1	D	389	PRO	3.3
1	A	263	TYR	3.3
1	C	591	PHE	3.3
1	D	493	TYR	3.3
1	E	398	PHE	3.3
1	F	503	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	244	TYR	3.3
1	H	226	PHE	3.3
1	H	291	THR	3.3
1	I	115	TYR	3.3
1	J	103	TYR	3.3
1	J	289	PHE	3.3
1	A	452	THR	3.3
1	C	248	THR	3.3
1	K	350	TYR	3.3
1	B	125	GLU	3.3
1	B	215	HIS	3.3
1	L	124	GLU	3.3
1	A	498	SER	3.3
1	C	93	SER	3.3
1	C	314	ALA	3.3
1	C	447	ALA	3.3
1	C	557	VAL	3.3
1	E	123	VAL	3.3
1	G	557	VAL	3.3
1	H	295	SER	3.3
1	C	414	GLY	3.3
1	D	442	GLY	3.3
1	A	506	ASN	3.3
1	C	272	ASN	3.3
1	E	568	ASN	3.3
1	G	582	ASN	3.3
1	K	459	ASP	3.3
1	D	487	LEU	3.3
1	F	527	LEU	3.3
1	I	94	LEU	3.3
1	K	466	LEU	3.3
1	H	556	ILE	3.3
1	K	144	ILE	3.3
1	K	445	ILE	3.3
1	K	576	ILE	3.3
1	C	238	PHE	3.3
1	A	246	TYR	3.3
1	A	411	TYR	3.3
1	D	244	TYR	3.3
1	I	288	TYR	3.3
1	B	218	LYS	3.3
1	C	311	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	554	SER	3.3
1	H	204	LYS	3.3
1	I	353	LYS	3.3
1	H	190	VAL	3.3
1	I	520	SER	3.3
1	I	550	SER	3.3
1	J	517	SER	3.3
1	L	436	LYS	3.3
1	E	153	VAL	3.3
1	E	330	VAL	3.3
1	E	585	ALA	3.3
1	F	153	VAL	3.3
1	G	153	VAL	3.3
1	K	187	VAL	3.3
1	K	207	VAL	3.3
1	K	308	VAL	3.3
1	L	187	VAL	3.3
1	F	568	ASN	3.3
1	H	180	ASP	3.3
1	H	479	ASP	3.3
1	I	159	ASP	3.3
1	I	479	ASP	3.3
1	J	352	ASN	3.3
1	K	139	ASN	3.3
1	G	210	LEU	3.3
1	G	242	LEU	3.3
1	H	487	LEU	3.3
1	H	595	LEU	3.3
1	I	595	LEU	3.3
1	K	219	LEU	3.3
1	B	110	ILE	3.3
1	H	510	ILE	3.3
1	H	547	ILE	3.3
1	I	327	ILE	3.3
1	K	444	ILE	3.3
1	L	107	ILE	3.3
1	L	418	PRO	3.3
1	B	205	ARG	3.3
1	B	124	GLU	3.3
1	F	102	GLU	3.3
1	F	227	GLU	3.3
1	F	279	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	508	GLU	3.3
1	A	130	PHE	3.3
1	C	97	THR	3.3
1	F	266	HIS	3.3
1	F	289	PHE	3.3
1	I	226	PHE	3.3
1	G	386	LYS	3.3
1	B	480	TYR	3.3
1	B	499	TYR	3.3
1	E	115	TYR	3.3
1	E	359	TYR	3.3
1	I	411	TYR	3.3
1	L	103	TYR	3.3
1	B	154	SER	3.3
1	B	348	SER	3.3
1	G	348	SER	3.3
1	G	429	VAL	3.3
1	H	112	VAL	3.3
1	J	471	VAL	3.3
1	L	230	VAL	3.3
1	L	388	ALA	3.3
1	E	150	ASP	3.3
1	F	521	ASN	3.3
1	J	364	ASP	3.3
1	A	601	LEU	3.3
1	D	198	LEU	3.3
1	G	239	LEU	3.3
1	I	127	LEU	3.3
1	J	466	LEU	3.3
1	K	297	LEU	3.3
1	K	595	LEU	3.3
1	L	210	LEU	3.3
1	C	228	ILE	3.3
1	C	307	PRO	3.3
1	D	393	ILE	3.3
1	F	100	PRO	3.3
1	F	107	ILE	3.3
1	H	110	ILE	3.3
1	C	507	GLU	3.3
1	E	584	LYS	3.3
1	H	518	LYS	3.3
1	J	105	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	488	THR	3.3
1	L	128	THR	3.3
1	E	354	PHE	3.3
1	J	226	PHE	3.3
1	G	567	GLN	3.3
1	C	246	TYR	3.3
1	E	391	SER	3.3
1	H	571	TRP	3.3
1	A	148	VAL	3.3
1	E	294	ALA	3.2
1	G	421	VAL	3.3
1	G	524	VAL	3.3
1	H	372	VAL	3.3
1	I	112	VAL	3.3
1	I	142	VAL	3.3
1	K	186	ALA	3.2
1	K	566	VAL	3.3
1	D	456	GLY	3.2
1	E	477	GLY	3.2
1	A	322	ASN	3.2
1	C	468	ASP	3.2
1	J	511	ASN	3.2
1	J	568	ASN	3.2
1	L	437	ASN	3.2
1	J	205	ARG	3.2
1	B	210	LEU	3.2
1	C	94	LEU	3.2
1	C	169	LEU	3.2
1	F	169	LEU	3.2
1	I	323	LEU	3.2
1	B	552	LYS	3.2
1	C	135	PRO	3.2
1	I	279	GLU	3.2
1	E	101	ILE	3.2
1	F	174	HIS	3.2
1	J	366	LYS	3.2
1	J	481	ILE	3.2
1	F	248	THR	3.2
1	I	458	THR	3.2
1	L	536	THR	3.2
1	A	292	TYR	3.2
1	B	439	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	287	TYR	3.2
1	G	541	TYR	3.2
1	I	176	TYR	3.2
1	I	261	MET	3.2
1	K	270	TYR	3.2
1	K	349	MET	3.2
1	A	274	ALA	3.2
1	B	365	VAL	3.2
1	B	566	VAL	3.2
1	D	299	ALA	3.2
1	D	502	VAL	3.2
1	E	91	VAL	3.2
1	F	224	VAL	3.2
1	G	294	ALA	3.2
1	G	455	VAL	3.2
1	J	482	VAL	3.2
1	K	413	VAL	3.2
1	K	434	VAL	3.2
1	J	120	GLY	3.2
1	J	390	GLY	3.2
1	C	197	ASP	3.2
1	C	322	ASN	3.2
1	D	322	ASN	3.2
1	D	394	ASP	3.2
1	F	134	ASN	3.2
1	B	366	LYS	3.2
1	B	451	LYS	3.2
1	B	507	GLU	3.2
1	B	532	GLU	3.2
1	F	173	LYS	3.2
1	J	147	LYS	3.2
1	B	214	LEU	3.2
1	H	127	LEU	3.2
1	I	357	LEU	3.2
1	J	214	LEU	3.2
1	J	89	PRO	3.2
1	A	99	ILE	3.2
1	B	510	ILE	3.2
1	B	574	ILE	3.2
1	G	99	ILE	3.2
1	K	453	ILE	3.2
1	K	481	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	113	GLN	3.2
1	B	276	THR	3.2
1	B	415	THR	3.2
1	H	569	THR	3.2
1	L	248	THR	3.2
1	D	243	PHE	3.2
1	B	247	MET	3.2
1	F	209	SER	3.2
1	G	146	SER	3.2
1	A	187	VAL	3.2
1	B	551	VAL	3.2
1	C	225	VAL	3.2
1	C	533	TYR	3.2
1	F	411	TYR	3.2
1	G	499	TYR	3.2
1	G	577	ALA	3.2
1	H	91	VAL	3.2
1	H	308	VAL	3.2
1	I	350	TYR	3.2
1	L	411	TYR	3.2
1	A	139	ASN	3.2
1	A	245	GLU	3.2
1	A	257	LYS	3.2
1	A	384	ASN	3.2
1	C	443	ASP	3.2
1	D	204	LYS	3.2
1	G	260	ASN	3.2
1	H	124	GLU	3.2
1	H	147	LYS	3.2
1	J	95	ASP	3.2
1	J	164	LYS	3.2
1	L	111	LYS	3.2
1	F	407	LEU	3.2
1	H	601	LEU	3.2
1	E	89	PRO	3.2
1	F	106	PRO	3.2
1	I	141	PRO	3.2
1	B	484	ILE	3.2
1	E	529	ILE	3.2
1	H	453	ILE	3.2
1	B	412	CYS	3.2
1	F	536	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	569	THR	3.2
1	L	465	THR	3.2
1	B	243	PHE	3.2
1	H	368	LYS	3.2
1	J	331	LYS	3.2
1	J	552	LYS	3.2
1	A	474	GLU	3.2
1	C	428	ALA	3.2
1	D	318	ALA	3.2
1	F	262	GLU	3.2
1	G	124	GLU	3.2
1	D	439	TYR	3.2
1	E	95	ASP	3.2
1	E	270	TYR	3.2
1	F	115	TYR	3.2
1	F	126	GLY	3.2
1	G	316	GLU	3.2
1	H	363	GLY	3.2
1	H	566	VAL	3.2
1	I	467	ALA	3.2
1	J	125	GLU	3.2
1	L	316	GLU	3.2
1	B	602	ASN	3.2
1	F	359	TYR	3.2
1	H	95	ASP	3.2
1	I	116	ASP	3.2
1	I	439	TYR	3.2
1	K	103	TYR	3.2
1	K	211	VAL	3.2
1	L	224	VAL	3.2
1	C	297	LEU	3.2
1	E	601	LEU	3.2
1	H	297	LEU	3.2
1	H	596	LEU	3.2
1	L	131	LEU	3.2
1	B	228	ILE	3.2
1	D	544	ILE	3.2
1	E	99	ILE	3.2
1	E	110	ILE	3.2
1	H	107	ILE	3.2
1	L	327	ILE	3.2
1	F	415	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	105	THR	3.2
1	A	400	MET	3.2
1	D	518	LYS	3.1
1	E	137	LYS	3.1
1	B	130	PHE	3.1
1	C	549	SER	3.1
1	D	178	PHE	3.1
1	G	503	PHE	3.1
1	H	172	SER	3.1
1	J	498	SER	3.1
1	E	124	GLU	3.1
1	G	87	GLU	3.1
1	H	102	GLU	3.1
1	H	160	GLU	3.1
1	I	508	GLU	3.1
1	A	186	ALA	3.1
1	B	329	GLY	3.1
1	A	230	VAL	3.1
1	B	557	VAL	3.1
1	C	233	ASN	3.1
1	C	370	ALA	3.1
1	E	373	GLY	3.1
1	I	390	GLY	3.1
1	I	577	ALA	3.1
1	K	496	GLY	3.1
1	D	231	ASP	3.1
1	D	273	ASN	3.1
1	D	406	VAL	3.1
1	E	600	VAL	3.1
1	G	434	VAL	3.1
1	H	207	VAL	3.1
1	H	230	VAL	3.1
1	I	185	VAL	3.1
1	I	429	VAL	3.1
1	J	181	ASN	3.1
1	J	269	VAL	3.1
1	J	579	VAL	3.1
1	B	115	TYR	3.1
1	C	411	TYR	3.1
1	E	383	TYR	3.1
1	H	115	TYR	3.1
1	B	470	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	323	LEU	3.1
1	C	416	LEU	3.1
1	F	523	PRO	3.1
1	K	106	PRO	3.1
1	K	601	LEU	3.1
1	J	571	TRP	3.1
1	A	327	ILE	3.1
1	G	101	ILE	3.1
1	L	529	ILE	3.1
1	B	151	LYS	3.1
1	I	212	THR	3.1
1	E	419	GLU	3.1
1	G	226	PHE	3.1
1	G	235	PHE	3.1
1	I	146	SER	3.1
1	J	86	SER	3.1
1	H	356	HIS	3.1
1	B	314	ALA	3.1
1	B	340	ALA	3.1
1	C	161	ASN	3.1
1	D	181	ASN	3.1
1	E	159	ASP	3.1
1	E	467	ALA	3.1
1	I	179	ASN	3.1
1	I	256	ASP	3.1
1	I	447	ALA	3.1
1	D	551	VAL	3.1
1	H	557	VAL	3.1
1	L	225	VAL	3.1
1	A	198	LEU	3.1
1	A	277	TYR	3.1
1	A	389	PRO	3.1
1	C	476	LEU	3.1
1	D	464	LEU	3.1
1	E	210	LEU	3.1
1	E	493	TYR	3.1
1	F	242	LEU	3.1
1	F	493	TYR	3.1
1	F	601	LEU	3.1
1	H	533	TYR	3.1
1	I	407	LEU	3.1
1	J	297	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	328	LEU	3.1
1	E	440	ARG	3.1
1	A	107	ILE	3.1
1	A	162	MET	3.1
1	B	129	ILE	3.1
1	C	110	ILE	3.1
1	C	271	ILE	3.1
1	E	298	ILE	3.1
1	G	264	ILE	3.1
1	H	228	ILE	3.1
1	H	264	ILE	3.1
1	H	584	LYS	3.1
1	J	396	MET	3.1
1	K	417	LYS	3.1
1	K	248	THR	3.1
1	G	138	GLU	3.1
1	G	200	GLU	3.1
1	I	125	GLU	3.1
1	J	280	GLU	3.1
1	K	324	GLU	3.1
1	L	335	GLU	3.1
1	A	194	SER	3.1
1	D	427	SER	3.1
1	H	427	SER	3.1
1	I	215	HIS	3.1
1	A	583	PHE	3.1
1	G	130	PHE	3.1
1	G	583	PHE	3.1
1	A	140	GLY	3.1
1	A	191	GLY	3.1
1	A	272	ASN	3.1
1	A	399	ASP	3.1
1	A	450	GLY	3.1
1	F	229	ASN	3.1
1	H	504	GLY	3.1
1	J	449	ASN	3.1
1	K	134	ASN	3.1
1	K	159	ASP	3.1
1	K	217	ASN	3.1
1	L	149	ASN	3.1
1	G	300	ALA	3.1
1	J	485	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	201	ALA	3.1
1	B	308	VAL	3.1
1	G	123	VAL	3.1
1	J	132	VAL	3.1
1	K	123	VAL	3.1
1	A	342	LEU	3.1
1	A	476	LEU	3.1
1	A	537	LEU	3.1
1	D	342	LEU	3.1
1	E	342	LEU	3.1
1	D	168	LYS	3.1
1	E	293	TYR	3.1
1	F	285	ARG	3.1
1	I	395	LEU	3.1
1	J	239	LEU	3.1
1	K	407	LEU	3.1
1	L	407	LEU	3.1
1	B	436	LYS	3.1
1	F	325	TYR	3.1
1	F	350	TYR	3.1
1	F	439	TYR	3.1
1	G	350	TYR	3.1
1	H	118	LYS	3.1
1	I	263	TYR	3.1
1	I	480	TYR	3.1
1	D	392	MET	3.1
1	B	107	ILE	3.1
1	B	376	ILE	3.1
1	F	369	ILE	3.1
1	C	124	GLU	3.1
1	C	160	GLU	3.1
1	D	227	GLU	3.1
1	F	163	GLU	3.1
1	I	160	GLU	3.1
1	C	415	THR	3.1
1	L	223	THR	3.1
1	B	555	SER	3.1
1	C	438	SER	3.1
1	G	93	SER	3.1
1	G	194	SER	3.1
1	H	146	SER	3.1
1	K	401	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	180	ASP	3.1
1	A	456	GLY	3.1
1	H	140	GLY	3.1
1	H	296	GLN	3.1
1	I	191	GLY	3.1
1	K	165	PHE	3.1
1	L	237	PHE	3.1
1	C	258	ASN	3.1
1	F	545	ASN	3.1
1	G	134	ASN	3.1
1	J	216	ASP	3.1
1	K	384	ASN	3.1
1	A	318	ALA	3.1
1	E	314	ALA	3.1
1	F	447	ALA	3.1
1	I	318	ALA	3.1
1	K	314	ALA	3.1
1	K	469	ALA	3.1
1	B	173	LYS	3.1
1	C	367	LYS	3.1
1	C	566	VAL	3.1
1	D	232	LYS	3.1
1	D	330	VAL	3.1
1	E	315	VAL	3.1
1	E	344	VAL	3.1
1	I	372	VAL	3.1
1	K	206	VAL	3.1
1	K	482	VAL	3.1
1	F	198	LEU	3.1
1	L	292	TYR	3.0
1	A	522	GLU	3.0
1	F	282	GLU	3.0
1	C	445	ILE	3.0
1	D	369	ILE	3.0
1	L	355	ILE	3.0
1	A	241	THR	3.0
1	B	209	SER	3.0
1	F	199	SER	3.0
1	J	295	SER	3.0
1	K	361	SER	3.0
1	L	559	SER	3.0
1	B	113	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	531	ASN	3.0
1	D	538	ASN	3.0
1	E	289	PHE	3.0
1	G	95	ASP	3.0
1	H	120	GLY	3.0
1	I	122	ASN	3.0
1	I	165	PHE	3.0
1	I	289	PHE	3.0
1	I	398	PHE	3.0
1	J	290	GLY	3.0
1	K	273	ASN	3.0
1	L	188	GLY	3.0
1	A	168	LYS	3.0
1	B	360	LYS	3.0
1	I	331	LYS	3.0
1	E	274	ALA	3.0
1	F	387	ALA	3.0
1	H	585	ALA	3.0
1	I	186	ALA	3.0
1	E	528	PRO	3.0
1	F	441	PRO	3.0
1	K	89	PRO	3.0
1	A	478	VAL	3.0
1	B	433	MET	3.0
1	E	222	LEU	3.0
1	F	421	VAL	3.0
1	G	142	VAL	3.0
1	G	371	LEU	3.0
1	G	385	LEU	3.0
1	H	333	LEU	3.0
1	H	338	MET	3.0
1	J	157	LEU	3.0
1	J	206	VAL	3.0
1	J	595	LEU	3.0
1	K	210	LEU	3.0
1	K	416	LEU	3.0
1	L	234	LEU	3.0
1	L	495	LEU	3.0
1	A	102	GLU	3.0
1	D	262	GLU	3.0
1	E	279	GLU	3.0
1	K	160	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	316	GLU	3.0
1	A	103	TYR	3.0
1	A	189	TYR	3.0
1	E	292	TYR	3.0
1	F	292	TYR	3.0
1	G	263	TYR	3.0
1	A	576	ILE	3.0
1	G	298	ILE	3.0
1	G	369	ILE	3.0
1	H	444	ILE	3.0
1	B	108	HIS	3.0
1	B	358	THR	3.0
1	E	452	THR	3.0
1	I	488	THR	3.0
1	K	348	SER	3.0
1	L	552	LYS	3.0
1	A	275	ASP	3.0
1	A	457	ASN	3.0
1	B	578	GLY	3.0
1	C	122	ASN	3.0
1	C	149	ASN	3.0
1	D	197	ASP	3.0
1	G	364	ASP	3.0
1	H	590	GLY	3.0
1	I	568	ASN	3.0
1	J	150	ASP	3.0
1	J	339	GLY	3.0
1	J	450	GLY	3.0
1	K	390	GLY	3.0
1	L	116	ASP	3.0
1	L	339	GLY	3.0
1	A	178	PHE	3.0
1	F	165	PHE	3.0
1	F	398	PHE	3.0
1	I	237	PHE	3.0
1	B	203	MET	3.0
1	J	542	ALA	3.0
1	L	340	ALA	3.0
1	A	88	VAL	3.0
1	A	466	LEU	3.0
1	B	280	GLU	3.0
1	B	601	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	208	LEU	3.0
1	I	413	VAL	3.0
1	J	112	VAL	3.0
1	J	167	VAL	3.0
1	J	478	VAL	3.0
1	J	507	GLU	3.0
1	K	560	LEU	3.0
1	L	317	LEU	3.0
1	L	336	LEU	3.0
1	E	472	TYR	3.0
1	F	530	ILE	3.0
1	K	325	TYR	3.0
1	L	472	TYR	3.0
1	L	547	ILE	3.0
1	J	377	THR	3.0
1	E	221	LYS	3.0
1	H	182	LYS	3.0
1	H	374	LYS	3.0
1	L	353	LYS	3.0
1	E	172	SER	3.0
1	F	145	SER	3.0
1	G	517	SER	3.0
1	B	384	ASN	3.0
1	F	363	GLY	3.0
1	F	525	TRP	3.0
1	G	109	ASP	3.0
1	H	394	ASP	3.0
1	I	521	ASN	3.0
1	J	322	ASN	3.0
1	F	338	MET	3.0
1	H	141	PRO	3.0
1	B	192	CYS	3.0
1	A	281	VAL	3.0
1	B	464	LEU	3.0
1	D	385	LEU	3.0
1	E	328	LEU	3.0
1	I	471	VAL	3.0
1	J	153	VAL	3.0
1	L	328	LEU	3.0
1	I	266	HIS	3.0
1	J	573	HIS	3.0
1	C	547	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	143	LYS	3.0
1	I	257	LYS	3.0
1	J	360	LYS	3.0
1	L	451	LYS	3.0
1	A	248	THR	3.0
1	A	270	TYR	3.0
1	A	341	TYR	3.0
1	D	536	THR	3.0
1	H	212	THR	3.0
1	I	541	TYR	3.0
1	J	350	TYR	3.0
1	L	189	TYR	3.0
1	A	348	SER	3.0
1	A	494	SER	3.0
1	B	498	SER	3.0
1	D	86	SER	3.0
1	F	448	SER	3.0
1	F	555	SER	3.0
1	G	498	SER	3.0
1	H	311	SER	3.0
1	K	295	SER	3.0
1	L	254	SER	3.0
1	A	364	ASP	3.0
1	C	95	ASP	3.0
1	D	275	ASP	3.0
1	G	122	ASN	3.0
1	I	217	ASN	3.0
1	J	119	GLY	3.0
1	H	177	MET	3.0
1	F	335	GLU	3.0
1	K	335	GLU	3.0
1	L	581	TRP	3.0
1	H	301	PRO	3.0
1	I	425	PHE	2.9
1	J	591	PHE	2.9
1	D	447	ALA	2.9
1	I	201	ALA	2.9
1	I	284	ALA	2.9
1	I	553	ALA	2.9
1	A	595	LEU	2.9
1	E	310	LEU	2.9
1	G	127	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	208	LEU	2.9
1	L	333	LEU	2.9
1	C	315	VAL	2.9
1	D	112	VAL	2.9
1	D	308	VAL	2.9
1	E	187	VAL	2.9
1	E	269	VAL	2.9
1	G	566	VAL	2.9
1	H	330	VAL	2.9
1	I	573	HIS	2.9
1	K	148	VAL	2.9
1	G	584	LYS	2.9
1	A	453	ILE	2.9
1	F	547	ILE	2.9
1	I	264	ILE	2.9
1	A	536	THR	2.9
1	C	358	THR	2.9
1	E	97	THR	2.9
1	F	488	THR	2.9
1	G	270	TYR	2.9
1	J	244	TYR	2.9
1	K	293	TYR	2.9
1	L	533	TYR	2.9
1	L	555	SER	2.9
1	B	109	ASP	2.9
1	E	394	ASP	2.9
1	G	322	ASN	2.9
1	H	125	GLU	2.9
1	J	431	GLU	2.9
1	J	538	ASN	2.9
1	L	392	MET	2.9
1	F	238	PHE	2.9
1	H	378	PHE	2.9
1	A	299	ALA	2.9
1	A	572	ALA	2.9
1	B	284	ALA	2.9
1	B	476	LEU	2.9
1	C	387	ALA	2.9
1	F	577	ALA	2.9
1	G	323	LEU	2.9
1	G	387	ALA	2.9
1	H	388	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	336	LEU	2.9
1	K	404	ALA	2.9
1	L	186	ALA	2.9
1	L	214	LEU	2.9
1	L	460	ALA	2.9
1	L	485	ALA	2.9
1	A	118	LYS	2.9
1	B	148	VAL	2.9
1	B	524	VAL	2.9
1	B	584	LYS	2.9
1	C	153	VAL	2.9
1	D	92	VAL	2.9
1	F	269	VAL	2.9
1	F	436	LYS	2.9
1	I	579	VAL	2.9
1	J	344	VAL	2.9
1	J	421	VAL	2.9
1	L	368	LYS	2.9
1	L	502	VAL	2.9
1	E	409	CYS	2.9
1	I	99	ILE	2.9
1	I	271	ILE	2.9
1	J	271	ILE	2.9
1	K	355	ILE	2.9
1	G	415	THR	2.9
1	A	568	ASN	2.9
1	B	580	SER	2.9
1	C	270	TYR	2.9
1	C	277	TYR	2.9
1	C	520	SER	2.9
1	D	359	TYR	2.9
1	D	161	ASN	2.9
1	E	580	SER	2.9
1	I	383	TYR	2.9
1	I	493	TYR	2.9
1	J	480	TYR	2.9
1	K	246	TYR	2.9
1	B	373	GLY	2.9
1	F	322	ASN	2.9
1	G	229	ASN	2.9
1	H	531	ASN	2.9
1	I	119	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	109	ASP	2.9
1	K	119	GLY	2.9
1	L	140	GLY	2.9
1	C	96	PRO	2.9
1	L	389	PRO	2.9
1	B	168	LYS	2.9
1	C	204	LYS	2.9
1	I	366	LYS	2.9
1	A	313	ALA	2.9
1	A	467	ALA	2.9
1	B	285	ARG	2.9
1	F	214	LEU	2.9
1	F	466	LEU	2.9
1	H	428	ALA	2.9
1	I	234	LEU	2.9
1	J	285	ARG	2.9
1	C	567	GLN	2.9
1	H	113	GLN	2.9
1	K	546	GLN	2.9
1	D	195	VAL	2.9
1	D	224	VAL	2.9
1	D	365	VAL	2.9
1	G	315	VAL	2.9
1	H	281	VAL	2.9
1	I	421	VAL	2.9
1	J	88	VAL	2.9
1	J	365	VAL	2.9
1	B	101	ILE	2.9
1	B	117	ILE	2.9
1	B	423	ILE	2.9
1	E	547	ILE	2.9
1	F	298	ILE	2.9
1	H	369	ILE	2.9
1	K	101	ILE	2.9
1	L	510	ILE	2.9
1	K	396	MET	2.9
1	K	422	GLU	2.9
1	K	497	THR	2.9
1	A	159	ASP	2.9
1	A	361	SER	2.9
1	A	543	ASP	2.9
1	C	348	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	180	ASP	2.9
1	G	181	ASN	2.9
1	G	580	SER	2.9
1	H	194	SER	2.9
1	H	231	ASP	2.9
1	I	199	SER	2.9
1	L	199	SER	2.9
1	K	462	GLY	2.9
1	K	538	ASN	2.9
1	B	325	TYR	2.9
1	C	244	TYR	2.9
1	C	439	TYR	2.9
1	D	341	TYR	2.9
1	D	100	PRO	2.9
1	J	518	LYS	2.9
1	B	495	LEU	2.9
1	C	243	PHE	2.9
1	E	318	ALA	2.9
1	F	152	GLN	2.9
1	H	208	LEU	2.9
1	H	404	ALA	2.9
1	I	354	PHE	2.9
1	J	398	PHE	2.9
1	K	492	LEU	2.9
1	K	577	ALA	2.9
1	L	300	ALA	2.9
1	L	387	ALA	2.9
1	L	553	ALA	2.9
1	A	581	TRP	2.9
1	B	132	VAL	2.9
1	E	557	VAL	2.9
1	F	112	VAL	2.9
1	G	600	VAL	2.9
1	J	195	VAL	2.9
1	K	344	VAL	2.9
1	L	92	VAL	2.9
1	I	335	GLU	2.9
1	L	507	GLU	2.9
1	A	212	THR	2.9
1	C	400	MET	2.9
1	D	99	ILE	2.9
1	E	358	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	444	ILE	2.9
1	F	446	THR	2.9
1	G	530	ILE	2.9
1	I	355	ILE	2.9
1	J	392	MET	2.9
1	A	184	SER	2.8
1	B	199	SER	2.8
1	C	183	ASN	2.9
1	D	302	SER	2.8
1	E	180	ASP	2.9
1	E	209	SER	2.8
1	F	109	ASP	2.9
1	F	348	SER	2.8
1	H	179	ASN	2.9
1	H	379	ASP	2.9
1	I	249	ASP	2.9
1	K	202	ASP	2.9
1	K	568	ASN	2.9
1	G	347	GLY	2.8
1	H	151	LYS	2.8
1	L	158	LYS	2.8
1	L	204	LYS	2.8
1	B	189	TYR	2.8
1	E	277	TYR	2.8
1	F	103	TYR	2.8
1	F	189	TYR	2.8
1	F	341	TYR	2.8
1	H	287	TYR	2.8
1	H	293	TYR	2.8
1	I	246	TYR	2.8
1	I	304	TYR	2.8
1	J	215	HIS	2.8
1	J	341	TYR	2.8
1	K	541	TYR	2.8
1	H	567	GLN	2.8
1	A	242	LEU	2.8
1	B	169	LEU	2.8
1	D	267	LEU	2.8
1	D	537	LEU	2.8
1	G	234	LEU	2.8
1	A	410	ALA	2.8
1	B	410	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	467	ALA	2.8
1	C	425	PHE	2.8
1	D	398	PHE	2.8
1	F	467	ALA	2.8
1	H	467	ALA	2.8
1	J	447	ALA	2.8
1	K	583	PHE	2.8
1	A	551	VAL	2.8
1	A	593	VAL	2.8
1	B	190	VAL	2.8
1	B	281	VAL	2.8
1	D	225	VAL	2.8
1	D	421	VAL	2.8
1	D	557	VAL	2.8
1	G	211	VAL	2.8
1	G	225	VAL	2.8
1	H	153	VAL	2.8
1	A	571	TRP	2.8
1	B	155	GLU	2.8
1	H	422	GLU	2.8
1	B	298	ILE	2.8
1	B	369	ILE	2.8
1	C	171	THR	2.8
1	D	412	CYS	2.8
1	E	241	THR	2.8
1	I	544	ILE	2.8
1	J	403	CYS	2.8
1	E	366	LYS	2.8
1	G	168	LYS	2.8
1	A	216	ASP	2.8
1	C	437	ASN	2.8
1	F	582	ASN	2.8
1	K	543	ASP	2.8
1	L	233	ASN	2.8
1	L	420	ASN	2.8
1	B	442	GLY	2.8
1	C	120	GLY	2.8
1	E	520	SER	2.8
1	F	548	SER	2.8
1	G	309	SER	2.8
1	H	309	SER	2.8
1	H	456	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	580	SER	2.8
1	L	220	SER	2.8
1	L	343	SER	2.8
1	L	462	GLY	2.8
1	F	356	HIS	2.8
1	H	307	PRO	2.8
1	A	350	TYR	2.8
1	C	480	TYR	2.8
1	F	499	TYR	2.8
1	G	292	TYR	2.8
1	I	244	TYR	2.8
1	I	270	TYR	2.8
1	J	304	TYR	2.8
1	L	263	TYR	2.8
1	B	94	LEU	2.8
1	C	317	LEU	2.8
1	D	426	LEU	2.8
1	D	596	LEU	2.8
1	I	317	LEU	2.8
1	J	333	LEU	2.8
1	L	601	LEU	2.8
1	A	387	ALA	2.8
1	B	387	ALA	2.8
1	C	583	PHE	2.8
1	D	226	PHE	2.8
1	E	178	PHE	2.8
1	F	201	ALA	2.8
1	H	354	PHE	2.8
1	E	431	GLU	2.8
1	A	203	MET	2.8
1	B	88	VAL	2.8
1	B	91	VAL	2.8
1	B	471	VAL	2.8
1	B	478	VAL	2.8
1	E	593	VAL	2.8
1	G	281	VAL	2.8
1	K	406	VAL	2.8
1	L	162	MET	2.8
1	L	213	MET	2.8
1	L	269	VAL	2.8
1	L	434	VAL	2.8
1	B	182	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	552	LYS	2.8
1	D	581	TRP	2.8
1	E	337	LYS	2.8
1	J	362	LYS	2.8
1	L	168	LYS	2.8
1	G	291	THR	2.8
1	I	393	ILE	2.8
1	J	248	THR	2.8
1	J	376	ILE	2.8
1	J	556	ILE	2.8
1	K	547	ILE	2.8
1	L	241	THR	2.8
1	A	545	ASN	2.8
1	D	303	ASN	2.8
1	E	590	GLY	2.8
1	F	108	HIS	2.8
1	H	459	ASP	2.8
1	I	139	ASN	2.8
1	I	582	ASN	2.8
1	J	379	ASP	2.8
1	A	325	TYR	2.8
1	H	244	TYR	2.8
1	J	263	TYR	2.8
1	A	310	LEU	2.8
1	B	336	LEU	2.8
1	C	595	LEU	2.8
1	D	492	LEU	2.8
1	H	495	LEU	2.8
1	J	210	LEU	2.8
1	J	407	LEU	2.8
1	C	316	GLU	2.8
1	D	334	GLU	2.8
1	E	200	GLU	2.8
1	H	532	GLU	2.8
1	L	279	GLU	2.8
1	A	405	ALA	2.8
1	F	405	ALA	2.8
1	I	274	ALA	2.8
1	L	313	ALA	2.8
1	A	165	PHE	2.8
1	C	378	PHE	2.8
1	F	130	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	591	PHE	2.8
1	J	354	PHE	2.8
1	D	331	LYS	2.8
1	E	367	LYS	2.8
1	I	417	LYS	2.8
1	K	587	LYS	2.8
1	A	185	VAL	2.8
1	B	114	VAL	2.8
1	E	112	VAL	2.8
1	G	88	VAL	2.8
1	G	230	VAL	2.8
1	G	286	VAL	2.8
1	H	413	VAL	2.8
1	I	88	VAL	2.8
1	I	236	ARG	2.8
1	L	440	ARG	2.8
1	A	129	ILE	2.8
1	A	556	ILE	2.8
1	B	355	ILE	2.8
1	C	355	ILE	2.8
1	D	228	ILE	2.8
1	D	358	THR	2.8
1	G	488	THR	2.8
1	I	228	ILE	2.8
1	I	423	ILE	2.8
1	J	291	THR	2.8
1	K	271	ILE	2.8
1	K	415	THR	2.8
1	D	139	ASN	2.8
1	E	526	TRP	2.8
1	L	484	ILE	2.8
1	J	116	ASP	2.8
1	K	545	ASN	2.8
1	B	152	GLN	2.8
1	B	345	GLY	2.8
1	D	145	SER	2.8
1	E	498	SER	2.8
1	F	136	GLY	2.8
1	H	435	SER	2.8
1	I	343	SER	2.8
1	I	515	GLN	2.8
1	I	578	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	102	GLU	2.8
1	F	124	GLU	2.8
1	J	160	GLU	2.8
1	A	222	LEU	2.8
1	A	287	TYR	2.8
1	A	304	TYR	2.8
1	A	470	LEU	2.8
1	B	562	LEU	2.8
1	D	222	LEU	2.8
1	G	287	TYR	2.8
1	G	395	LEU	2.8
1	H	385	LEU	2.8
1	I	277	TYR	2.8
1	J	470	LEU	2.8
1	L	244	TYR	2.8
1	L	476	LEU	2.8
1	F	204	LYS	2.8
1	H	218	LYS	2.8
1	I	162	MET	2.8
1	I	540	LYS	2.8
1	J	158	LYS	2.8
1	J	314	ALA	2.8
1	E	175	PHE	2.8
1	H	235	PHE	2.8
1	H	398	PHE	2.8
1	I	378	PHE	2.8
1	K	205	ARG	2.8
1	A	211	VAL	2.8
1	C	429	VAL	2.8
1	D	91	VAL	2.8
1	D	207	VAL	2.8
1	D	372	VAL	2.8
1	I	502	VAL	2.8
1	B	174	HIS	2.7
1	B	544	ILE	2.7
1	C	446	THR	2.7
1	D	117	ILE	2.7
1	D	446	THR	2.7
1	C	229	ASN	2.7
1	E	161	ASN	2.7
1	F	538	ASN	2.7
1	G	256	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	443	ASP	2.7
1	J	249	ASP	2.7
1	J	298	ILE	2.7
1	B	145	SER	2.7
1	B	311	SER	2.7
1	C	309	SER	2.7
1	E	581	TRP	2.7
1	K	409	CYS	2.7
1	A	138	GLU	2.7
1	B	250	GLU	2.7
1	J	102	GLU	2.7
1	J	422	GLU	2.7
1	B	337	LYS	2.7
1	B	417	LYS	2.7
1	G	368	LYS	2.7
1	K	118	LYS	2.7
1	F	222	LEU	2.7
1	A	314	ALA	2.7
1	B	440	ARG	2.7
1	C	205	ARG	2.7
1	C	325	TYR	2.7
1	D	270	TYR	2.7
1	E	325	TYR	2.7
1	G	246	TYR	2.7
1	G	493	TYR	2.7
1	I	410	ALA	2.7
1	I	440	ARG	2.7
1	K	176	TYR	2.7
1	L	201	ALA	2.7
1	C	289	PHE	2.7
1	A	206	VAL	2.7
1	C	330	VAL	2.7
1	F	434	VAL	2.7
1	I	434	VAL	2.7
1	C	90	GLN	2.7
1	A	369	ILE	2.7
1	A	379	ASP	2.7
1	B	128	THR	2.7
1	H	171	THR	2.7
1	J	152	GLN	2.7
1	A	445	ILE	2.7
1	D	216	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	602	ASN	2.7
1	E	275	ASP	2.7
1	G	149	ASN	2.7
1	J	458	THR	2.7
1	I	510	ILE	2.7
1	J	144	ILE	2.7
1	J	272	ASN	2.7
1	B	191	GLY	2.7
1	B	462	GLY	2.7
1	B	477	GLY	2.7
1	G	126	GLY	2.7
1	L	450	GLY	2.7
1	C	498	SER	2.7
1	E	295	SER	2.7
1	J	93	SER	2.7
1	L	154	SER	2.7
1	J	588	PRO	2.7
1	K	389	PRO	2.7
1	D	121	CYS	2.7
1	D	431	GLU	2.7
1	F	332	GLU	2.7
1	I	419	GLU	2.7
1	C	182	LYS	2.7
1	C	203	MET	2.7
1	C	537	LEU	2.7
1	D	336	LEU	2.7
1	E	537	LEU	2.7
1	J	336	LEU	2.7
1	J	342	LEU	2.7
1	K	157	LEU	2.7
1	L	416	LEU	2.7
1	A	473	ALA	2.7
1	D	350	TYR	2.7
1	E	499	TYR	2.7
1	F	472	TYR	2.7
1	H	490	ALA	2.7
1	I	473	ALA	2.7
1	K	533	TYR	2.7
1	K	572	ALA	2.7
1	K	585	ALA	2.7
1	C	573	HIS	2.7
1	G	573	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	591	PHE	2.7
1	D	156	PHE	2.7
1	I	238	PHE	2.7
1	A	546	GLN	2.7
1	D	429	VAL	2.7
1	E	195	VAL	2.7
1	K	600	VAL	2.7
1	L	206	VAL	2.7
1	L	365	VAL	2.7
1	A	303	ASN	2.7
1	B	249	ASP	2.7
1	B	291	THR	2.7
1	B	519	THR	2.7
1	D	180	ASP	2.7
1	D	249	ASP	2.7
1	E	133	ASN	2.7
1	E	483	ASP	2.7
1	F	452	THR	2.7
1	F	531	ASN	2.7
1	I	233	ASN	2.7
1	I	575	ASP	2.7
1	J	122	ASN	2.7
1	K	322	ASN	2.7
1	A	414	GLY	2.7
1	A	574	ILE	2.7
1	C	513	ILE	2.7
1	E	423	ILE	2.7
1	H	339	GLY	2.7
1	J	513	ILE	2.7
1	L	376	ILE	2.7
1	A	326	LYS	2.7
1	A	516	SER	2.7
1	B	158	LYS	2.7
1	B	283	LYS	2.7
1	B	295	SER	2.7
1	E	427	SER	2.7
1	E	518	LYS	2.7
1	E	550	SER	2.7
1	F	218	LYS	2.7
1	I	351	PRO	2.7
1	J	232	LYS	2.7
1	J	548	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	168	LYS	2.7
1	L	125	GLU	2.7
1	L	209	SER	2.7
1	L	295	SER	2.7
1	L	391	SER	2.7
1	A	430	CYS	2.7
1	E	321	LEU	2.7
1	G	321	LEU	2.7
1	G	601	LEU	2.7
1	H	222	LEU	2.7
1	H	323	LEU	2.7
1	H	395	LEU	2.7
1	I	157	LEU	2.7
1	I	385	LEU	2.7
1	J	267	LEU	2.7
1	J	476	LEU	2.7
1	B	196	ALA	2.7
1	B	300	ALA	2.7
1	C	388	ALA	2.7
1	C	572	ALA	2.7
1	G	318	ALA	2.7
1	H	266	HIS	2.7
1	I	460	ALA	2.7
1	L	535	ALA	2.7
1	A	115	TYR	2.7
1	A	383	TYR	2.7
1	C	115	TYR	2.7
1	D	277	TYR	2.7
1	H	515	GLN	2.7
1	L	152	GLN	2.7
1	D	175	PHE	2.7
1	D	354	PHE	2.7
1	D	378	PHE	2.7
1	H	561	PHE	2.7
1	I	599	PHE	2.7
1	K	378	PHE	2.7
1	K	599	PHE	2.7
1	C	502	VAL	2.7
1	A	155	GLU	2.7
1	A	227	GLU	2.7
1	B	105	THR	2.7
1	B	137	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	488	THR	2.7
1	C	511	ASN	2.7
1	E	167	VAL	2.7
1	F	95	ASP	2.7
1	F	206	VAL	2.7
1	F	281	VAL	2.7
1	D	377	THR	2.7
1	F	511	ASN	2.7
1	G	202	ASP	2.7
1	G	365	VAL	2.7
1	H	166	ASN	2.7
1	H	221	LYS	2.7
1	H	306	ASN	2.7
1	H	524	VAL	2.7
1	I	206	VAL	2.7
1	I	269	VAL	2.7
1	E	155	GLU	2.7
1	F	518	LYS	2.7
1	K	432	ASN	2.7
1	L	137	LYS	2.7
1	L	531	ASN	2.7
1	I	564	GLU	2.7
1	C	170	GLY	2.7
1	D	107	ILE	2.7
1	D	327	ILE	2.7
1	E	369	ILE	2.7
1	E	453	ILE	2.7
1	G	590	GLY	2.7
1	H	578	GLY	2.7
1	J	408	GLY	2.7
1	J	444	ILE	2.7
1	B	86	SER	2.7
1	B	141	PRO	2.7
1	B	550	SER	2.7
1	K	302	SER	2.7
1	C	157	LEU	2.7
1	C	581	TRP	2.7
1	E	131	LEU	2.7
1	F	487	LEU	2.7
1	H	336	LEU	2.7
1	F	215	HIS	2.6
1	D	313	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	428	ALA	2.6
1	J	404	ALA	2.6
1	A	541	TYR	2.6
1	B	503	PHE	2.6
1	D	252	PHE	2.6
1	D	353	LYS	2.6
1	D	540	LYS	2.6
1	E	243	PHE	2.6
1	F	244	TYR	2.6
1	H	278	LYS	2.6
1	I	221	LYS	2.6
1	J	599	PHE	2.6
1	K	411	TYR	2.6
1	L	235	PHE	2.6
1	L	354	PHE	2.6
1	L	359	TYR	2.6
1	A	282	GLU	2.6
1	B	150	ASP	2.6
1	B	160	GLU	2.6
1	B	303	ASN	2.6
1	B	531	ASN	2.6
1	C	179	ASN	2.6
1	C	457	ASN	2.6
1	F	273	ASN	2.6
1	G	231	ASP	2.6
1	G	568	ASN	2.6
1	H	104	ASN	2.6
1	H	250	GLU	2.6
1	I	102	GLU	2.6
1	J	564	GLU	2.6
1	I	315	VAL	2.6
1	I	524	VAL	2.6
1	J	230	VAL	2.6
1	B	446	THR	2.6
1	I	223	THR	2.6
1	J	519	THR	2.6
1	B	414	GLY	2.6
1	C	327	ILE	2.6
1	C	369	ILE	2.6
1	C	501	GLY	2.6
1	E	381	GLY	2.6
1	C	440	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	481	ILE	2.6
1	G	355	ILE	2.6
1	G	453	ILE	2.6
1	G	544	ILE	2.6
1	H	327	ILE	2.6
1	L	193	GLY	2.6
1	I	86	SER	2.6
1	I	588	PRO	2.6
1	L	586	ARG	2.6
1	C	209	SER	2.6
1	F	302	SER	2.6
1	K	254	SER	2.6
1	F	162	MET	2.6
1	A	509	LEU	2.6
1	F	476	LEU	2.6
1	J	305	CYS	2.6
1	J	371	LEU	2.6
1	L	514	LEU	2.6
1	B	525	TRP	2.6
1	J	113	GLN	2.6
1	L	113	GLN	2.6
1	D	360	LYS	2.6
1	E	320	LYS	2.6
1	F	331	LYS	2.6
1	H	337	LYS	2.6
1	I	278	LYS	2.6
1	K	265	LYS	2.6
1	L	362	LYS	2.6
1	L	512	LYS	2.6
1	L	447	ALA	2.6
1	A	279	GLU	2.6
1	B	282	GLU	2.6
1	E	240	GLU	2.6
1	E	564	GLU	2.6
1	G	245	GLU	2.6
1	G	250	GLU	2.6
1	J	419	GLU	2.6
1	L	598	GLU	2.6
1	A	231	ASP	2.6
1	B	468	ASP	2.6
1	C	503	PHE	2.6
1	D	364	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	104	ASN	2.6
1	E	506	ASN	2.6
1	F	150	ASP	2.6
1	F	565	PHE	2.6
1	G	252	PHE	2.6
1	H	243	PHE	2.6
1	G	439	TYR	2.6
1	I	258	ASN	2.6
1	I	325	TYR	2.6
1	I	538	ASN	2.6
1	J	180	ASP	2.6
1	J	420	ASN	2.6
1	K	178	PHE	2.6
1	K	352	ASN	2.6
1	K	505	ASN	2.6
1	K	591	PHE	2.6
1	L	226	PHE	2.6
1	C	176	TYR	2.6
1	L	288	TYR	2.6
1	L	399	ASP	2.6
1	C	594	ARG	2.6
1	D	205	ARG	2.6
1	A	167	VAL	2.6
1	D	187	VAL	2.6
1	D	524	VAL	2.6
1	E	207	VAL	2.6
1	H	88	VAL	2.6
1	H	92	VAL	2.6
1	H	600	VAL	2.6
1	I	91	VAL	2.6
1	J	148	VAL	2.6
1	J	281	VAL	2.6
1	J	315	VAL	2.6
1	L	167	VAL	2.6
1	L	372	VAL	2.6
1	A	135	PRO	2.6
1	A	298	ILE	2.6
1	A	309	SER	2.6
1	C	427	SER	2.6
1	E	484	ILE	2.6
1	E	556	ILE	2.6
1	F	435	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	172	SER	2.6
1	G	548	SER	2.6
1	J	154	SER	2.6
1	J	199	SER	2.6
1	K	484	ILE	2.6
1	K	556	ILE	2.6
1	L	86	SER	2.6
1	L	266	HIS	2.6
1	B	385	LEU	2.6
1	G	198	LEU	2.6
1	G	527	LEU	2.6
1	J	475	LYS	2.6
1	A	332	GLU	2.6
1	F	419	GLU	2.6
1	G	526	TRP	2.6
1	I	155	GLU	2.6
1	L	332	GLU	2.6
1	A	535	ALA	2.6
1	D	467	ALA	2.6
1	H	370	ALA	2.6
1	C	521	ASN	2.6
1	D	217	ASN	2.6
1	G	133	ASN	2.6
1	G	249	ASP	2.6
1	H	399	ASP	2.6
1	I	432	ASN	2.6
1	L	159	ASP	2.6
1	A	398	PHE	2.6
1	B	591	PHE	2.6
1	D	289	PHE	2.6
1	J	503	PHE	2.6
1	B	224	VAL	2.6
1	B	287	TYR	2.6
1	B	292	TYR	2.6
1	C	486	THR	2.6
1	E	281	VAL	2.6
1	E	339	GLY	2.6
1	E	377	THR	2.6
1	H	263	TYR	2.6
1	I	408	GLY	2.6
1	I	593	VAL	2.6
1	J	488	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	171	THR	2.6
1	K	96	PRO	2.6
1	L	207	VAL	2.6
1	B	513	ILE	2.6
1	C	556	ILE	2.6
1	D	380	SER	2.6
1	E	548	SER	2.6
1	F	498	SER	2.6
1	F	513	ILE	2.6
1	J	327	ILE	2.6
1	K	327	ILE	2.6
1	K	391	SER	2.6
1	L	435	SER	2.6
1	L	448	SER	2.6
1	L	556	ILE	2.6
1	A	424	HIS	2.6
1	D	118	LYS	2.6
1	I	137	LYS	2.6
1	J	204	LYS	2.6
1	E	267	LEU	2.6
1	E	407	LEU	2.6
1	G	562	LEU	2.6
1	H	426	LEU	2.6
1	I	333	LEU	2.6
1	J	509	LEU	2.6
1	K	208	LEU	2.6
1	L	371	LEU	2.6
1	A	419	GLU	2.6
1	B	163	GLU	2.6
1	E	125	GLU	2.6
1	F	280	GLU	2.6
1	H	240	GLU	2.6
1	I	332	GLU	2.6
1	J	200	GLU	2.6
1	B	542	ALA	2.6
1	C	469	ALA	2.6
1	D	460	ALA	2.6
1	F	284	ALA	2.6
1	I	585	ALA	2.6
1	K	581	TRP	2.6
1	A	352	ASN	2.6
1	B	511	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	273	ASN	2.6
1	E	166	ASN	2.6
1	F	506	ASN	2.6
1	H	229	ASN	2.6
1	H	545	ASN	2.6
1	K	483	ASP	2.6
1	C	349	MET	2.6
1	A	458	THR	2.6
1	B	237	PHE	2.6
1	C	354	PHE	2.6
1	E	165	PHE	2.6
1	E	171	THR	2.6
1	E	235	PHE	2.6
1	F	171	THR	2.6
1	F	188	GLY	2.6
1	A	372	VAL	2.6
1	B	482	VAL	2.6
1	C	185	VAL	2.6
1	F	389	PRO	2.6
1	G	452	THR	2.6
1	H	377	THR	2.6
1	J	276	THR	2.6
1	J	425	PHE	2.6
1	K	519	THR	2.6
1	F	429	VAL	2.6
1	F	455	VAL	2.6
1	F	551	VAL	2.6
1	G	330	VAL	2.6
1	H	471	VAL	2.6
1	I	455	VAL	2.6
1	K	224	VAL	2.6
1	K	286	VAL	2.6
1	K	528	PRO	2.6
1	K	588	PRO	2.6
1	L	524	VAL	2.6
1	A	220	SER	2.6
1	B	293	TYR	2.6
1	C	189	TYR	2.6
1	E	539	SER	2.6
1	F	484	ILE	2.6
1	J	264	ILE	2.6
1	K	439	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	559	SER	2.6
1	L	246	TYR	2.6
1	L	549	SER	2.6
1	A	143	LYS	2.6
1	D	158	LYS	2.6
1	D	552	LYS	2.6
1	F	368	LYS	2.6
1	G	218	LYS	2.6
1	G	587	LYS	2.6
1	I	111	LYS	2.6
1	K	436	LYS	2.6
1	B	87	GLU	2.5
1	B	595	LEU	2.5
1	C	426	LEU	2.5
1	C	464	LEU	2.5
1	C	560	LEU	2.5
1	D	210	LEU	2.5
1	D	297	LEU	2.5
1	F	127	LEU	2.5
1	F	470	LEU	2.5
1	F	509	LEU	2.5
1	H	282	GLU	2.5
1	H	332	GLU	2.5
1	H	371	LEU	2.5
1	I	527	LEU	2.5
1	K	102	GLU	2.5
1	L	297	LEU	2.5
1	F	586	ARG	2.5
1	G	205	ARG	2.5
1	B	553	ALA	2.5
1	C	485	ALA	2.5
1	D	409	CYS	2.5
1	E	186	ALA	2.5
1	J	274	ALA	2.5
1	K	410	ALA	2.5
1	C	247	MET	2.5
1	C	392	MET	2.5
1	D	261	MET	2.5
1	E	217	ASN	2.5
1	F	159	ASP	2.5
1	F	379	ASP	2.5
1	G	538	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	134	ASN	2.5
1	I	216	ASP	2.5
1	J	261	MET	2.5
1	K	531	ASN	2.5
1	I	525	TRP	2.5
1	J	526	TRP	2.5
1	B	188	GLY	2.5
1	C	252	PHE	2.5
1	C	523	PRO	2.5
1	F	307	PRO	2.5
1	F	456	GLY	2.5
1	G	442	GLY	2.5
1	I	120	GLY	2.5
1	E	252	PHE	2.5
1	I	130	PHE	2.5
1	J	446	THR	2.5
1	L	565	PHE	2.5
1	A	529	ILE	2.5
1	C	576	ILE	2.5
1	D	172	SER	2.5
1	D	254	SER	2.5
1	F	559	SER	2.5
1	G	86	SER	2.5
1	G	367	LYS	2.5
1	H	360	LYS	2.5
1	H	366	LYS	2.5
1	K	218	LYS	2.5
1	K	475	LYS	2.5
1	L	190	VAL	2.5
1	G	144	ILE	2.5
1	G	327	ILE	2.5
1	J	574	ILE	2.5
1	K	107	ILE	2.5
1	A	439	TYR	2.5
1	B	288	TYR	2.5
1	C	288	TYR	2.5
1	D	541	TYR	2.5
1	E	439	TYR	2.5
1	G	359	TYR	2.5
1	L	383	TYR	2.5
1	D	280	GLU	2.5
1	D	522	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	279	GLU	2.5
1	H	419	GLU	2.5
1	K	532	GLU	2.5
1	C	267	LEU	2.5
1	C	310	LEU	2.5
1	C	336	LEU	2.5
1	C	385	LEU	2.5
1	F	385	LEU	2.5
1	F	495	LEU	2.5
1	G	267	LEU	2.5
1	G	426	LEU	2.5
1	I	210	LEU	2.5
1	I	219	LEU	2.5
1	I	310	LEU	2.5
1	J	357	LEU	2.5
1	B	490	ALA	2.5
1	F	384	ASN	2.5
1	G	233	ASN	2.5
1	G	275	ASP	2.5
1	G	469	ALA	2.5
1	G	505	ASN	2.5
1	G	521	ASN	2.5
1	I	305	CYS	2.5
1	I	511	ASN	2.5
1	K	249	ASP	2.5
1	K	340	ALA	2.5
1	A	204	LYS	2.5
1	A	329	GLY	2.5
1	A	584	LYS	2.5
1	B	170	GLY	2.5
1	B	418	PRO	2.5
1	D	347	GLY	2.5
1	G	381	GLY	2.5
1	H	290	GLY	2.5
1	H	367	LYS	2.5
1	I	164	LYS	2.5
1	K	253	LYS	2.5
1	K	477	GLY	2.5
1	L	307	PRO	2.5
1	L	523	PRO	2.5
1	E	446	THR	2.5
1	H	415	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	128	THR	2.5
1	A	503	PHE	2.5
1	E	565	PHE	2.5
1	F	378	PHE	2.5
1	F	526	TRP	2.5
1	I	581	TRP	2.5
1	A	199	SER	2.5
1	B	438	SER	2.5
1	B	567	GLN	2.5
1	C	190	VAL	2.5
1	C	494	SER	2.5
1	D	315	VAL	2.5
1	D	515	GLN	2.5
1	E	254	SER	2.5
1	F	391	SER	2.5
1	F	517	SER	2.5
1	G	401	SER	2.5
1	G	515	GLN	2.5
1	I	190	VAL	2.5
1	J	343	SER	2.5
1	K	184	SER	2.5
1	K	199	SER	2.5
1	L	515	GLN	2.5
1	L	520	SER	2.5
1	B	393	ILE	2.5
1	B	444	ILE	2.5
1	C	264	ILE	2.5
1	B	454	GLU	2.5
1	C	304	TYR	2.5
1	C	508	GLU	2.5
1	F	598	GLU	2.5
1	G	522	GLU	2.5
1	J	533	TYR	2.5
1	K	359	TYR	2.5
1	C	328	LEU	2.5
1	D	333	LEU	2.5
1	E	157	LEU	2.5
1	F	131	LEU	2.5
1	I	169	LEU	2.5
1	J	208	LEU	2.5
1	L	509	LEU	2.5
1	B	396	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	392	MET	2.5
1	E	433	MET	2.5
1	C	216	ASP	2.5
1	D	272	ASN	2.5
1	D	437	ASN	2.5
1	E	353	LYS	2.5
1	E	368	LYS	2.5
1	E	410	ALA	2.5
1	E	511	ASN	2.5
1	E	531	ASN	2.5
1	F	294	ALA	2.5
1	G	467	ALA	2.5
1	G	589	LYS	2.5
1	H	473	ALA	2.5
1	I	275	ASP	2.5
1	I	326	LYS	2.5
1	I	384	ASN	2.5
1	J	585	ALA	2.5
1	J	602	ASN	2.5
1	K	542	ALA	2.5
1	L	104	ASN	2.5
1	A	504	GLY	2.5
1	C	119	GLY	2.5
1	C	268	GLY	2.5
1	D	96	PRO	2.5
1	D	301	PRO	2.5
1	E	441	PRO	2.5
1	H	89	PRO	2.5
1	H	381	GLY	2.5
1	I	504	GLY	2.5
1	L	430	CYS	2.5
1	G	458	THR	2.5
1	I	446	THR	2.5
1	K	291	THR	2.5
1	B	206	VAL	2.5
1	B	211	VAL	2.5
1	B	559	SER	2.5
1	C	199	SER	2.5
1	C	454	GLU	2.5
1	D	123	VAL	2.5
1	F	125	GLU	2.5
1	F	154	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	207	VAL	2.5
1	J	332	GLU	2.5
1	K	145	SER	2.5
1	K	235	PHE	2.5
1	K	565	PHE	2.5
1	D	144	ILE	2.5
1	D	376	ILE	2.5
1	E	513	ILE	2.5
1	F	524	VAL	2.5
1	G	190	VAL	2.5
1	I	148	VAL	2.5
1	L	163	GLU	2.5
1	L	227	GLU	2.5
1	L	308	VAL	2.5
1	D	103	TYR	2.5
1	I	341	TYR	2.5
1	J	270	TYR	2.5
1	J	325	TYR	2.5
1	B	466	LEU	2.5
1	J	131	LEU	2.5
1	I	392	MET	2.5
1	C	331	LYS	2.5
1	D	218	LYS	2.5
1	G	512	LYS	2.5
1	H	158	LYS	2.5
1	E	202	ASP	2.5
1	H	543	ASP	2.5
1	L	322	ASN	2.5
1	A	577	ALA	2.5
1	C	410	ALA	2.5
1	F	318	ALA	2.5
1	G	196	ALA	2.5
1	G	201	ALA	2.5
1	I	299	ALA	2.5
1	J	424	HIS	2.5
1	K	174	HIS	2.5
1	A	136	GLY	2.5
1	B	390	GLY	2.5
1	D	418	PRO	2.5
1	F	290	GLY	2.5
1	J	462	GLY	2.5
1	K	501	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	290	GLY	2.5
1	L	329	GLY	2.5
1	L	414	GLY	2.5
1	A	403	CYS	2.4
1	C	569	THR	2.4
1	C	597	THR	2.4
1	D	597	THR	2.4
1	G	305	CYS	2.4
1	H	305	CYS	2.4
1	H	446	THR	2.4
1	I	431	GLU	2.4
1	J	97	THR	2.4
1	J	536	THR	2.4
1	K	87	GLU	2.4
1	K	276	THR	2.4
1	A	146	SER	2.4
1	A	175	PHE	2.4
1	C	91	VAL	2.4
1	C	398	PHE	2.4
1	J	184	SER	2.4
1	J	185	VAL	2.4
1	K	132	VAL	2.4
1	K	252	PHE	2.4
1	K	548	SER	2.4
1	K	555	SER	2.4
1	D	481	ILE	2.4
1	E	88	VAL	2.4
1	H	206	VAL	2.4
1	H	393	ILE	2.4
1	I	551	VAL	2.4
1	L	88	VAL	2.4
1	L	591	PHE	2.4
1	B	526	TRP	2.4
1	B	581	TRP	2.4
1	A	562	LEU	2.4
1	B	246	TYR	2.4
1	D	214	LEU	2.4
1	F	246	TYR	2.4
1	F	317	LEU	2.4
1	H	292	TYR	2.4
1	J	169	LEU	2.4
1	J	310	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	321	LEU	2.4
1	J	426	LEU	2.4
1	J	487	LEU	2.4
1	K	357	LEU	2.4
1	K	480	TYR	2.4
1	C	232	LYS	2.4
1	C	396	MET	2.4
1	E	177	MET	2.4
1	F	283	LYS	2.4
1	G	177	MET	2.4
1	G	278	LYS	2.4
1	J	320	LYS	2.4
1	L	247	MET	2.4
1	B	104	ASN	2.4
1	C	303	ASN	2.4
1	C	545	ASN	2.4
1	E	306	ASN	2.4
1	H	505	ASN	2.4
1	I	399	ASP	2.4
1	K	231	ASP	2.4
1	K	424	HIS	2.4
1	L	179	ASN	2.4
1	E	567	GLN	2.4
1	A	469	ALA	2.4
1	K	313	ALA	2.4
1	A	124	GLU	2.4
1	C	522	GLU	2.4
1	D	489	GLY	2.4
1	D	496	GLY	2.4
1	E	227	GLU	2.4
1	F	390	GLY	2.4
1	G	419	GLU	2.4
1	K	227	GLU	2.4
1	H	465	THR	2.4
1	I	291	THR	2.4
1	B	430	CYS	2.4
1	F	409	CYS	2.4
1	H	412	CYS	2.4
1	I	559	SER	2.4
1	C	237	PHE	2.4
1	D	298	ILE	2.4
1	D	574	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	129	ILE	2.4
1	E	355	ILE	2.4
1	E	510	ILE	2.4
1	E	544	ILE	2.4
1	F	190	VAL	2.4
1	I	129	ILE	2.4
1	K	429	VAL	2.4
1	K	503	PHE	2.4
1	L	599	PHE	2.4
1	B	164	LYS	2.4
1	E	232	LYS	2.4
1	I	362	LYS	2.4
1	I	367	LYS	2.4
1	F	571	TRP	2.4
1	H	349	MET	2.4
1	L	571	TRP	2.4
1	A	214	LEU	2.4
1	A	234	LEU	2.4
1	B	333	LEU	2.4
1	E	198	LEU	2.4
1	E	371	LEU	2.4
1	G	297	LEU	2.4
1	H	321	LEU	2.4
1	I	131	LEU	2.4
1	B	103	TYR	2.4
1	B	411	TYR	2.4
1	D	176	TYR	2.4
1	G	304	TYR	2.4
1	I	359	TYR	2.4
1	A	202	ASP	2.4
1	A	394	ASP	2.4
1	C	249	ASP	2.4
1	C	543	ASP	2.4
1	D	420	ASN	2.4
1	H	312	ASN	2.4
1	I	180	ASP	2.4
1	I	183	ASN	2.4
1	I	273	ASN	2.4
1	J	179	ASN	2.4
1	K	166	ASN	2.4
1	L	432	ASN	2.4
1	E	335	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	200	GLU	2.4
1	A	558	ALA	2.4
1	D	588	PRO	2.4
1	E	141	PRO	2.4
1	E	126	GLY	2.4
1	E	542	ALA	2.4
1	E	570	ALA	2.4
1	F	450	GLY	2.4
1	F	553	ALA	2.4
1	I	106	PRO	2.4
1	G	140	GLY	2.4
1	H	442	GLY	2.4
1	I	592	GLY	2.4
1	J	370	ALA	2.4
1	K	294	ALA	2.4
1	K	447	ALA	2.4
1	L	382	GLY	2.4
1	C	458	THR	2.4
1	J	128	THR	2.4
1	A	311	SER	2.4
1	B	517	SER	2.4
1	H	93	SER	2.4
1	H	494	SER	2.4
1	I	554	SER	2.4
1	J	539	SER	2.4
1	L	539	SER	2.4
1	A	101	ILE	2.4
1	A	142	VAL	2.4
1	A	484	ILE	2.4
1	B	252	PHE	2.4
1	B	327	ILE	2.4
1	C	563	LYS	2.4
1	D	264	ILE	2.4
1	D	281	VAL	2.4
1	D	355	ILE	2.4
1	D	366	LYS	2.4
1	E	147	LYS	2.4
1	E	403	CYS	2.4
1	B	434	VAL	2.4
1	B	599	PHE	2.4
1	G	237	PHE	2.4
1	G	579	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	298	ILE	2.4
1	I	232	LYS	2.4
1	J	397	LYS	2.4
1	C	269	VAL	2.4
1	D	434	VAL	2.4
1	E	230	VAL	2.4
1	E	471	VAL	2.4
1	H	482	VAL	2.4
1	I	123	VAL	2.4
1	I	478	VAL	2.4
1	J	423	ILE	2.4
1	J	576	ILE	2.4
1	K	92	VAL	2.4
1	K	112	VAL	2.4
1	L	315	VAL	2.4
1	J	213	MET	2.4
1	D	317	LEU	2.4
1	E	416	LEU	2.4
1	E	464	LEU	2.4
1	I	514	LEU	2.4
1	A	525	TRP	2.4
1	J	581	TRP	2.4
1	A	215	HIS	2.4
1	E	304	TYR	2.4
1	G	215	HIS	2.4
1	L	424	HIS	2.4
1	I	251	ARG	2.4
1	I	586	ARG	2.4
1	A	161	ASN	2.4
1	A	437	ASN	2.4
1	C	155	GLU	2.4
1	D	166	ASN	2.4
1	D	179	ASN	2.4
1	D	332	GLU	2.4
1	D	582	ASN	2.4
1	E	149	ASN	2.4
1	E	508	GLU	2.4
1	H	384	ASN	2.4
1	J	233	ASN	2.4
1	J	479	ASP	2.4
1	K	507	GLU	2.4
1	L	245	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	389	PRO	2.4
1	B	126	GLY	2.4
1	D	558	ALA	2.4
1	E	363	GLY	2.4
1	F	388	ALA	2.4
1	G	274	ALA	2.4
1	G	408	GLY	2.4
1	H	414	GLY	2.4
1	I	500	ALA	2.4
1	A	451	LYS	2.4
1	E	360	LYS	2.4
1	F	360	LYS	2.4
1	G	563	LYS	2.4
1	I	589	LYS	2.4
1	K	128	THR	2.4
1	K	320	LYS	2.4
1	K	465	THR	2.4
1	K	569	THR	2.4
1	G	145	SER	2.4
1	H	448	SER	2.4
1	I	154	SER	2.4
1	I	348	SER	2.4
1	I	498	SER	2.4
1	L	93	SER	2.4
1	A	252	PHE	2.4
1	A	286	VAL	2.4
1	A	330	VAL	2.4
1	C	156	PHE	2.4
1	D	566	VAL	2.4
1	D	591	PHE	2.4
1	E	228	ILE	2.4
1	F	243	PHE	2.4
1	F	392	MET	2.4
1	F	396	MET	2.4
1	F	591	PHE	2.4
1	G	107	ILE	2.4
1	G	114	VAL	2.4
1	I	203	MET	2.4
1	I	252	PHE	2.4
1	I	396	MET	2.4
1	I	503	PHE	2.4
1	J	91	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	101	ILE	2.4
1	J	593	VAL	2.4
1	K	225	VAL	2.4
1	K	243	PHE	2.4
1	L	425	PHE	2.4
1	C	242	LEU	2.4
1	C	466	LEU	2.4
1	E	476	LEU	2.4
1	F	357	LEU	2.4
1	F	562	LEU	2.4
1	H	466	LEU	2.4
1	I	416	LEU	2.4
1	L	127	LEU	2.4
1	L	242	LEU	2.4
1	B	586	ARG	2.4
1	G	594	ARG	2.4
1	B	546	GLN	2.4
1	F	319	GLN	2.4
1	A	262	GLU	2.4
1	F	532	GLU	2.4
1	G	454	GLU	2.4
1	A	582	ASN	2.3
1	B	568	ASN	2.3
1	C	263	TYR	2.3
1	E	263	TYR	2.3
1	F	480	TYR	2.3
1	H	350	TYR	2.3
1	I	506	ASN	2.3
1	J	411	TYR	2.3
1	J	499	TYR	2.3
1	K	312	ASN	2.3
1	J	301	PRO	2.3
1	K	418	PRO	2.3
1	A	173	LYS	2.3
1	B	347	GLY	2.3
1	A	201	ALA	2.3
1	C	221	LYS	2.3
1	C	375	GLY	2.3
1	D	584	LYS	2.3
1	F	404	ALA	2.3
1	F	451	LYS	2.3
1	J	126	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	542	ALA	2.3
1	G	340	ALA	2.3
1	H	460	ALA	2.3
1	K	221	LYS	2.3
1	L	278	LYS	2.3
1	C	465	THR	2.3
1	E	569	THR	2.3
1	H	488	THR	2.3
1	L	171	THR	2.3
1	L	446	THR	2.3
1	L	486	THR	2.3
1	D	295	SER	2.3
1	D	343	SER	2.3
1	D	517	SER	2.3
1	F	438	SER	2.3
1	H	209	SER	2.3
1	I	494	SER	2.3
1	K	209	SER	2.3
1	L	302	SER	2.3
1	C	162	MET	2.3
1	I	349	MET	2.3
1	C	226	PHE	2.3
1	D	132	VAL	2.3
1	D	153	VAL	2.3
1	E	156	PHE	2.3
1	E	566	VAL	2.3
1	G	129	ILE	2.3
1	G	175	PHE	2.3
1	G	185	VAL	2.3
1	G	591	PHE	2.3
1	J	369	ILE	2.3
1	K	330	VAL	2.3
1	L	413	VAL	2.3
1	B	356	HIS	2.3
1	C	266	HIS	2.3
1	I	174	HIS	2.3
1	A	567	GLN	2.3
1	C	234	LEU	2.3
1	G	470	LEU	2.3
1	H	470	LEU	2.3
1	J	567	GLN	2.3
1	K	242	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	596	LEU	2.3
1	C	279	GLU	2.3
1	E	316	GLU	2.3
1	G	262	GLU	2.3
1	L	324	GLU	2.3
1	C	166	ASN	2.3
1	K	180	ASP	2.3
1	L	273	ASN	2.3
1	L	459	ASP	2.3
1	B	263	TYR	2.3
1	C	164	LYS	2.3
1	D	263	TYR	2.3
1	D	383	TYR	2.3
1	E	588	PRO	2.3
1	F	151	LYS	2.3
1	F	353	LYS	2.3
1	F	417	LYS	2.3
1	G	89	PRO	2.3
1	H	418	PRO	2.3
1	I	265	LYS	2.3
1	K	244	TYR	2.3
1	K	288	TYR	2.3
1	L	325	TYR	2.3
1	B	402	GLY	2.3
1	F	170	GLY	2.3
1	L	442	GLY	2.3
1	G	388	ALA	2.3
1	H	294	ALA	2.3
1	K	473	ALA	2.3
1	B	458	THR	2.3
1	G	97	THR	2.3
1	I	105	THR	2.3
1	I	241	THR	2.3
1	B	427	SER	2.3
1	C	254	SER	2.3
1	D	361	SER	2.3
1	G	254	SER	2.3
1	H	498	SER	2.3
1	H	517	SER	2.3
1	J	172	SER	2.3
1	K	172	SER	2.3
1	K	380	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	123	VAL	2.3
1	B	424	HIS	2.3
1	C	107	ILE	2.3
1	I	110	ILE	2.3
1	I	376	ILE	2.3
1	K	129	ILE	2.3
1	B	522	GLU	2.3
1	C	206	VAL	2.3
1	C	235	PHE	2.3
1	C	471	VAL	2.3
1	D	599	PHE	2.3
1	G	207	VAL	2.3
1	G	561	PHE	2.3
1	H	227	GLU	2.3
1	H	245	GLU	2.3
1	I	583	PHE	2.3
1	J	238	PHE	2.3
1	K	245	GLU	2.3
1	K	478	VAL	2.3
1	K	593	VAL	2.3
1	L	429	VAL	2.3
1	A	219	LEU	2.3
1	A	385	LEU	2.3
1	B	242	LEU	2.3
1	B	514	LEU	2.3
1	C	495	LEU	2.3
1	D	328	LEU	2.3
1	F	514	LEU	2.3
1	G	310	LEU	2.3
1	G	328	LEU	2.3
1	H	476	LEU	2.3
1	I	371	LEU	2.3
1	J	409	CYS	2.3
1	L	310	LEU	2.3
1	C	118	LYS	2.3
1	C	320	LYS	2.3
1	E	116	ASP	2.3
1	H	326	LYS	2.3
1	I	322	ASN	2.3
1	I	518	LYS	2.3
1	K	95	ASP	2.3
1	L	133	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	582	ASN	2.3
1	A	441	PRO	2.3
1	E	96	PRO	2.3
1	I	89	PRO	2.3
1	I	389	PRO	2.3
1	D	287	TYR	2.3
1	E	103	TYR	2.3
1	E	191	GLY	2.3
1	F	496	GLY	2.3
1	G	193	GLY	2.3
1	I	477	GLY	2.3
1	J	501	GLY	2.3
1	K	499	TYR	2.3
1	L	350	TYR	2.3
1	L	525	TRP	2.3
1	B	388	ALA	2.3
1	B	570	ALA	2.3
1	C	300	ALA	2.3
1	E	299	ALA	2.3
1	J	162	MET	2.3
1	K	274	ALA	2.3
1	D	276	THR	2.3
1	F	486	THR	2.3
1	L	488	THR	2.3
1	D	209	SER	2.3
1	G	199	SER	2.3
1	G	311	SER	2.3
1	G	448	SER	2.3
1	H	285	ARG	2.3
1	A	240	GLU	2.3
1	C	113	GLN	2.3
1	C	335	GLU	2.3
1	J	522	GLU	2.3
1	L	564	GLU	2.3
1	B	99	ILE	2.3
1	B	481	ILE	2.3
1	E	271	ILE	2.3
1	I	547	ILE	2.3
1	B	238	PHE	2.3
1	B	406	VAL	2.3
1	B	425	PHE	2.3
1	E	130	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	211	VAL	2.3
1	G	167	VAL	2.3
1	G	406	VAL	2.3
1	H	148	VAL	2.3
1	J	235	PHE	2.3
1	L	289	PHE	2.3
1	A	283	LYS	2.3
1	A	337	LYS	2.3
1	A	407	LEU	2.3
1	B	265	LYS	2.3
1	E	214	LEU	2.3
1	F	182	LYS	2.3
1	G	509	LEU	2.3
1	G	518	LYS	2.3
1	H	164	LYS	2.3
1	I	368	LYS	2.3
1	J	416	LEU	2.3
1	I	412	CYS	2.3
1	A	197	ASP	2.3
1	A	249	ASP	2.3
1	A	306	ASN	2.3
1	B	179	ASN	2.3
1	C	150	ASP	2.3
1	D	479	ASP	2.3
1	D	543	ASP	2.3
1	G	399	ASP	2.3
1	J	543	ASP	2.3
1	K	272	ASN	2.3
1	K	457	ASN	2.3
1	E	135	PRO	2.3
1	J	106	PRO	2.3
1	K	307	PRO	2.3
1	D	329	GLY	2.3
1	K	290	GLY	2.3
1	A	293	TYR	2.3
1	B	541	TYR	2.3
1	G	383	TYR	2.3
1	K	341	TYR	2.3
1	L	293	TYR	2.3
1	L	439	TYR	2.3
1	C	577	ALA	2.3
1	D	340	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	526	TRP	2.3
1	C	536	THR	2.3
1	E	415	THR	2.3
1	J	241	THR	2.3
1	L	519	THR	2.3
1	C	539	SER	2.3
1	H	154	SER	2.3
1	H	554	SER	2.3
1	A	507	GLU	2.3
1	C	282	GLU	2.3
1	D	163	GLU	2.3
1	G	324	GLU	2.3
1	H	279	GLU	2.3
1	C	278	LYS	2.3
1	D	556	ILE	2.3
1	F	168	LYS	2.3
1	F	376	ILE	2.3
1	K	368	LYS	2.3
1	L	481	ILE	2.3
1	A	114	VAL	2.3
1	A	190	VAL	2.3
1	A	207	VAL	2.3
1	B	357	LEU	2.2
1	D	237	PHE	2.2
1	D	455	VAL	2.3
1	F	328	LEU	2.2
1	F	599	PHE	2.2
1	G	169	LEU	2.2
1	G	565	PHE	2.2
1	H	94	LEU	2.2
1	J	92	VAL	2.3
1	J	557	VAL	2.3
1	J	596	LEU	2.2
1	K	198	LEU	2.2
1	K	238	PHE	2.2
1	L	211	VAL	2.3
1	L	583	PHE	2.2
1	B	180	ASP	2.2
1	D	183	ASN	2.2
1	E	303	ASN	2.2
1	E	312	ASN	2.2
1	K	181	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	141	PRO	2.2
1	A	496	GLY	2.2
1	D	290	GLY	2.2
1	E	188	GLY	2.2
1	F	373	GLY	2.2
1	F	375	GLY	2.2
1	G	373	GLY	2.2
1	H	440	ARG	2.2
1	H	592	GLY	2.2
1	J	382	GLY	2.2
1	K	440	ARG	2.2
1	L	491	MET	2.2
1	E	163	GLU	2.2
1	E	341	TYR	2.2
1	E	577	ALA	2.2
1	F	485	ALA	2.2
1	G	569	THR	2.2
1	G	597	THR	2.2
1	H	341	TYR	2.2
1	H	500	ALA	2.2
1	I	313	ALA	2.2
1	I	558	ALA	2.2
1	A	152	GLN	2.2
1	E	486	THR	2.2
1	F	546	GLN	2.2
1	G	105	THR	2.2
1	J	288	TYR	2.2
1	H	90	GLN	2.2
1	L	291	THR	2.2
1	D	571	TRP	2.2
1	E	343	SER	2.2
1	G	98	SER	2.2
1	I	361	SER	2.2
1	E	397	LYS	2.2
1	F	118	LYS	2.2
1	J	182	LYS	2.2
1	K	204	LYS	2.2
1	D	453	ILE	2.2
1	F	101	ILE	2.2
1	H	529	ILE	2.2
1	K	423	ILE	2.2
1	A	308	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	502	VAL	2.2
1	C	175	PHE	2.2
1	C	224	VAL	2.2
1	C	372	VAL	2.2
1	E	509	LEU	2.2
1	E	524	VAL	2.2
1	E	560	LEU	2.2
1	F	297	LEU	2.2
1	D	561	PHE	2.2
1	E	425	PHE	2.2
1	F	235	PHE	2.2
1	G	92	VAL	2.2
1	G	222	LEU	2.2
1	J	562	LEU	2.2
1	K	333	LEU	2.2
1	K	426	LEU	2.2
1	G	243	PHE	2.2
1	H	252	PHE	2.2
1	L	482	VAL	2.2
1	A	449	ASN	2.2
1	A	505	ASN	2.2
1	E	543	ASP	2.2
1	F	202	ASP	2.2
1	F	420	ASN	2.2
1	G	394	ASP	2.2
1	A	261	MET	2.2
1	A	307	PRO	2.2
1	B	213	MET	2.2
1	C	100	PRO	2.2
1	E	162	MET	2.2
1	E	389	PRO	2.2
1	F	205	ARG	2.2
1	F	400	MET	2.2
1	G	441	PRO	2.2
1	B	120	GLY	2.2
1	E	456	GLY	2.2
1	H	188	GLY	2.2
1	J	329	GLY	2.2
1	J	578	GLY	2.2
1	L	345	GLY	2.2
1	L	590	GLY	2.2
1	L	419	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	147	LYS	2.2
1	D	386	LYS	2.2
1	I	152	GLN	2.2
1	B	212	THR	2.2
1	B	241	THR	2.2
1	D	388	ALA	2.2
1	I	346	LYS	2.2
1	J	340	ALA	2.2
1	L	164	LYS	2.2
1	I	597	THR	2.2
1	K	358	THR	2.2
1	K	486	THR	2.2
1	L	105	THR	2.2
1	A	472	TYR	2.2
1	A	555	SER	2.2
1	C	98	SER	2.2
1	D	246	TYR	2.2
1	E	533	TYR	2.2
1	H	359	TYR	2.2
1	J	209	SER	2.2
1	A	444	ILE	2.2
1	E	107	ILE	2.2
1	E	445	ILE	2.2
1	E	574	ILE	2.2
1	G	271	ILE	2.2
1	G	510	ILE	2.2
1	I	484	ILE	2.2
1	J	484	ILE	2.2
1	C	514	LEU	2.2
1	D	169	LEU	2.2
1	D	234	LEU	2.2
1	D	357	LEU	2.2
1	E	297	LEU	2.2
1	G	208	LEU	2.2
1	H	464	LEU	2.2
1	J	385	LEU	2.2
1	J	560	LEU	2.2
1	K	487	LEU	2.2
1	L	222	LEU	2.2
1	A	413	VAL	2.2
1	A	455	VAL	2.2
1	D	413	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	92	VAL	2.2
1	F	330	VAL	2.2
1	G	148	VAL	2.2
1	H	211	VAL	2.2
1	I	557	VAL	2.2
1	J	434	VAL	2.2
1	L	406	VAL	2.2
1	E	238	PHE	2.2
1	F	156	PHE	2.2
1	B	449	ASN	2.2
1	D	312	ASN	2.2
1	E	249	ASP	2.2
1	F	352	ASN	2.2
1	G	116	ASP	2.2
1	G	468	ASP	2.2
1	H	420	ASN	2.2
1	J	440	ARG	2.2
1	J	506	ASN	2.2
1	L	150	ASP	2.2
1	L	202	ASP	2.2
1	L	205	ARG	2.2
1	L	231	ASP	2.2
1	D	203	MET	2.2
1	D	349	MET	2.2
1	G	203	MET	2.2
1	G	338	MET	2.2
1	J	338	MET	2.2
1	B	504	GLY	2.2
1	C	339	GLY	2.2
1	C	382	GLY	2.2
1	C	462	GLY	2.2
1	C	504	GLY	2.2
1	D	120	GLY	2.2
1	J	140	GLY	2.2
1	J	412	CYS	2.2
1	C	240	GLU	2.2
1	F	422	GLU	2.2
1	G	102	GLU	2.2
1	B	111	LYS	2.2
1	E	436	LYS	2.2
1	H	424	HIS	2.2
1	I	320	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	128	THR	2.2
1	A	255	THR	2.2
1	A	585	ALA	2.2
1	B	97	THR	2.2
1	D	553	ALA	2.2
1	F	460	ALA	2.2
1	B	343	SER	2.2
1	E	302	SER	2.2
1	F	520	SER	2.2
1	F	597	THR	2.2
1	G	410	ALA	2.2
1	G	154	SER	2.2
1	H	452	THR	2.2
1	I	438	SER	2.2
1	J	448	SER	2.2
1	A	288	TYR	2.2
1	J	277	TYR	2.2
1	G	525	TRP	2.2
1	A	481	ILE	2.2
1	B	297	LEU	2.2
1	B	537	LEU	2.2
1	C	357	LEU	2.2
1	D	527	LEU	2.2
1	E	336	LEU	2.2
1	F	423	ILE	2.2
1	H	560	LEU	2.2
1	I	481	ILE	2.2
1	J	99	ILE	2.2
1	J	198	LEU	2.2
1	J	547	ILE	2.2
1	J	534	ARG	2.2
1	A	338	MET	2.2
1	C	104	ASN	2.2
1	C	116	ASP	2.2
1	C	413	VAL	2.2
1	D	202	ASP	2.2
1	D	432	ASN	2.2
1	D	503	PHE	2.2
1	D	545	ASN	2.2
1	E	197	ASP	2.2
1	E	434	VAL	2.2
1	E	437	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	91	VAL	2.2
1	G	511	ASN	2.2
1	H	224	VAL	2.2
1	H	502	VAL	2.2
1	H	237	PHE	2.2
1	H	599	PHE	2.2
1	I	420	ASN	2.2
1	J	211	VAL	2.2
1	E	599	PHE	2.2
1	K	582	ASN	2.2
1	G	100	PRO	2.2
1	H	96	PRO	2.2
1	I	441	PRO	2.2
1	A	324	GLU	2.2
1	A	564	GLU	2.2
1	C	138	GLU	2.2
1	C	475	LYS	2.2
1	H	353	LYS	2.2
1	H	475	LYS	2.2
1	I	334	GLU	2.2
1	J	111	LYS	2.2
1	J	143	LYS	2.2
1	K	125	GLU	2.2
1	E	152	GLN	2.2
1	G	496	GLY	2.2
1	G	501	GLY	2.2
1	I	108	HIS	2.2
1	E	192	CYS	2.2
1	F	305	CYS	2.2
1	J	430	CYS	2.2
1	A	553	ALA	2.2
1	C	516	SER	2.2
1	C	553	ALA	2.2
1	D	199	SER	2.2
1	D	404	ALA	2.2
1	D	580	SER	2.2
1	E	340	ALA	2.2
1	G	572	ALA	2.2
1	H	401	SER	2.2
1	H	469	ALA	2.2
1	I	302	SER	2.2
1	I	452	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	452	THR	2.2
1	J	467	ALA	2.2
1	J	473	ALA	2.2
1	J	569	THR	2.2
1	D	440	ARG	2.1
1	G	534	ARG	2.1
1	J	292	TYR	2.1
1	B	445	ILE	2.1
1	B	547	ILE	2.1
1	C	509	LEU	2.1
1	C	544	ILE	2.1
1	E	94	LEU	2.1
1	E	487	LEU	2.1
1	F	537	LEU	2.1
1	G	423	ILE	2.1
1	G	481	ILE	2.1
1	H	537	LEU	2.1
1	J	445	ILE	2.1
1	B	312	ASN	2.1
1	G	217	ASN	2.1
1	G	400	MET	2.1
1	C	207	VAL	2.1
1	F	406	VAL	2.1
1	F	413	VAL	2.1
1	G	91	VAL	2.1
1	I	92	VAL	2.1
1	I	330	VAL	2.1
1	K	161	ASN	2.1
1	L	275	ASP	2.1
1	A	147	LYS	2.1
1	A	346	LYS	2.1
1	A	366	LYS	2.1
1	C	326	LYS	2.1
1	D	316	GLU	2.1
1	D	475	LYS	2.1
1	E	417	LYS	2.1
1	B	96	PRO	2.1
1	F	160	GLU	2.1
1	F	351	PRO	2.1
1	F	583	PHE	2.1
1	H	598	GLU	2.1
1	J	316	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	334	GLU	2.1
1	K	397	LYS	2.1
1	I	418	PRO	2.1
1	K	425	PHE	2.1
1	L	243	PHE	2.1
1	C	174	HIS	2.1
1	C	215	HIS	2.1
1	E	573	HIS	2.1
1	K	319	GLN	2.1
1	A	347	GLY	2.1
1	B	290	GLY	2.1
1	C	191	GLY	2.1
1	D	363	GLY	2.1
1	E	170	GLY	2.1
1	E	408	GLY	2.1
1	F	489	GLY	2.1
1	K	347	GLY	2.1
1	F	403	CYS	2.1
1	A	284	ALA	2.1
1	A	415	THR	2.1
1	A	486	THR	2.1
1	A	597	THR	2.1
1	B	186	ALA	2.1
1	B	220	SER	2.1
1	C	295	SER	2.1
1	C	318	ALA	2.1
1	C	380	SER	2.1
1	G	438	SER	2.1
1	I	519	THR	2.1
1	I	535	ALA	2.1
1	I	572	ALA	2.1
1	J	490	ALA	2.1
1	K	388	ALA	2.1
1	L	358	THR	2.1
1	L	585	ALA	2.1
1	C	463	ARG	2.1
1	G	285	ARG	2.1
1	G	396	MET	2.1
1	H	304	TYR	2.1
1	K	472	TYR	2.1
1	A	321	LEU	2.1
1	B	530	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	99	ILE	2.1
1	C	342	LEU	2.1
1	C	484	ILE	2.1
1	C	596	LEU	2.1
1	D	371	LEU	2.1
1	E	218	LYS	2.1
1	E	393	ILE	2.1
1	E	589	LYS	2.1
1	F	137	LYS	2.1
1	F	264	ILE	2.1
1	G	232	LYS	2.1
1	I	369	ILE	2.1
1	I	513	ILE	2.1
1	J	368	LYS	2.1
1	K	264	ILE	2.1
1	K	298	ILE	2.1
1	L	513	ILE	2.1
1	A	256	ASP	2.1
1	B	432	ASN	2.1
1	D	511	ASN	2.1
1	E	233	ASN	2.1
1	G	545	ASN	2.1
1	K	197	ASP	2.1
1	K	275	ASP	2.1
1	L	280	GLU	2.1
1	A	132	VAL	2.1
1	A	471	VAL	2.1
1	B	429	VAL	2.1
1	C	230	VAL	2.1
1	B	354	PHE	2.1
1	B	565	PHE	2.1
1	C	389	PRO	2.1
1	E	413	VAL	2.1
1	H	100	PRO	2.1
1	L	108	HIS	2.1
1	L	215	HIS	2.1
1	D	235	PHE	2.1
1	D	339	GLY	2.1
1	E	193	GLY	2.1
1	E	462	GLY	2.1
1	F	120	GLY	2.1
1	G	191	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	592	GLY	2.1
1	H	501	GLY	2.1
1	J	363	GLY	2.1
1	L	456	GLY	2.1
1	L	501	GLY	2.1
1	F	192	CYS	2.1
1	A	98	SER	2.1
1	A	570	ALA	2.1
1	B	520	SER	2.1
1	C	212	THR	2.1
1	E	497	THR	2.1
1	J	586	ARG	2.1
1	B	572	ALA	2.1
1	F	410	ALA	2.1
1	G	380	SER	2.1
1	H	340	ALA	2.1
1	I	314	ALA	2.1
1	J	299	ALA	2.1
1	J	494	SER	2.1
1	K	98	SER	2.1
1	L	294	ALA	2.1
1	L	554	SER	2.1
1	C	111	LYS	2.1
1	C	362	LYS	2.1
1	C	397	LYS	2.1
1	D	326	LYS	2.1
1	F	349	MET	2.1
1	G	360	LYS	2.1
1	G	366	LYS	2.1
1	I	400	MET	2.1
1	J	203	MET	2.1
1	K	111	LYS	2.1
1	L	151	LYS	2.1
1	L	338	MET	2.1
1	A	416	LEU	2.1
1	E	239	LEU	2.1
1	F	240	GLU	2.1
1	H	499	TYR	2.1
1	I	189	TYR	2.1
1	I	298	ILE	2.1
1	J	129	ILE	2.1
1	J	495	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	131	LEU	2.1
1	L	445	ILE	2.1
1	L	466	LEU	2.1
1	B	134	ASN	2.1
1	B	244	TYR	2.1
1	B	457	ASN	2.1
1	C	103	TYR	2.1
1	D	483	ASP	2.1
1	D	533	TYR	2.1
1	F	166	ASN	2.1
1	K	292	TYR	2.1
1	K	394	ASP	2.1
1	L	530	ILE	2.1
1	A	90	GLN	2.1
1	G	152	GLN	2.1
1	I	356	HIS	2.1
1	L	356	HIS	2.1
1	C	211	VAL	2.1
1	C	455	VAL	2.1
1	D	211	VAL	2.1
1	F	593	VAL	2.1
1	G	206	VAL	2.1
1	I	96	PRO	2.1
1	L	471	VAL	2.1
1	B	571	TRP	2.1
1	E	561	PHE	2.1
1	E	450	GLY	2.1
1	F	329	GLY	2.1
1	L	268	GLY	2.1
1	A	465	THR	2.1
1	B	248	THR	2.1
1	B	380	SER	2.1
1	B	488	THR	2.1
1	C	105	THR	2.1
1	C	192	CYS	2.1
1	D	154	SER	2.1
1	D	223	THR	2.1
1	F	458	THR	2.1
1	G	516	SER	2.1
1	H	223	THR	2.1
1	H	403	CYS	2.1
1	I	549	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	559	SER	2.1
1	K	520	SER	2.1
1	A	374	LYS	2.1
1	C	299	ALA	2.1
1	C	313	ALA	2.1
1	C	490	ALA	2.1
1	D	572	ALA	2.1
1	E	563	LYS	2.1
1	G	447	ALA	2.1
1	H	314	ALA	2.1
1	J	337	LYS	2.1
1	K	535	ALA	2.1
1	D	87	GLU	2.1
1	G	160	GLU	2.1
1	G	422	GLU	2.1
1	A	169	LEU	2.1
1	C	562	LEU	2.1
1	C	601	LEU	2.1
1	D	356	HIS	2.1
1	D	470	LEU	2.1
1	E	127	LEU	2.1
1	G	219	LEU	2.1
1	H	174	HIS	2.1
1	I	222	LEU	2.1
1	I	319	GLN	2.1
1	I	426	LEU	2.1
1	K	214	LEU	2.1
1	A	510	ILE	2.1
1	D	505	ASN	2.1
1	E	468	ASP	2.1
1	F	483	ASP	2.1
1	F	510	ILE	2.1
1	F	574	ILE	2.1
1	F	576	ILE	2.1
1	H	303	ASN	2.1
1	I	437	ASN	2.1
1	I	483	ASP	2.1
1	J	399	ASP	2.1
1	J	459	ASP	2.1
1	K	228	ILE	2.1
1	K	233	ASN	2.1
1	K	530	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	575	ASP	2.1
1	L	298	ILE	2.1
1	A	351	PRO	2.1
1	A	359	TYR	2.1
1	B	383	TYR	2.1
1	H	441	PRO	2.1
1	H	528	PRO	2.1
1	J	472	TYR	2.1
1	K	277	TYR	2.1
1	A	421	VAL	2.1
1	B	92	VAL	2.1
1	D	269	VAL	2.1
1	E	185	VAL	2.1
1	K	167	VAL	2.1
1	K	502	VAL	2.1
1	A	402	GLY	2.1
1	B	583	PHE	2.1
1	C	450	GLY	2.1
1	F	504	GLY	2.1
1	G	390	GLY	2.1
1	J	477	GLY	2.1
1	A	586	ARG	2.1
1	B	236	ARG	2.1
1	C	236	ARG	2.1
1	E	205	ARG	2.1
1	E	586	ARG	2.1
1	F	440	ARG	2.1
1	K	236	ARG	2.1
1	A	158	LYS	2.0
1	B	326	LYS	2.0
1	C	353	LYS	2.0
1	E	540	LYS	2.0
1	G	417	LYS	2.0
1	J	353	LYS	2.0
1	L	118	LYS	2.0
1	A	172	SER	2.0
1	A	302	SER	2.0
1	C	361	SER	2.0
1	D	497	THR	2.0
1	D	516	SER	2.0
1	F	580	SER	2.0
1	I	415	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	435	SER	2.0
1	K	194	SER	2.0
1	A	409	CYS	2.0
1	B	428	ALA	2.0
1	D	284	ALA	2.0
1	G	335	GLU	2.0
1	H	558	ALA	2.0
1	I	340	ALA	2.0
1	K	203	MET	2.0
1	K	213	MET	2.0
1	E	305	CYS	2.0
1	J	192	CYS	2.0
1	K	279	GLU	2.0
1	D	90	GLN	2.0
1	D	113	GLN	2.0
1	K	215	HIS	2.0
1	A	131	LEU	2.0
1	A	134	ASN	2.0
1	D	595	LEU	2.0
1	E	443	ASP	2.0
1	F	426	LEU	2.0
1	G	466	LEU	2.0
1	G	514	LEU	2.0
1	G	596	LEU	2.0
1	I	312	ASN	2.0
1	I	470	LEU	2.0
1	J	127	LEU	2.0
1	F	453	ILE	2.0
1	J	355	ILE	2.0
1	K	544	ILE	2.0
1	A	106	PRO	2.0
1	D	89	PRO	2.0
1	F	301	PRO	2.0
1	G	141	PRO	2.0
1	B	493	TYR	2.0
1	D	115	TYR	2.0
1	D	325	TYR	2.0
1	E	176	TYR	2.0
1	K	263	TYR	2.0
1	A	315	VAL	2.0
1	C	112	VAL	2.0
1	F	372	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	502	VAL	2.0
1	G	344	VAL	2.0
1	G	372	VAL	2.0
1	G	440	ARG	2.0
1	I	211	VAL	2.0
1	J	524	VAL	2.0
1	K	285	ARG	2.0
1	K	463	ARG	2.0
1	K	557	VAL	2.0
1	G	504	GLY	2.0
1	J	237	PHE	2.0
1	B	320	LYS	2.0
1	F	589	LYS	2.0
1	G	265	LYS	2.0
1	H	552	LYS	2.0
1	L	283	LYS	2.0
1	H	526	TRP	2.0
1	A	377	THR	2.0
1	A	446	THR	2.0
1	A	532	GLU	2.0
1	B	422	GLU	2.0
1	C	177	MET	2.0
1	D	162	MET	2.0
1	D	433	MET	2.0
1	J	349	MET	2.0
1	B	448	SER	2.0
1	E	105	THR	2.0
1	F	494	SER	2.0
1	G	520	SER	2.0
1	G	539	SER	2.0
1	H	380	SER	2.0
1	I	172	SER	2.0
1	J	311	SER	2.0
1	K	564	GLU	2.0
1	L	334	GLU	2.0
1	B	473	ALA	2.0
1	E	553	ALA	2.0
1	J	186	ALA	2.0
1	J	201	ALA	2.0
1	G	424	HIS	2.0
1	J	356	HIS	2.0
1	K	121	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	495	LEU	2.0
1	B	239	LEU	2.0
1	B	426	LEU	2.0
1	C	312	ASN	2.0
1	D	562	LEU	2.0
1	F	303	ASN	2.0
1	F	459	ASP	2.0
1	G	273	ASN	2.0
1	G	407	LEU	2.0
1	G	449	ASN	2.0
1	H	210	LEU	2.0
1	I	303	ASN	2.0
1	I	509	LEU	2.0
1	J	531	ASN	2.0
1	L	443	ASP	2.0
1	A	547	ILE	2.0
1	C	101	ILE	2.0
1	C	141	PRO	2.0
1	D	307	PRO	2.0
1	E	307	PRO	2.0
1	G	445	ILE	2.0
1	I	453	ILE	2.0
1	K	251	ARG	2.0
1	F	512	LYS	2.0
1	L	366	LYS	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($\text{\AA}^2$)	Q<0.9
7	SO4	C	708	5/5	0.03	0.35	53,57,64,72	0
5	1PE	A	706	12/16	0.09	0.31	33,46,50,51	0
5	1PE	B	706	10/16	0.19	0.27	41,45,54,56	0
7	SO4	A	709	5/5	0.26	0.37	53,57,75,78	0
5	1PE	D	705	10/16	0.29	0.28	27,37,45,48	0
5	1PE	G	707	6/16	0.31	0.27	31,35,39,39	0
7	SO4	C	711	5/5	0.32	0.80	41,45,53,55	0
5	1PE	J	706	11/16	0.34	0.26	36,43,47,52	0
5	1PE	J	705	11/16	0.35	0.28	33,40,50,52	0
5	1PE	C	705	13/16	0.35	0.26	27,41,52,52	0
5	1PE	L	705	7/16	0.35	0.37	30,34,39,41	0
2	CO3	L	701	4/4	0.37	0.23	16,17,18,19	0
5	1PE	H	705	10/16	0.37	0.25	35,44,50,53	0
7	SO4	K	708	5/5	0.38	0.29	58,60,74,75	0
5	1PE	B	705	10/16	0.39	0.28	36,40,51,51	0
5	1PE	F	705	10/16	0.41	0.23	26,37,45,52	0
5	1PE	H	706	10/16	0.41	0.24	30,40,46,47	0
7	SO4	F	707	5/5	0.41	0.46	55,57,61,75	0
5	1PE	E	705	12/16	0.41	0.26	29,39,44,45	0
6	GOL	A	707	6/6	0.43	0.29	37,37,45,54	0
7	SO4	I	708	5/5	0.44	0.21	74,74,83,91	0
5	1PE	I	705	12/16	0.46	0.25	35,40,43,47	0
5	1PE	G	705	9/16	0.46	0.23	25,32,39,40	0
7	SO4	E	709	5/5	0.46	0.40	47,51,64,76	0
7	SO4	C	710	5/5	0.47	0.45	34,38,58,62	0
7	SO4	G	711	5/5	0.47	0.39	46,48,51,55	0
5	1PE	C	706	9/16	0.48	0.20	26,29,35,36	0
5	1PE	D	706	10/16	0.49	0.20	27,36,40,41	0
7	SO4	A	711	5/5	0.50	0.36	56,56,63,81	0
7	SO4	C	707	5/5	0.51	0.27	57,57,57,58	0
5	1PE	I	706	11/16	0.53	0.24	26,35,48,53	0
7	SO4	C	709	5/5	0.54	0.48	55,55,63,82	0
2	CO3	C	701	4/4	0.56	0.24	15,16,18,18	0
5	1PE	L	706	10/16	0.56	0.23	31,38,45,48	0
5	1PE	K	705	12/16	0.56	0.22	29,41,46,47	0
7	SO4	I	707	5/5	0.58	0.23	52,58,61,64	0
7	SO4	G	710	5/5	0.59	0.17	35,43,55,58	0
2	CO3	F	701	4/4	0.60	0.20	19,19,19,20	0
5	1PE	G	706	6/16	0.61	0.21	34,37,41,42	0
2	CO3	G	701	4/4	0.61	0.20	13,14,17,19	0
5	1PE	J	707	10/16	0.61	0.22	27,34,42,52	0
5	1PE	E	706	12/16	0.62	0.19	25,33,43,44	0
5	1PE	K	706	12/16	0.63	0.23	26,36,43,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	A	708	5/5	0.65	0.27	44,47,50,58	0
7	SO4	A	712	5/5	0.65	0.49	36,42,50,54	0
5	1PE	A	705	9/16	0.66	0.22	25,32,36,39	0
7	SO4	F	706	5/5	0.66	0.24	44,46,54,58	0
7	SO4	L	707	5/5	0.67	0.28	62,63,64,66	0
7	SO4	E	708	5/5	0.68	0.26	42,42,54,56	0
7	SO4	K	707	5/5	0.68	0.28	53,54,58,71	0
2	CO3	A	701	4/4	0.69	0.23	15,18,19,20	0
4	4ZN	D	704	20/20	0.70	0.21	13,20,27,31	3
7	SO4	A	710	5/5	0.71	0.17	36,40,54,59	0
4	4ZN	B	704	16/20	0.77	0.23	11,19,24,31	3
4	4ZN	L	704	16/20	0.78	0.19	14,18,23,27	3
7	SO4	J	709	5/5	0.78	0.38	30,33,41,44	5
2	CO3	K	701	4/4	0.78	0.23	19,19,19,21	0
2	CO3	H	701	4/4	0.78	0.15	15,16,17,19	0
4	4ZN	E	704	20/20	0.78	0.23	16,20,27,28	7
4	4ZN	K	704	14/20	0.79	0.19	14,20,28,33	0
7	SO4	D	707	5/5	0.79	0.20	42,43,57,58	0
2	CO3	D	701	4/4	0.80	0.21	16,17,18,18	0
2	CO3	I	701	4/4	0.80	0.15	15,15,16,17	0
4	4ZN	F	704	16/20	0.81	0.18	17,21,27,31	3
3	ZN	J	703	1/1	0.82	0.07	15,15,15,15	0
7	SO4	B	707	5/5	0.83	0.15	17,19,23,24	0
4	4ZN	H	704	16/20	0.83	0.20	12,18,28,32	3
4	4ZN	J	704	16/20	0.83	0.16	14,17,21,27	3
3	ZN	J	702	1/1	0.83	0.05	19,19,19,19	0
3	ZN	C	703	1/1	0.83	0.06	15,15,15,15	0
7	SO4	G	708	5/5	0.83	0.21	41,43,46,58	0
3	ZN	E	702	1/1	0.83	0.07	17,17,17,17	0
3	ZN	L	703	1/1	0.84	0.07	17,17,17,17	0
3	ZN	K	703	1/1	0.84	0.09	16,16,16,16	0
3	ZN	I	702	1/1	0.85	0.07	19,19,19,19	0
3	ZN	F	703	1/1	0.86	0.05	18,18,18,18	0
4	4ZN	C	704	16/20	0.86	0.17	15,18,23,24	4
4	4ZN	G	704	16/20	0.87	0.16	14,17,22,23	4
2	CO3	E	701	4/4	0.87	0.21	16,18,18,21	0
3	ZN	L	702	1/1	0.88	0.04	18,18,18,18	0
4	4ZN	A	704	16/20	0.89	0.16	15,17,22,23	3
3	ZN	E	703	1/1	0.89	0.06	17,17,17,17	0
4	4ZN	I	704	12/20	0.89	0.15	16,18,22,23	0
3	ZN	F	702	1/1	0.90	0.10	22,22,22,22	0
2	CO3	B	701	4/4	0.91	0.13	16,16,16,20	0

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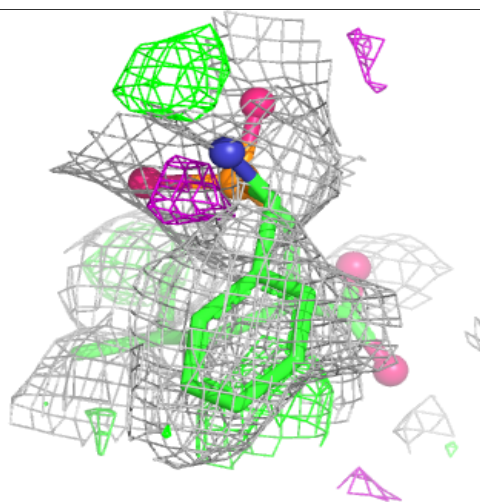
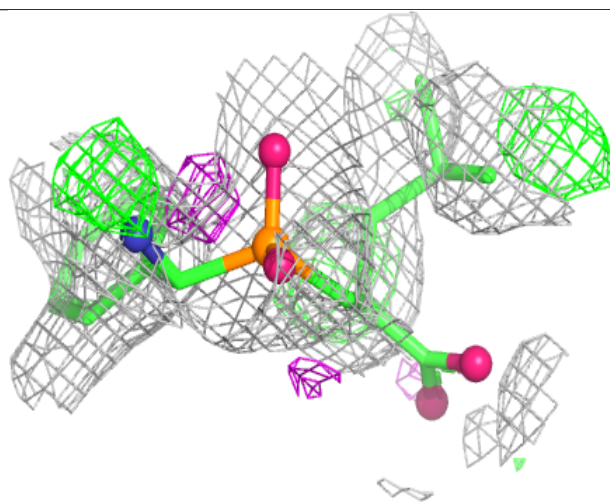
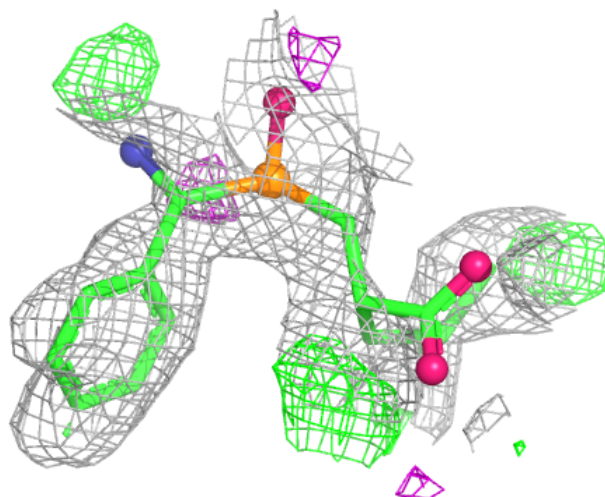
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	H	703	1/1	0.91	0.08	15,15,15,15	0
2	CO3	J	701	4/4	0.91	0.10	15,16,17,20	0
7	SO4	G	709	5/5	0.91	0.13	16,19,20,22	0
7	SO4	E	707	5/5	0.92	0.15	21,21,23,24	0
3	ZN	K	702	1/1	0.92	0.04	19,19,19,19	0
3	ZN	C	702	1/1	0.92	0.09	19,19,19,19	0
3	ZN	B	702	1/1	0.93	0.04	17,17,17,17	0
3	ZN	D	702	1/1	0.93	0.07	17,17,17,17	0
3	ZN	G	702	1/1	0.93	0.06	18,18,18,18	0
7	SO4	J	708	5/5	0.93	0.10	21,22,24,25	0
3	ZN	H	702	1/1	0.94	0.07	17,17,17,17	0
3	ZN	A	702	1/1	0.95	0.04	18,18,18,18	0
3	ZN	D	703	1/1	0.95	0.05	17,17,17,17	0
3	ZN	I	703	1/1	0.95	0.02	19,19,19,19	0
3	ZN	A	703	1/1	0.96	0.07	14,14,14,14	0
3	ZN	B	703	1/1	0.97	0.06	15,15,15,15	0
3	ZN	G	703	1/1	0.98	0.05	15,15,15,15	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.

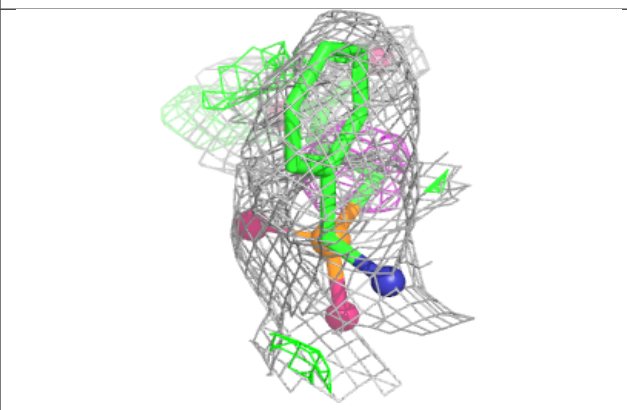
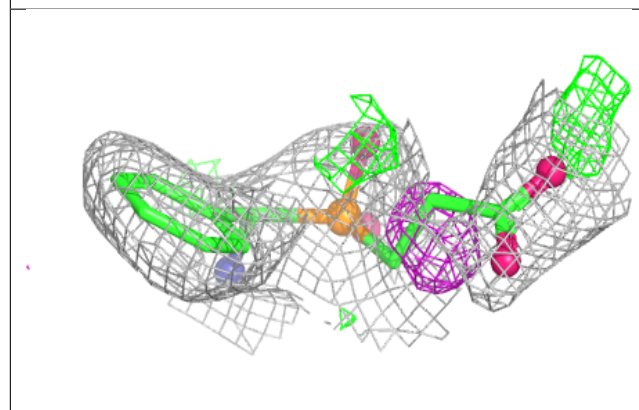
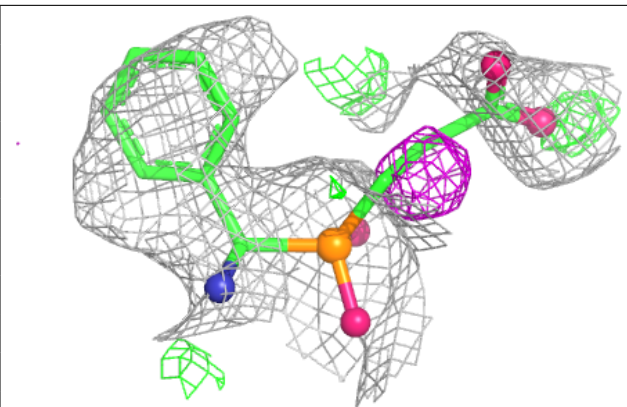
Electron density around 4ZN D 704:

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



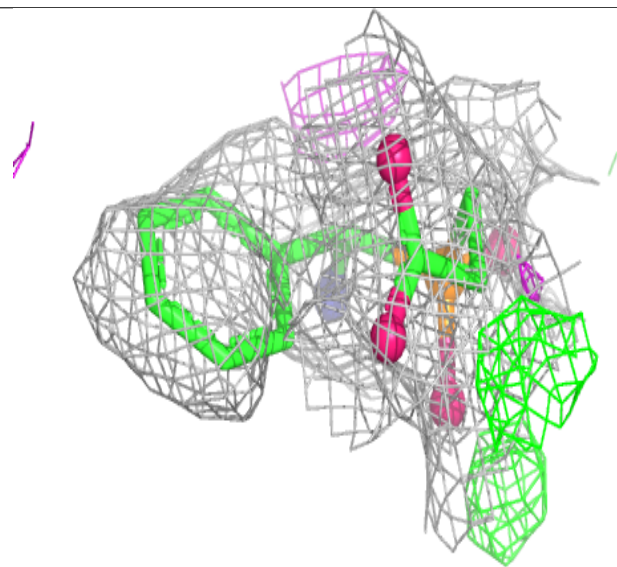
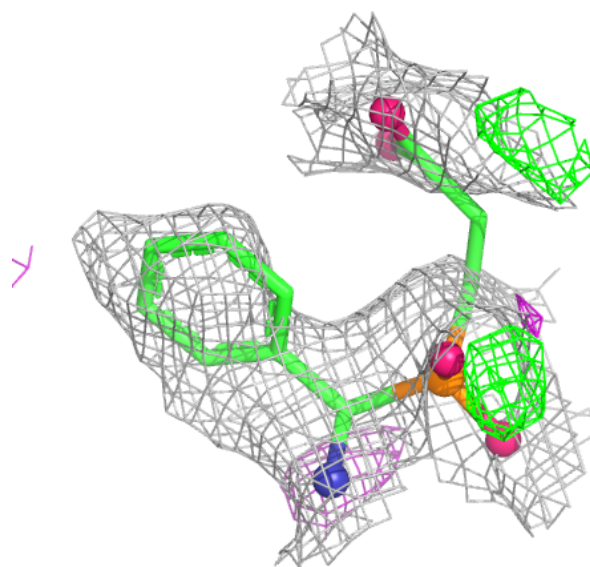
Electron density around 4ZN B 704:

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



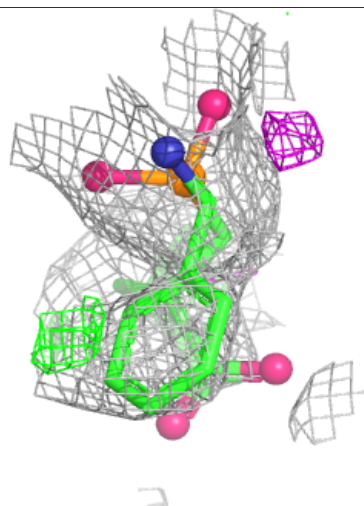
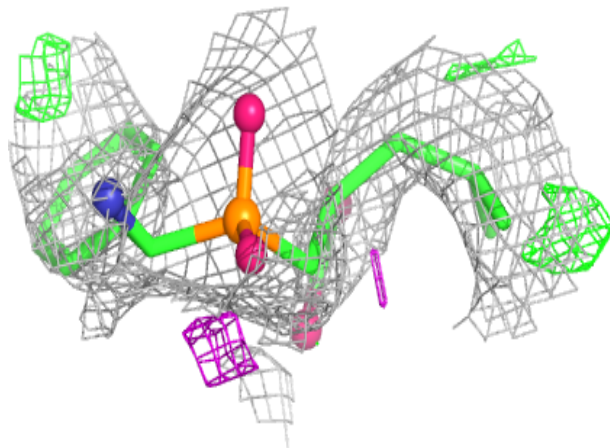
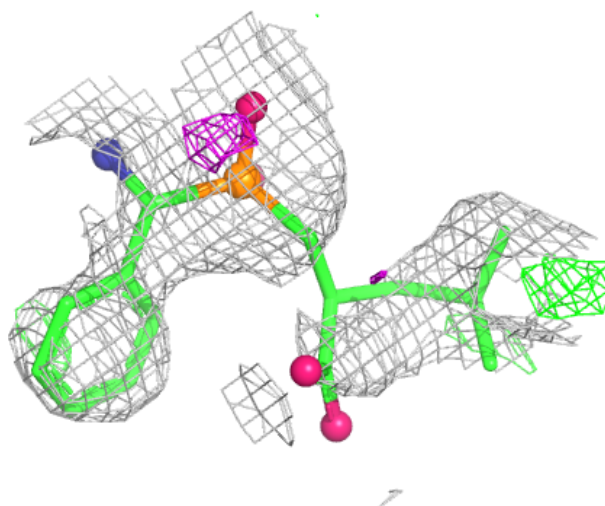
Electron density around 4ZN L 704:

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



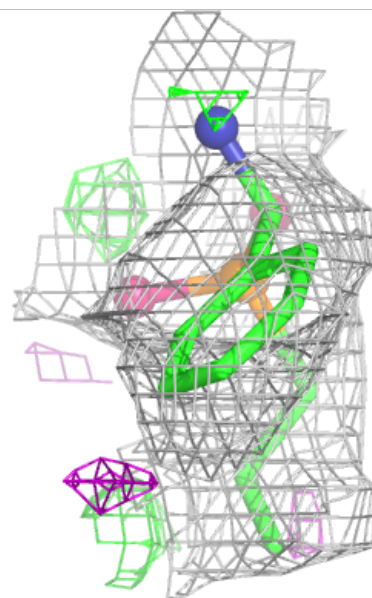
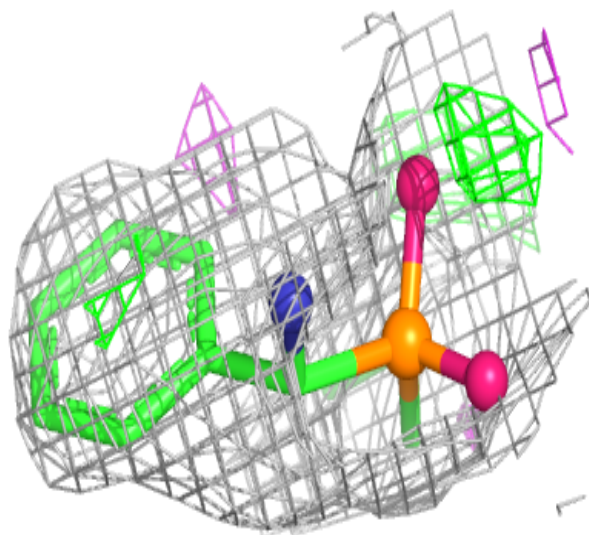
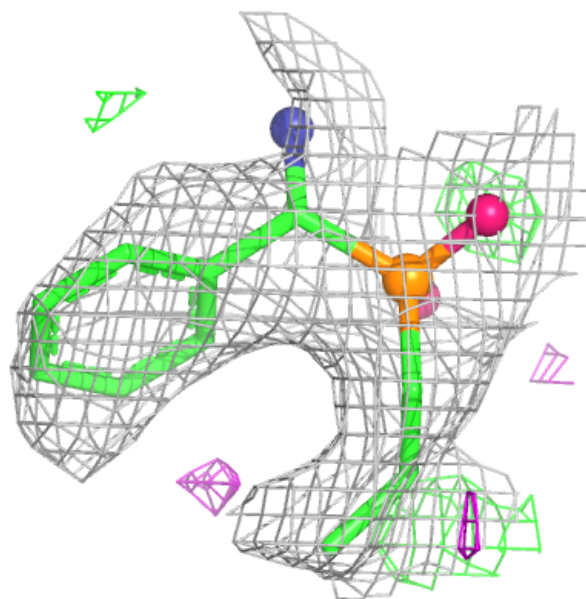
Electron density around 4ZN E 704:

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



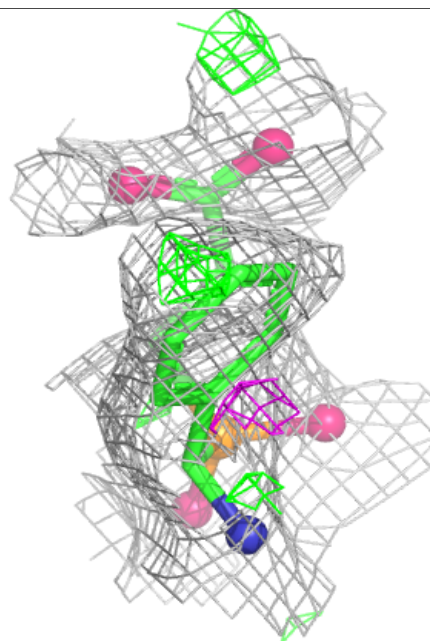
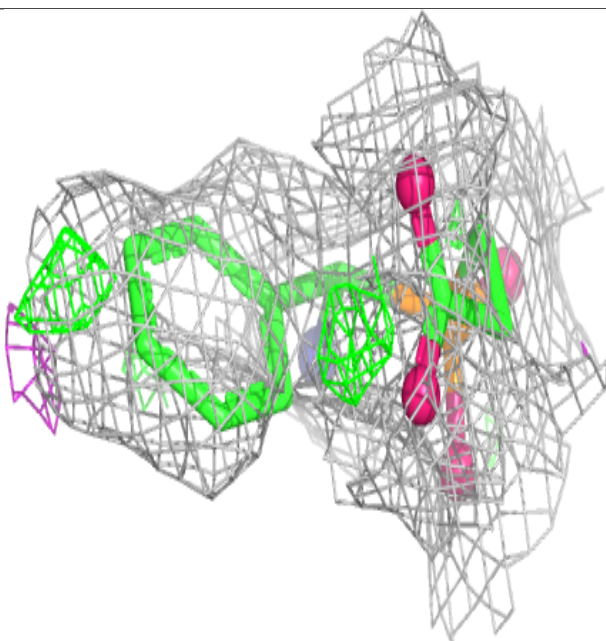
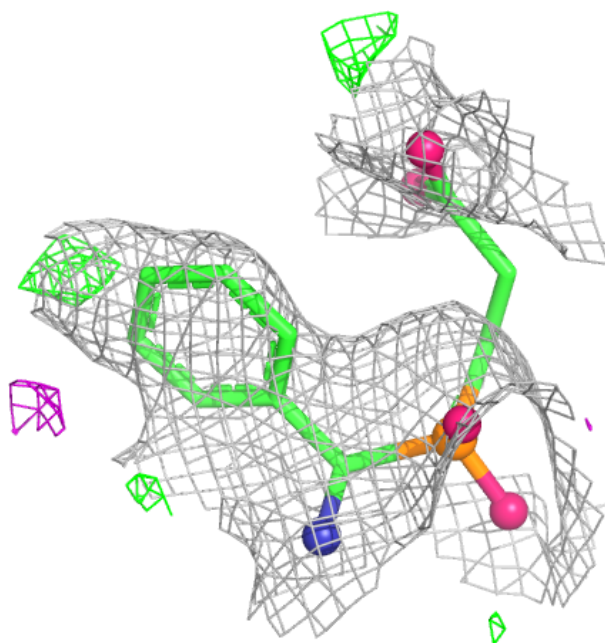
Electron density around 4ZN K 704:

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



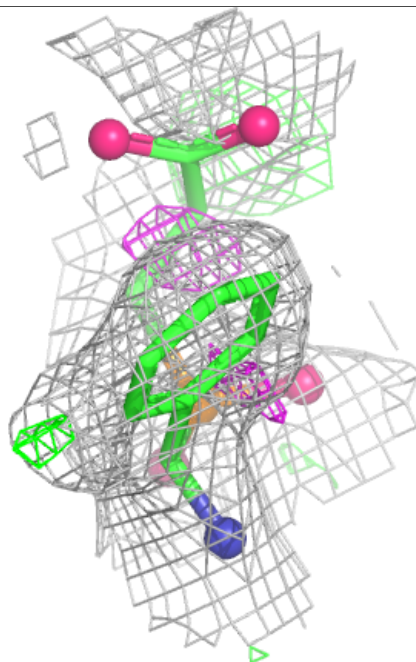
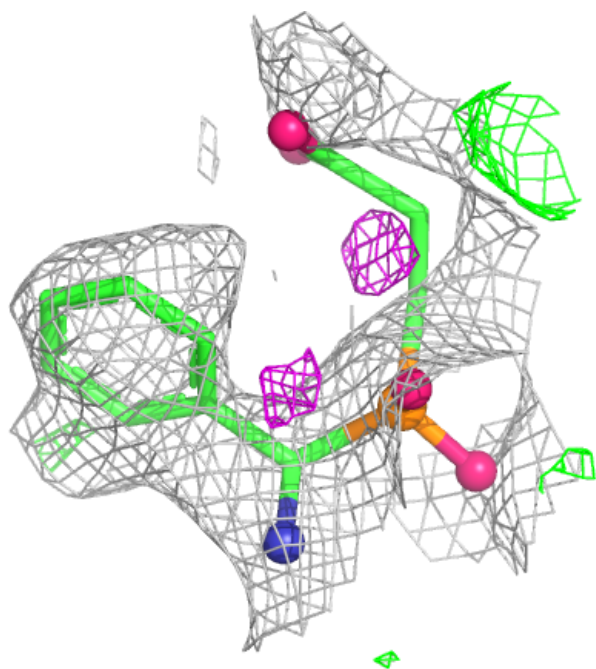
Electron density around 4ZN F 704:

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



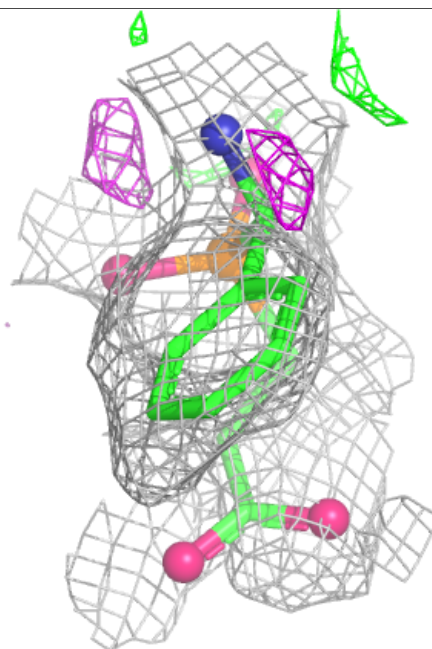
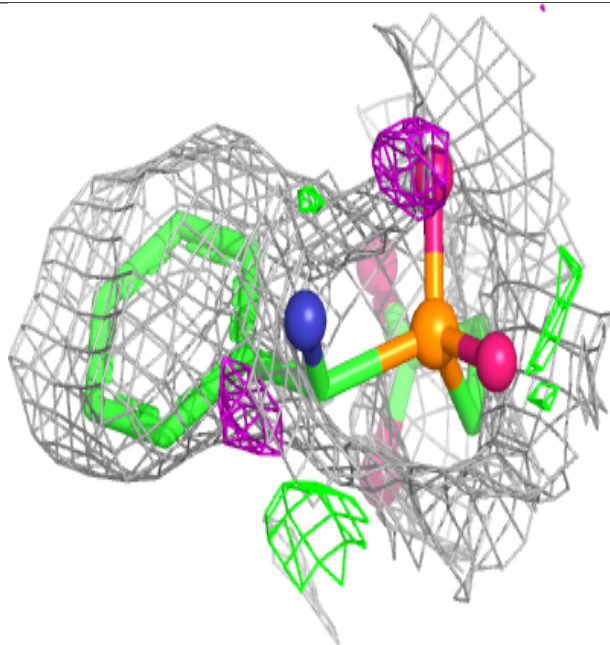
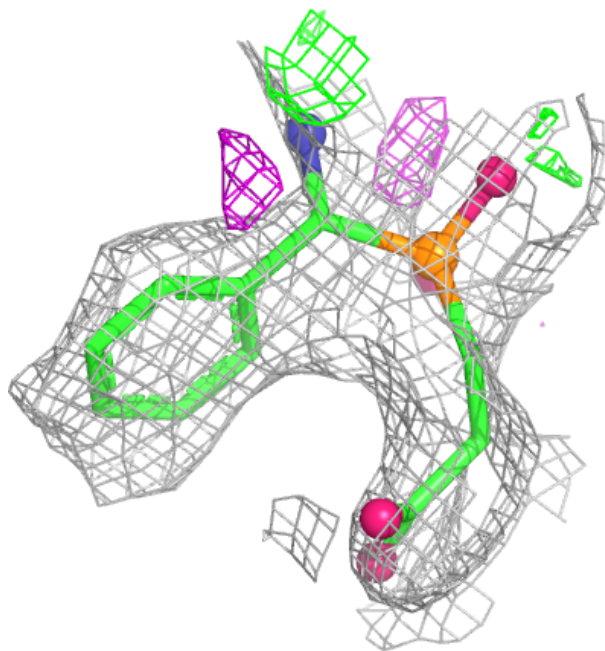
Electron density around 4ZN H 704:

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



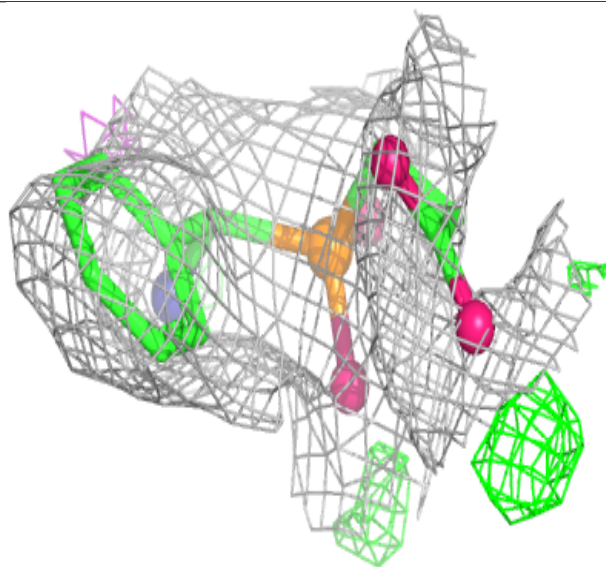
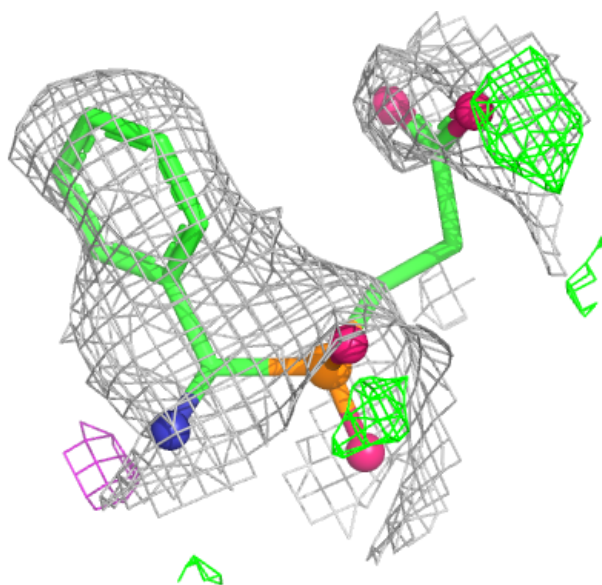
Electron density around 4ZN J 704:

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



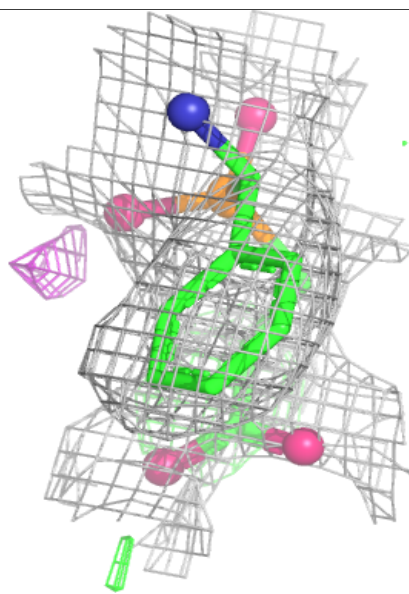
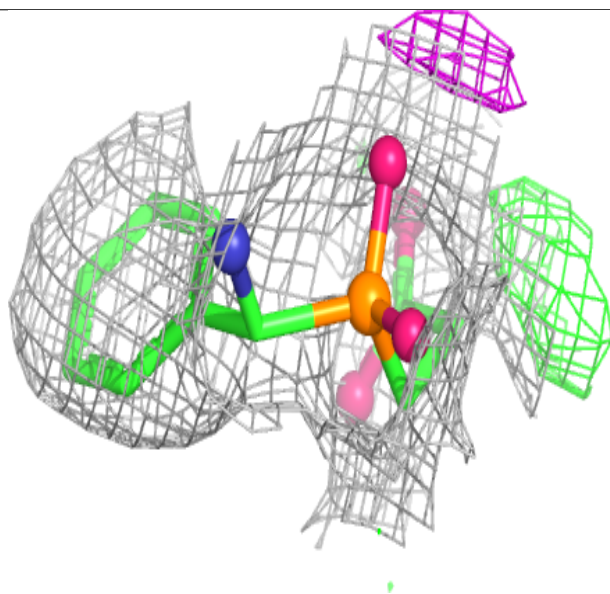
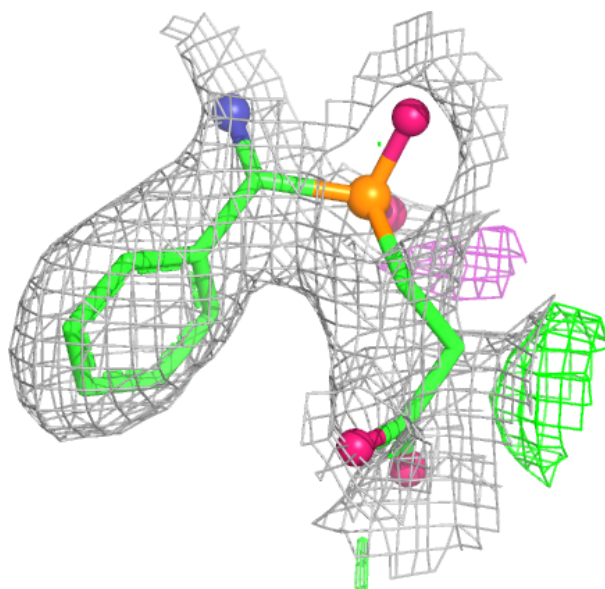
Electron density around 4ZN C 704:

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and green (positive)



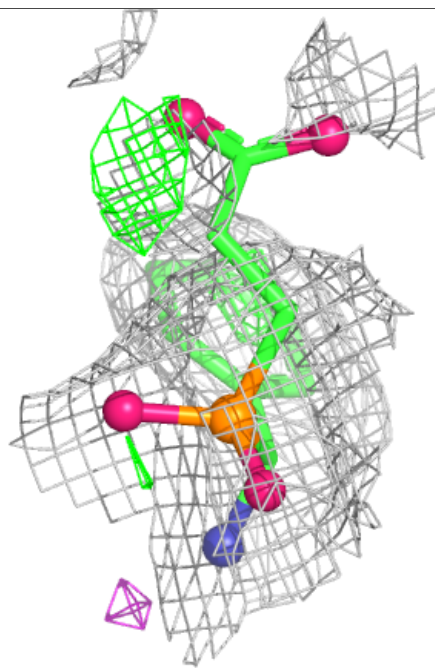
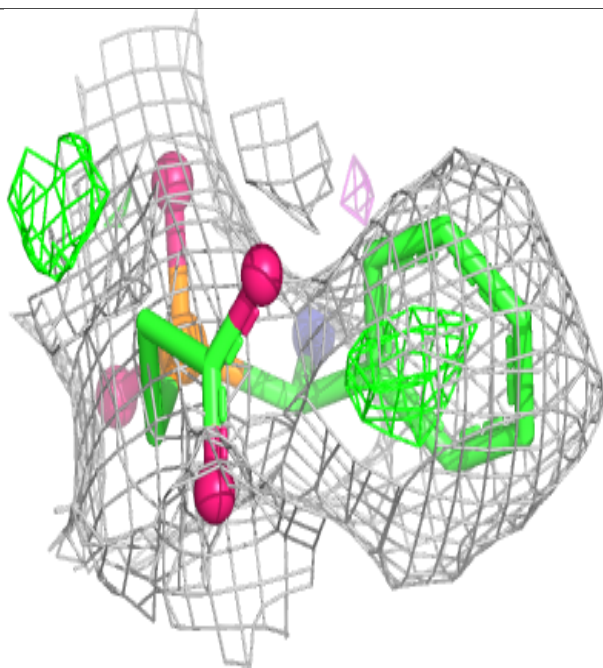
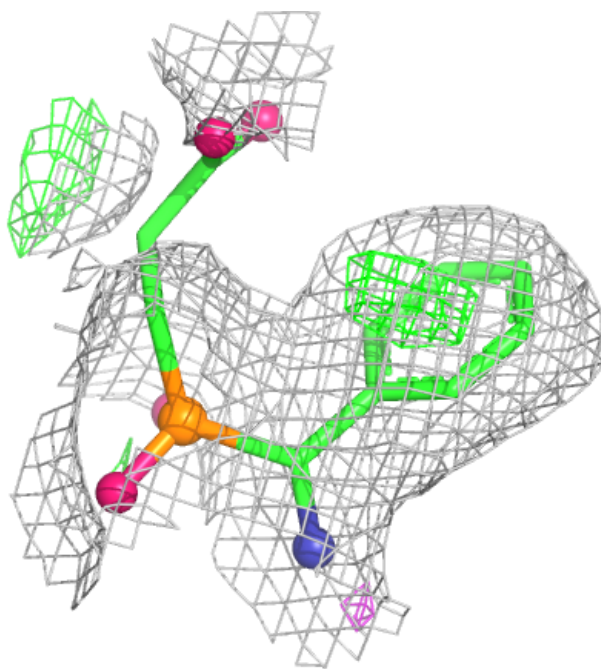
Electron density around 4ZN G 704:

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



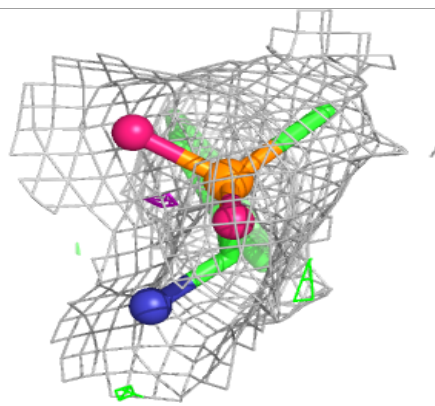
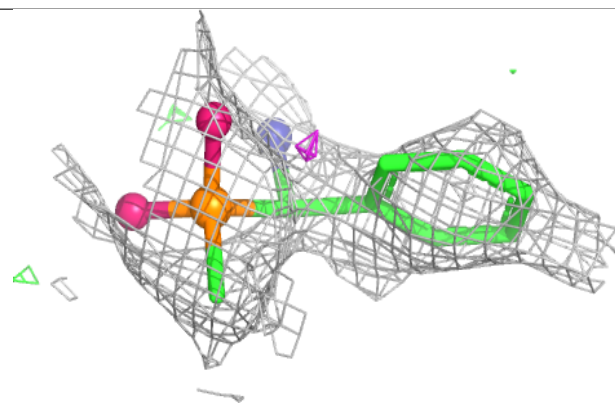
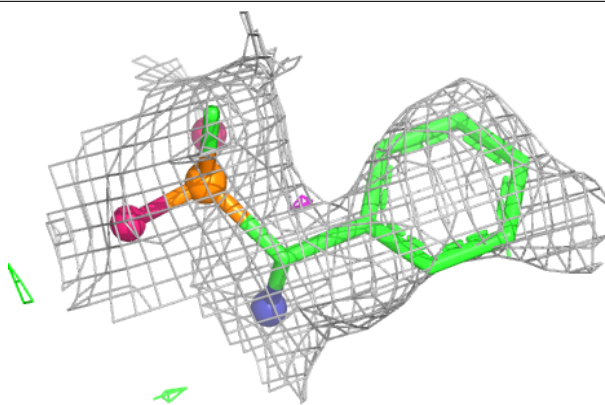
Electron density around 4ZN A 704:

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



Electron density around 4ZN I 704:

$2mF_o - DF_c$ (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.