



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 04:36 PM EST

PDB ID : 4QF0  
Title : Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains, quadruple mutant, P21212 form  
Authors : Lai, Y.-T.; Yeates, T.O.  
Deposited on : 2014-05-19  
Resolution : 6.49 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

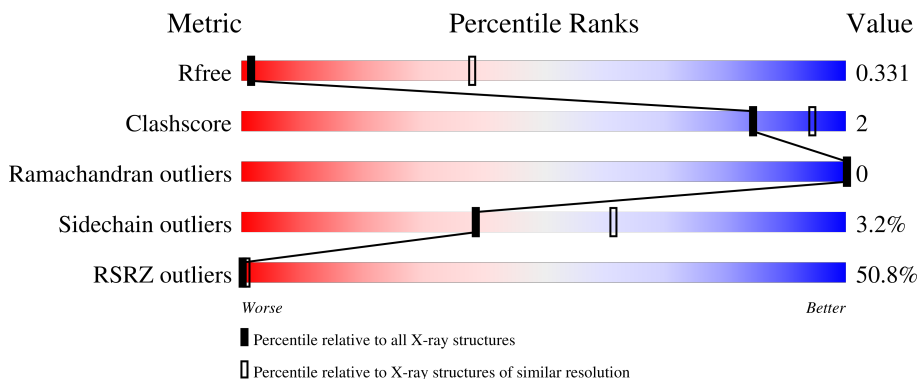
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.49 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))
$R_{free}$	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)
RSRZ outliers	127900	1002 (9.00-3.80)

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  $\geq 3$ , 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	456	
1	B	456	
1	C	456	
1	D	456	
1	E	456	

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Mol	Chain	Length	Quality of chain
1	F	456	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '46%', a green segment in the middle labeled '88%', and a yellow segment on the right labeled '9%'. A small grey dot is visible at the far right end of the bar.</p>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 20256 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 Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	441	3376	2151	569	648	8	0	0	0
1	B	441	3376	2151	569	648	8	0	0	0
1	C	441	3376	2151	569	648	8	0	0	0
1	D	441	3376	2151	569	648	8	0	0	0
1	E	441	3376	2151	569	648	8	0	0	0
1	F	441	3376	2151	569	648	8	0	0	0

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	GLN	engineered mutation	UNP P29715
A	51	ALA	TYR	engineered mutation	UNP P29715
A	118	ALA	LYS	engineered mutation	UNP P29715
A	278	ALA	-	linker	UNP P03485
A	279	GLN	-	linker	UNP P03485
A	280	GLU	-	linker	UNP P03485
A	281	ALA	-	linker	UNP P03485
A	282	GLN	-	linker	UNP P03485
A	283	LYS	-	linker	UNP P03485
A	284	GLN	-	linker	UNP P03485
A	285	LYS	-	linker	UNP P03485
A	448	LEU	-	expression tag	UNP P03485
A	449	GLU	-	expression tag	UNP P03485
A	450	HIS	-	expression tag	UNP P03485
A	451	HIS	-	expression tag	UNP P03485
A	452	HIS	-	expression tag	UNP P03485
A	453	HIS	-	expression tag	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
A	454	HIS	-	expression tag	UNP P03485
A	455	HIS	-	expression tag	UNP P03485
B	24	THR	GLN	engineered mutation	UNP P29715
B	51	ALA	TYR	engineered mutation	UNP P29715
B	118	ALA	LYS	engineered mutation	UNP P29715
B	278	ALA	-	linker	UNP P03485
B	279	GLN	-	linker	UNP P03485
B	280	GLU	-	linker	UNP P03485
B	281	ALA	-	linker	UNP P03485
B	282	GLN	-	linker	UNP P03485
B	283	LYS	-	linker	UNP P03485
B	284	GLN	-	linker	UNP P03485
B	285	LYS	-	linker	UNP P03485
B	448	LEU	-	expression tag	UNP P03485
B	449	GLU	-	expression tag	UNP P03485
B	450	HIS	-	expression tag	UNP P03485
B	451	HIS	-	expression tag	UNP P03485
B	452	HIS	-	expression tag	UNP P03485
B	453	HIS	-	expression tag	UNP P03485
B	454	HIS	-	expression tag	UNP P03485
B	455	HIS	-	expression tag	UNP P03485
C	24	THR	GLN	engineered mutation	UNP P29715
C	51	ALA	TYR	engineered mutation	UNP P29715
C	118	ALA	LYS	engineered mutation	UNP P29715
C	278	ALA	-	linker	UNP P03485
C	279	GLN	-	linker	UNP P03485
C	280	GLU	-	linker	UNP P03485
C	281	ALA	-	linker	UNP P03485
C	282	GLN	-	linker	UNP P03485
C	283	LYS	-	linker	UNP P03485
C	284	GLN	-	linker	UNP P03485
C	285	LYS	-	linker	UNP P03485
C	448	LEU	-	expression tag	UNP P03485
C	449	GLU	-	expression tag	UNP P03485
C	450	HIS	-	expression tag	UNP P03485
C	451	HIS	-	expression tag	UNP P03485
C	452	HIS	-	expression tag	UNP P03485
C	453	HIS	-	expression tag	UNP P03485
C	454	HIS	-	expression tag	UNP P03485
C	455	HIS	-	expression tag	UNP P03485
D	24	THR	GLN	engineered mutation	UNP P29715
D	51	ALA	TYR	engineered mutation	UNP P29715

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Chain	Residue	Modelled	Actual	Comment	Reference
D	118	ALA	LYS	engineered mutation	UNP P29715
D	278	ALA	-	linker	UNP P03485
D	279	GLN	-	linker	UNP P03485
D	280	GLU	-	linker	UNP P03485
D	281	ALA	-	linker	UNP P03485
D	282	GLN	-	linker	UNP P03485
D	283	LYS	-	linker	UNP P03485
D	284	GLN	-	linker	UNP P03485
D	285	LYS	-	linker	UNP P03485
D	448	LEU	-	expression tag	UNP P03485
D	449	GLU	-	expression tag	UNP P03485
D	450	HIS	-	expression tag	UNP P03485
D	451	HIS	-	expression tag	UNP P03485
D	452	HIS	-	expression tag	UNP P03485
D	453	HIS	-	expression tag	UNP P03485
D	454	HIS	-	expression tag	UNP P03485
D	455	HIS	-	expression tag	UNP P03485
E	24	THR	GLN	engineered mutation	UNP P29715
E	51	ALA	TYR	engineered mutation	UNP P29715
E	118	ALA	LYS	engineered mutation	UNP P29715
E	278	ALA	-	linker	UNP P03485
E	279	GLN	-	linker	UNP P03485
E	280	GLU	-	linker	UNP P03485
E	281	ALA	-	linker	UNP P03485
E	282	GLN	-	linker	UNP P03485
E	283	LYS	-	linker	UNP P03485
E	284	GLN	-	linker	UNP P03485
E	285	LYS	-	linker	UNP P03485
E	448	LEU	-	expression tag	UNP P03485
E	449	GLU	-	expression tag	UNP P03485
E	450	HIS	-	expression tag	UNP P03485
E	451	HIS	-	expression tag	UNP P03485
E	452	HIS	-	expression tag	UNP P03485
E	453	HIS	-	expression tag	UNP P03485
E	454	HIS	-	expression tag	UNP P03485
E	455	HIS	-	expression tag	UNP P03485
F	24	THR	GLN	engineered mutation	UNP P29715
F	51	ALA	TYR	engineered mutation	UNP P29715
F	118	ALA	LYS	engineered mutation	UNP P29715
F	278	ALA	-	linker	UNP P03485
F	279	GLN	-	linker	UNP P03485
F	280	GLU	-	linker	UNP P03485

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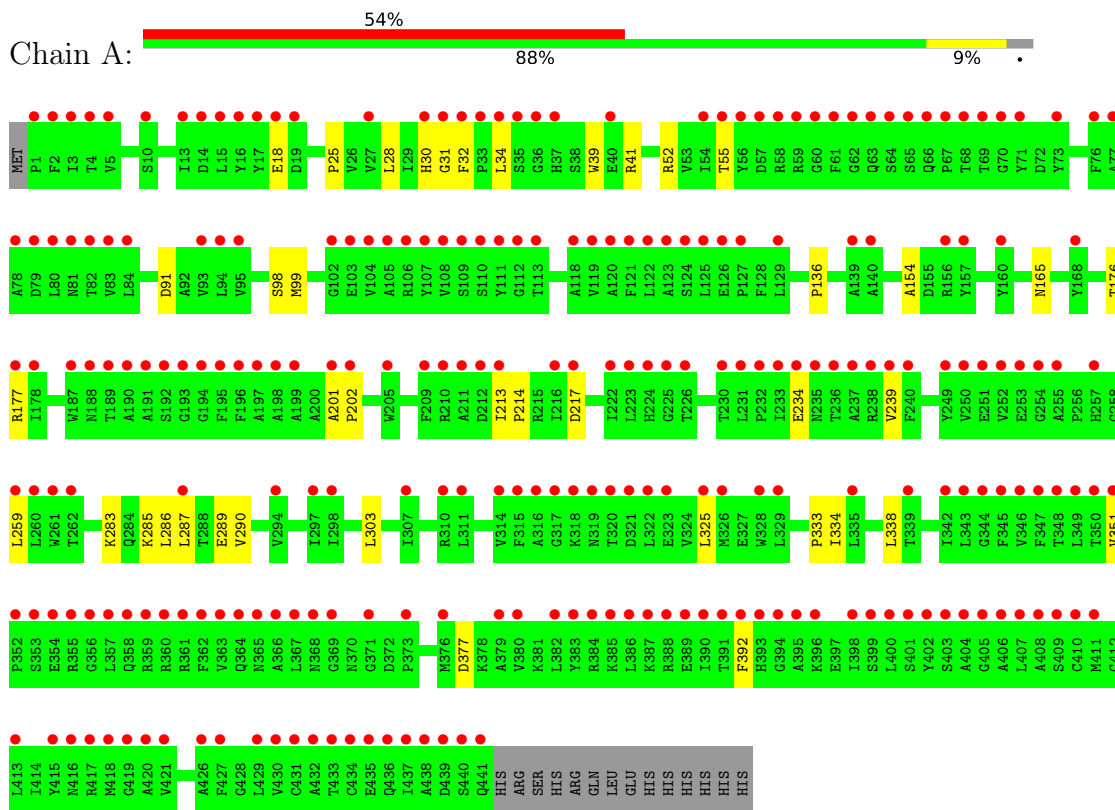
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Chain	Residue	Modelled	Actual	Comment	Reference
F	281	ALA	-	linker	UNP P03485
F	282	GLN	-	linker	UNP P03485
F	283	LYS	-	linker	UNP P03485
F	284	GLN	-	linker	UNP P03485
F	285	LYS	-	linker	UNP P03485
F	448	LEU	-	expression tag	UNP P03485
F	449	GLU	-	expression tag	UNP P03485
F	450	HIS	-	expression tag	UNP P03485
F	451	HIS	-	expression tag	UNP P03485
F	452	HIS	-	expression tag	UNP P03485
F	453	HIS	-	expression tag	UNP P03485
F	454	HIS	-	expression tag	UNP P03485
F	455	HIS	-	expression tag	UNP P03485

### 3 Residue-property plots i

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: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

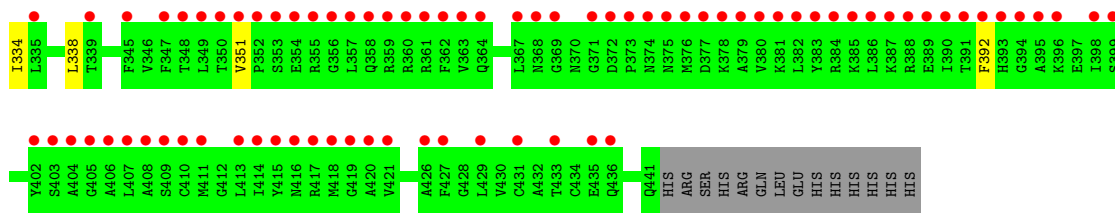


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

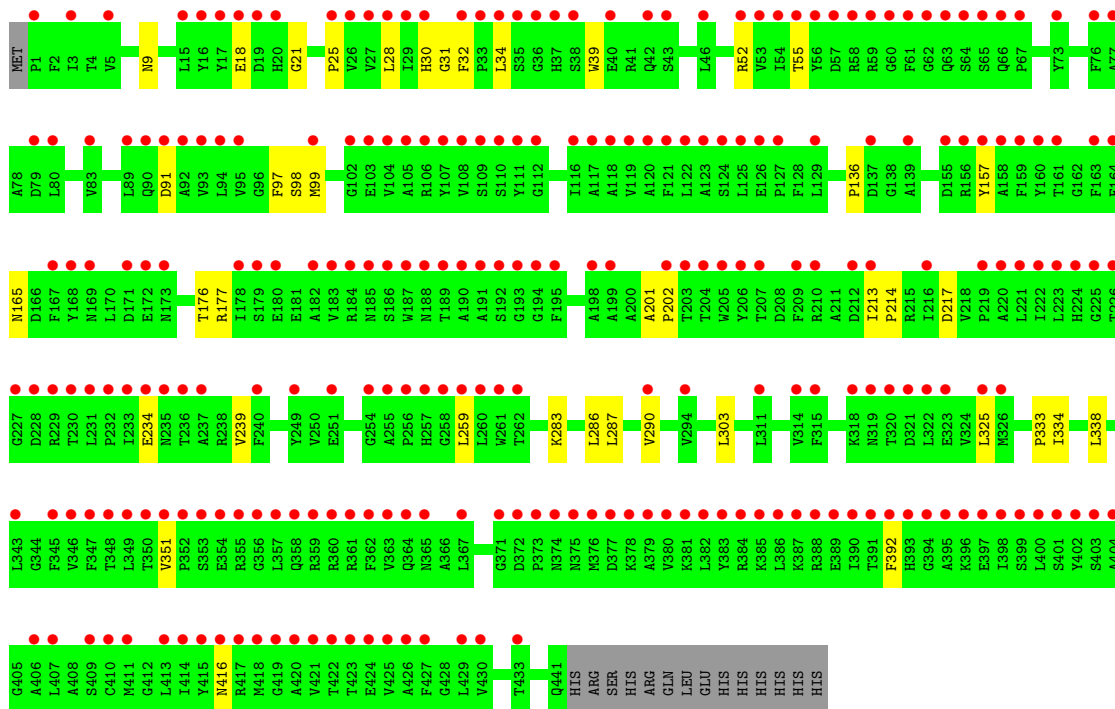
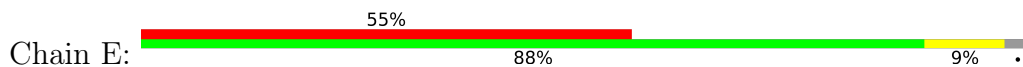




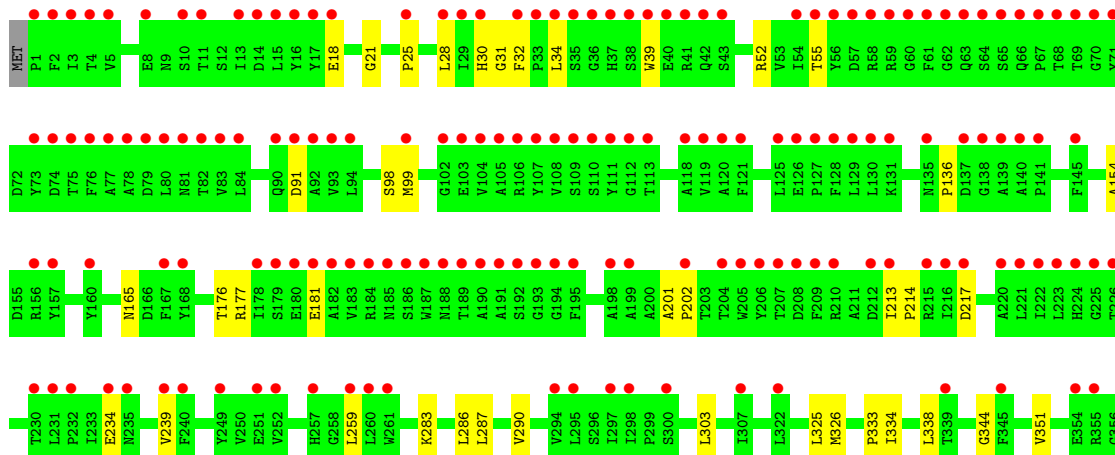
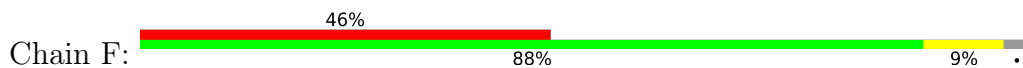


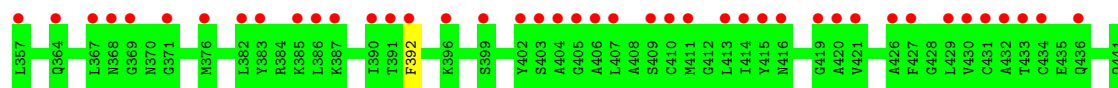


• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera



• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera





HIS
ARG
SER
HIS
HIS
ARG
GLN
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.50Å 147.73Å 167.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.71 – 6.49 93.71 – 6.49	Depositor EDS
% Data completeness (in resolution range)	99.6 (93.71-6.49) 99.6 (93.71-6.49)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 6.72Å)	Xtrriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.271 , 0.324 0.273 , 0.331	Depositor DCC
$R_{free}$ test set	451 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	398.2	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 410.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.003 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	20256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	313.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.41	0/3452	0.55	0/4702
1	B	0.40	0/3452	0.56	0/4702
1	C	0.41	0/3452	0.56	0/4702
1	D	0.40	0/3452	0.56	0/4702
1	E	0.40	0/3452	0.56	0/4702
1	F	0.41	0/3452	0.56	0/4702
All	All	0.40	0/20712	0.56	0/28212

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3376	0	3286	16	0
1	B	3376	0	3286	16	0
1	C	3376	0	3286	15	0
1	D	3376	0	3286	16	0
1	E	3376	0	3286	18	0
1	F	3376	0	3286	18	0
All	All	20256	0	19716	92	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 2.

All (92) 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:F:30:HIS:CE1	1:F:34:LEU:O	2.28	0.85
1:B:30:HIS:CE1	1:B:34:LEU:O	2.32	0.82
1:A:30:HIS:CE1	1:A:34:LEU:O	2.33	0.81
1:C:30:HIS:CE1	1:C:34:LEU:O	2.33	0.81
1:E:30:HIS:CE1	1:E:34:LEU:O	2.38	0.77
1:D:30:HIS:CE1	1:D:34:LEU:O	2.39	0.75
1:F:283:LYS:O	1:F:287:LEU:HG	1.92	0.69
1:E:283:LYS:O	1:E:287:LEU:HG	1.97	0.64
1:D:283:LYS:O	1:D:287:LEU:HG	1.98	0.64
1:A:283:LYS:O	1:A:287:LEU:HG	1.98	0.64
1:C:283:LYS:O	1:C:287:LEU:HG	1.99	0.62
1:A:286:LEU:O	1:A:290:VAL:HG23	2.02	0.59
1:B:286:LEU:O	1:B:290:VAL:HG23	2.02	0.59
1:D:333:PRO:O	1:D:334:ILE:HG12	2.02	0.59
1:B:333:PRO:O	1:B:334:ILE:HG12	2.02	0.59
1:D:286:LEU:O	1:D:290:VAL:HG23	2.03	0.59
1:E:286:LEU:O	1:E:290:VAL:HG23	2.02	0.59
1:F:286:LEU:O	1:F:290:VAL:HG23	2.02	0.59
1:A:333:PRO:O	1:A:334:ILE:HG12	2.03	0.59
1:B:283:LYS:O	1:B:287:LEU:HG	2.02	0.59
1:C:333:PRO:O	1:C:334:ILE:HG12	2.03	0.59
1:E:157:TYR:HB3	1:F:181:GLU:HB3	1.84	0.59
1:C:286:LEU:O	1:C:290:VAL:HG23	2.03	0.58
1:E:333:PRO:O	1:E:334:ILE:HG12	2.02	0.58
1:F:333:PRO:O	1:F:334:ILE:HG12	2.07	0.54
1:C:176:THR:HG22	1:C:177:ARG:HG3	1.93	0.51
1:D:176:THR:HG22	1:D:177:ARG:HG3	1.92	0.51
1:F:176:THR:HG22	1:F:177:ARG:HG3	1.93	0.51
1:E:176:THR:HG22	1:E:177:ARG:HG3	1.93	0.50
1:B:176:THR:HG22	1:B:177:ARG:HG3	1.93	0.50
1:A:176:THR:HG22	1:A:177:ARG:HG3	1.93	0.49
1:A:41:ARG:NH2	1:C:154:ALA:O	2.38	0.49
1:A:32:PHE:HB2	1:A:99:MET:SD	2.53	0.49
1:E:32:PHE:HB2	1:E:99:MET:SD	2.53	0.48
1:C:32:PHE:HB2	1:C:99:MET:SD	2.53	0.48
1:F:32:PHE:HB2	1:F:99:MET:SD	2.53	0.48
1:D:32:PHE:HB2	1:D:99:MET:SD	2.54	0.48
1:B:32:PHE:HB2	1:B:99:MET:SD	2.53	0.47
1:B:418:MET:SD	1:E:416:ASN:ND2	2.86	0.47
1:D:41:ARG:NH2	1:F:154:ALA:O	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:HIS:ND1	1:F:34:LEU:O	2.48	0.47
1:A:154:ALA:O	1:B:41:ARG:NH2	2.36	0.45
1:B:285:LYS:O	1:B:289:GLU:HG3	2.17	0.44
1:F:28:LEU:HB3	1:F:39:TRP:CE2	2.53	0.44
1:D:31:GLY:HA3	1:D:98:SER:HB3	2.00	0.44
1:B:213:ILE:N	1:B:214:PRO:CD	2.81	0.44
1:A:28:LEU:HB3	1:A:39:TRP:CE2	2.53	0.43
1:B:31:GLY:HA3	1:B:98:SER:HB3	2.00	0.43
1:A:213:ILE:N	1:A:214:PRO:CD	2.81	0.43
1:B:18:GLU:HB2	1:B:55:THR:OG1	2.18	0.43
1:E:31:GLY:HA3	1:E:98:SER:HB3	2.00	0.43
1:A:286:LEU:HD11	1:A:392:PHE:CG	2.53	0.43
1:C:18:GLU:HB2	1:C:55:THR:OG1	2.19	0.43
1:F:326:MET:HE1	1:F:344:GLY:HA2	2.01	0.43
1:A:18:GLU:HB2	1:A:55:THR:OG1	2.19	0.43
1:E:201:ALA:HB3	1:E:202:PRO:HD3	2.01	0.43
1:D:18:GLU:HB2	1:D:55:THR:OG1	2.19	0.43
1:B:28:LEU:HB3	1:B:39:TRP:CE2	2.53	0.43
1:E:18:GLU:HB2	1:E:55:THR:OG1	2.19	0.43
1:F:213:ILE:N	1:F:214:PRO:CD	2.82	0.43
1:A:25:PRO:HA	1:A:52:ARG:HB3	2.01	0.43
1:D:25:PRO:HA	1:D:52:ARG:HB3	2.01	0.43
1:D:286:LEU:HD11	1:D:392:PHE:CG	2.54	0.43
1:A:31:GLY:HA3	1:A:98:SER:HB3	2.01	0.43
1:D:201:ALA:HB3	1:D:202:PRO:HD3	2.01	0.43
1:D:28:LEU:HB3	1:D:39:TRP:CE2	2.54	0.42
1:E:28:LEU:HB3	1:E:39:TRP:CE2	2.53	0.42
1:F:286:LEU:HD11	1:F:392:PHE:CG	2.53	0.42
1:F:18:GLU:HB2	1:F:55:THR:OG1	2.19	0.42
1:F:25:PRO:HA	1:F:52:ARG:HB3	2.01	0.42
1:F:31:GLY:HA3	1:F:98:SER:HB3	2.01	0.42
1:C:28:LEU:HB3	1:C:39:TRP:CE2	2.54	0.42
1:D:213:ILE:N	1:D:214:PRO:CD	2.81	0.42
1:B:286:LEU:HD11	1:B:392:PHE:CG	2.55	0.42
1:A:201:ALA:HB3	1:A:202:PRO:HD3	2.02	0.42
1:C:31:GLY:HA3	1:C:98:SER:HB3	2.00	0.42
1:C:213:ILE:N	1:C:214:PRO:CD	2.82	0.42
1:E:213:ILE:N	1:E:214:PRO:CD	2.82	0.42
1:F:201:ALA:HB3	1:F:202:PRO:HD3	2.01	0.42
1:E:25:PRO:HA	1:E:52:ARG:HB3	2.02	0.42
1:D:9:ASN:ND2	1:E:21:GLY:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:ASN:ND2	1:F:21:GLY:O	2.51	0.41
1:B:201:ALA:HB3	1:B:202:PRO:HD3	2.01	0.41
1:C:201:ALA:HB3	1:C:202:PRO:HD3	2.01	0.41
1:B:25:PRO:HA	1:B:52:ARG:HB3	2.01	0.41
1:A:285:LYS:O	1:A:289:GLU:HG3	2.21	0.41
1:C:25:PRO:HA	1:C:52:ARG:HB3	2.02	0.41
1:C:286:LEU:HD11	1:C:392:PHE:CG	2.56	0.41
1:D:285:LYS:O	1:D:289:GLU:HG3	2.21	0.41
1:E:286:LEU:HD11	1:E:392:PHE:CG	2.55	0.41
1:E:97:PHE:O	1:E:98:SER:C	2.60	0.40
1:C:326:MET:HE1	1:C:344:GLY:HA2	2.03	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	439/456 (96%)	413 (94%)	26 (6%)	0	100	100
1	B	439/456 (96%)	413 (94%)	26 (6%)	0	100	100
1	C	439/456 (96%)	414 (94%)	25 (6%)	0	100	100
1	D	439/456 (96%)	413 (94%)	26 (6%)	0	100	100
1	E	439/456 (96%)	414 (94%)	25 (6%)	0	100	100
1	F	439/456 (96%)	414 (94%)	25 (6%)	0	100	100
All	All	2634/2736 (96%)	2481 (94%)	153 (6%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/369 (94%)	336 (97%)	12 (3%)	37	60
1	B	348/369 (94%)	337 (97%)	11 (3%)	39	61
1	C	348/369 (94%)	337 (97%)	11 (3%)	39	61
1	D	348/369 (94%)	337 (97%)	11 (3%)	39	61
1	E	348/369 (94%)	337 (97%)	11 (3%)	39	61
1	F	348/369 (94%)	337 (97%)	11 (3%)	39	61
All	All	2088/2214 (94%)	2021 (97%)	67 (3%)	39	61

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASP
1	A	136	PRO
1	A	165	ASN
1	A	217	ASP
1	A	234	GLU
1	A	239	VAL
1	A	259	LEU
1	A	303	LEU
1	A	325	LEU
1	A	338	LEU
1	A	351	VAL
1	A	377	ASP
1	B	91	ASP
1	B	136	PRO
1	B	165	ASN
1	B	217	ASP
1	B	234	GLU
1	B	239	VAL
1	B	259	LEU
1	B	303	LEU
1	B	325	LEU
1	B	338	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	351	VAL
1	C	91	ASP
1	C	136	PRO
1	C	165	ASN
1	C	217	ASP
1	C	234	GLU
1	C	239	VAL
1	C	259	LEU
1	C	303	LEU
1	C	325	LEU
1	C	338	LEU
1	C	351	VAL
1	D	91	ASP
1	D	136	PRO
1	D	165	ASN
1	D	217	ASP
1	D	234	GLU
1	D	239	VAL
1	D	259	LEU
1	D	303	LEU
1	D	325	LEU
1	D	338	LEU
1	D	351	VAL
1	E	91	ASP
1	E	136	PRO
1	E	165	ASN
1	E	217	ASP
1	E	234	GLU
1	E	239	VAL
1	E	259	LEU
1	E	303	LEU
1	E	325	LEU
1	E	338	LEU
1	E	351	VAL
1	F	91	ASP
1	F	136	PRO
1	F	165	ASN
1	F	217	ASP
1	F	234	GLU
1	F	239	VAL
1	F	259	LEU
1	F	303	LEU

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Mol	Chain	Res	Type
1	F	325	LEU
1	F	338	LEU
1	F	351	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	B	188	ASN
1	C	188	ASN
1	D	188	ASN
1	E	188	ASN
1	F	188	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	441/456 (96%)	2.63	244 (55%) 0 0	121, 325, 340, 340	0
1	B	441/456 (96%)	2.21	215 (48%) 0 1	122, 314, 340, 340	0
1	C	441/456 (96%)	1.87	169 (38%) 0 1	122, 313, 340, 340	0
1	D	441/456 (96%)	2.96	258 (58%) 0 0	122, 321, 340, 340	0
1	E	441/456 (96%)	2.71	251 (56%) 0 0	122, 320, 340, 340	0
1	F	441/456 (96%)	2.18	208 (47%) 0 1	121, 317, 340, 340	0
All	All	2646/2736 (96%)	2.43	1345 (50%) 0 1	121, 318, 340, 340	0

All (1345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	358	GLN	14.3
1	A	359	ARG	14.1
1	D	33	PRO	14.0
1	A	66	GLN	13.5
1	B	359	ARG	13.2
1	A	65	SER	12.8
1	D	359	ARG	12.8
1	E	419	GLY	12.6
1	A	59	ARG	12.2
1	D	193	GLY	12.1
1	A	358	GLN	12.0
1	E	359	ARG	11.6
1	D	59	ARG	11.5
1	E	55	THR	11.4
1	A	60	GLY	11.4
1	D	66	GLN	11.3
1	E	420	ALA	11.3
1	F	59	ARG	11.3
1	E	358	GLN	10.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	66	GLN	10.8
1	F	65	SER	10.8
1	A	33	PRO	10.8
1	A	251	GLU	10.7
1	F	33	PRO	10.5
1	D	58	ARG	10.4
1	D	37	HIS	10.2
1	D	60	GLY	10.0
1	D	357	LEU	9.8
1	B	358	GLN	9.8
1	D	191	ALA	9.8
1	D	34	LEU	9.5
1	D	113	THR	9.5
1	C	33	PRO	9.5
1	C	225	GLY	9.4
1	E	18	GLU	9.4
1	E	56	TYR	9.4
1	D	35	SER	9.3
1	C	59	ARG	9.3
1	A	62	GLY	9.3
1	D	194	GLY	9.2
1	E	421	VAL	9.1
1	D	61	PHE	9.0
1	A	67	PRO	8.9
1	D	224	HIS	8.7
1	C	56	TYR	8.7
1	E	418	MET	8.6
1	A	357	LEU	8.5
1	F	62	GLY	8.5
1	D	124	SER	8.5
1	D	62	GLY	8.5
1	E	124	SER	8.4
1	F	60	GLY	8.4
1	D	103	GLU	8.4
1	D	18	GLU	8.3
1	D	112	GLY	8.3
1	A	61	PHE	8.2
1	B	389	GLU	8.2
1	D	125	LEU	8.1
1	B	126	GLU	8.1
1	F	37	HIS	8.0
1	E	37	HIS	8.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	224	HIS	8.0
1	A	56	TYR	7.9
1	D	32	PHE	7.8
1	D	251	GLU	7.8
1	D	65	SER	7.8
1	D	30	HIS	7.7
1	A	224	HIS	7.7
1	C	419	GLY	7.6
1	D	31	GLY	7.6
1	D	108	VAL	7.6
1	A	58	ARG	7.6
1	E	57	ASP	7.5
1	F	139	ALA	7.5
1	D	1	PRO	7.5
1	F	140	ALA	7.4
1	C	226	THR	7.4
1	E	386	LEU	7.3
1	D	190	ALA	7.3
1	D	73	TYR	7.3
1	B	33	PRO	7.3
1	A	57	ASP	7.3
1	D	192	SER	7.3
1	E	399	SER	7.2
1	E	383	TYR	7.2
1	A	64	SER	7.2
1	E	125	LEU	7.2
1	E	357	LEU	7.2
1	D	55	THR	7.2
1	A	403	SER	7.2
1	A	417	ARG	7.1
1	D	57	ASP	7.1
1	B	357	LEU	7.0
1	E	126	GLU	7.0
1	B	235	ASN	6.9
1	C	58	ARG	6.9
1	F	67	PRO	6.9
1	D	416	ASN	6.9
1	D	419	GLY	6.9
1	D	56	TYR	6.9
1	B	354	GLU	6.9
1	C	57	ASP	6.9
1	A	436	GLN	6.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	261	TRP	6.9
1	E	320	THR	6.8
1	A	416	ASN	6.8
1	D	198	ALA	6.8
1	A	55	THR	6.8
1	B	193	GLY	6.8
1	F	403	SER	6.8
1	E	364	GLN	6.7
1	B	419	GLY	6.7
1	F	63	GLN	6.7
1	A	126	GLU	6.7
1	B	125	LEU	6.7
1	D	389	GLU	6.7
1	E	224	HIS	6.7
1	B	66	GLN	6.7
1	D	107	TYR	6.7
1	D	364	GLN	6.6
1	D	105	ALA	6.6
1	D	418	MET	6.6
1	B	420	ALA	6.6
1	A	194	GLY	6.5
1	C	65	SER	6.5
1	B	37	HIS	6.5
1	D	354	GLU	6.5
1	A	18	GLU	6.5
1	A	319	ASN	6.5
1	E	393	HIS	6.5
1	B	298	ILE	6.4
1	E	123	ALA	6.4
1	D	189	THR	6.4
1	B	391	THR	6.4
1	E	392	PHE	6.4
1	E	33	PRO	6.4
1	A	419	GLY	6.4
1	A	193	GLY	6.4
1	F	61	PHE	6.4
1	A	360	ARG	6.4
1	A	354	GLU	6.3
1	A	63	GLN	6.3
1	C	62	GLY	6.3
1	A	195	PHE	6.3
1	D	126	GLU	6.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	56	TYR	6.3
1	B	18	GLU	6.3
1	F	261	TRP	6.3
1	A	320	THR	6.3
1	F	129	LEU	6.3
1	C	18	GLU	6.3
1	B	62	GLY	6.2
1	B	386	LEU	6.2
1	F	192	SER	6.2
1	D	383	TYR	6.2
1	F	58	ARG	6.2
1	D	20	HIS	6.2
1	D	36	GLY	6.2
1	B	299	PRO	6.1
1	A	399	SER	6.1
1	A	389	GLU	6.1
1	E	65	SER	6.1
1	C	34	LEU	6.1
1	F	57	ASP	6.1
1	C	126	GLU	6.1
1	E	360	ARG	6.1
1	B	402	TYR	6.1
1	F	79	ASP	6.1
1	D	76	PHE	6.1
1	E	59	ARG	6.1
1	D	376	MET	6.1
1	A	124	SER	6.0
1	D	402	TYR	6.0
1	A	198	ALA	6.0
1	B	416	ASN	6.0
1	A	16	TYR	5.9
1	A	238	ARG	5.9
1	C	66	GLN	5.9
1	C	195	PHE	5.9
1	E	387	LYS	5.9
1	D	38	SER	5.9
1	E	66	GLN	5.9
1	F	141	PRO	5.9
1	A	109	SER	5.9
1	E	54	ILE	5.9
1	D	235	ASN	5.9
1	F	38	SER	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	250	VAL	5.9
1	D	356	GLY	5.8
1	C	55	THR	5.8
1	B	56	TYR	5.8
1	D	391	THR	5.8
1	A	32	PHE	5.8
1	B	40	GLU	5.8
1	E	382	LEU	5.8
1	E	416	ASN	5.8
1	E	222	ILE	5.8
1	D	156	ARG	5.8
1	F	404	ALA	5.8
1	A	212	ASP	5.7
1	C	168	TYR	5.7
1	C	32	PHE	5.7
1	C	418	MET	5.7
1	F	178	ILE	5.7
1	E	223	LEU	5.7
1	E	193	GLY	5.7
1	A	240	PHE	5.7
1	D	195	PHE	5.7
1	E	415	TYR	5.6
1	E	121	PHE	5.6
1	C	255	ALA	5.6
1	F	193	GLY	5.6
1	D	123	ALA	5.6
1	B	178	ILE	5.6
1	D	382	LEU	5.6
1	C	198	ALA	5.6
1	E	73	TYR	5.6
1	A	418	MET	5.6
1	F	5	VAL	5.6
1	B	415	TYR	5.6
1	D	104	VAL	5.6
1	D	420	ALA	5.5
1	D	225	GLY	5.5
1	D	16	TYR	5.5
1	A	34	LEU	5.5
1	D	63	GLN	5.5
1	E	204	THR	5.5
1	A	157	TYR	5.5
1	E	17	TYR	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	227	GLY	5.5
1	E	417	ARG	5.5
1	F	35	SER	5.5
1	F	34	LEU	5.4
1	E	16	TYR	5.4
1	A	79	ASP	5.4
1	E	385	LYS	5.4
1	D	392	PHE	5.4
1	D	205	TRP	5.4
1	D	417	ARG	5.4
1	E	190	ALA	5.4
1	D	17	TYR	5.4
1	F	73	TYR	5.4
1	A	237	ALA	5.4
1	B	417	ARG	5.4
1	D	79	ASP	5.4
1	E	350	THR	5.4
1	B	90	GLN	5.4
1	C	240	PHE	5.4
1	B	360	ARG	5.4
1	A	404	ALA	5.3
1	A	364	GLN	5.3
1	B	1	PRO	5.3
1	D	386	LEU	5.3
1	D	199	ALA	5.3
1	F	36	GLY	5.3
1	E	60	GLY	5.3
1	A	402	TYR	5.3
1	A	111	TYR	5.3
1	D	223	LEU	5.3
1	A	415	TYR	5.3
1	B	384	ARG	5.3
1	E	63	GLN	5.3
1	A	223	LEU	5.2
1	E	389	GLU	5.2
1	D	388	ARG	5.2
1	A	322	LEU	5.2
1	E	187	TRP	5.2
1	E	40	GLU	5.2
1	C	169	ASN	5.2
1	E	62	GLY	5.2
1	F	103	GLU	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	260	LEU	5.2
1	A	252	VAL	5.2
1	D	393	HIS	5.2
1	D	261	TRP	5.2
1	E	235	ASN	5.2
1	D	403	SER	5.2
1	F	433	THR	5.1
1	B	383	TYR	5.1
1	D	380	VAL	5.1
1	F	18	GLU	5.1
1	C	61	PHE	5.1
1	F	64	SER	5.1
1	E	58	ARG	5.1
1	C	60	GLY	5.1
1	D	111	TYR	5.1
1	D	206	TYR	5.1
1	F	130	LEU	5.1
1	B	127	PRO	5.1
1	F	386	LEU	5.1
1	D	106	ARG	5.1
1	D	394	GLY	5.1
1	D	415	TYR	5.1
1	D	114	ALA	5.1
1	E	120	ALA	5.1
1	B	168	TYR	5.1
1	B	124	SER	5.1
1	F	179	SER	5.1
1	D	188	ASN	5.1
1	A	352	PRO	5.0
1	E	15	LEU	5.0
1	C	171	ASP	5.0
1	B	390	ILE	5.0
1	A	225	GLY	5.0
1	A	356	GLY	5.0
1	B	387	LYS	5.0
1	E	384	ARG	5.0
1	A	68	THR	5.0
1	A	15	LEU	5.0
1	E	156	ARG	5.0
1	E	391	THR	5.0
1	E	61	PHE	5.0
1	A	348	THR	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	172	GLU	5.0
1	B	139	ALA	4.9
1	E	348	THR	4.9
1	D	29	ILE	4.9
1	F	212	ASP	4.9
1	F	190	ALA	4.9
1	C	67	PRO	4.9
1	E	195	PHE	4.9
1	D	260	LEU	4.9
1	D	64	SER	4.9
1	D	168	TYR	4.9
1	C	37	HIS	4.9
1	E	395	ALA	4.9
1	F	191	ALA	4.9
1	D	157	TYR	4.9
1	B	38	SER	4.9
1	D	102	GLY	4.9
1	E	194	GLY	4.9
1	E	394	GLY	4.9
1	A	226	THR	4.9
1	E	157	TYR	4.9
1	A	433	THR	4.9
1	E	398	ILE	4.9
1	C	178	ILE	4.9
1	A	106	ARG	4.9
1	A	350	THR	4.8
1	D	197	ALA	4.8
1	E	38	SER	4.8
1	D	230	THR	4.8
1	B	59	ARG	4.8
1	D	40	GLU	4.8
1	E	322	LEU	4.8
1	F	16	TYR	4.8
1	F	106	ARG	4.8
1	B	63	GLN	4.8
1	A	107	TYR	4.8
1	E	354	GLU	4.8
1	C	254	GLY	4.8
1	E	319	ASN	4.8
1	D	385	LYS	4.8
1	D	77	ALA	4.8
1	E	191	ALA	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	108	VAL	4.8
1	F	40	GLU	4.7
1	D	185	ASN	4.7
1	D	375	ASN	4.7
1	F	32	PHE	4.7
1	D	360	ARG	4.7
1	F	198	ALA	4.7
1	F	213	ILE	4.7
1	A	125	LEU	4.7
1	C	259	LEU	4.7
1	E	396	LYS	4.7
1	E	122	LEU	4.7
1	F	368	ASN	4.7
1	E	164	PHE	4.7
1	B	34	LEU	4.7
1	F	399	SER	4.7
1	C	63	GLN	4.7
1	B	364	GLN	4.6
1	B	61	PHE	4.6
1	B	392	PHE	4.6
1	E	3	ILE	4.6
1	E	160	TYR	4.6
1	B	20	HIS	4.6
1	A	69	THR	4.6
1	A	233	ILE	4.6
1	D	236	THR	4.6
1	F	1	PRO	4.6
1	F	14	ASP	4.6
1	C	173	ASN	4.6
1	D	404	ALA	4.6
1	D	421	VAL	4.6
1	D	299	PRO	4.6
1	A	197	ALA	4.6
1	C	229	ARG	4.6
1	C	185	ASN	4.6
1	D	3	ILE	4.5
1	E	119	VAL	4.5
1	F	235	ASN	4.6
1	A	156	ARG	4.5
1	E	257	HIS	4.5
1	D	19	ASP	4.5
1	C	194	GLY	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	192	SER	4.5
1	E	107	TYR	4.5
1	D	257	HIS	4.5
1	D	99	MET	4.5
1	B	320	THR	4.5
1	D	390	ILE	4.5
1	B	194	GLY	4.5
1	E	225	GLY	4.5
1	C	5	VAL	4.5
1	F	195	PHE	4.5
1	E	35	SER	4.5
1	B	35	SER	4.5
1	D	237	ALA	4.5
1	E	106	ARG	4.5
1	E	373	PRO	4.5
1	D	204	THR	4.5
1	E	198	ALA	4.5
1	F	76	PHE	4.5
1	F	107	TYR	4.4
1	B	388	ARG	4.4
1	B	17	TYR	4.4
1	E	212	ASP	4.4
1	F	189	THR	4.4
1	F	68	THR	4.4
1	B	57	ASP	4.4
1	D	384	ARG	4.4
1	F	55	THR	4.4
1	D	396	LYS	4.4
1	A	73	TYR	4.4
1	A	261	TRP	4.4
1	B	380	VAL	4.4
1	F	216	ILE	4.4
1	A	362	PHE	4.4
1	E	168	TYR	4.4
1	B	421	VAL	4.4
1	D	54	ILE	4.4
1	E	231	LEU	4.4
1	C	300	SER	4.4
1	B	58	ARG	4.4
1	F	131	LYS	4.4
1	A	437	ILE	4.4
1	A	192	SER	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	19	ASP	4.4
1	B	385	LYS	4.3
1	A	315	PHE	4.3
1	D	15	LEU	4.3
1	E	53	VAL	4.3
1	B	403	SER	4.3
1	C	260	LEU	4.3
1	C	15	LEU	4.3
1	B	55	THR	4.3
1	B	322	LEU	4.3
1	A	386	LEU	4.3
1	F	119	VAL	4.3
1	E	34	LEU	4.3
1	D	53	VAL	4.3
1	E	209	PHE	4.3
1	F	405	GLY	4.3
1	A	435	GLU	4.3
1	F	80	LEU	4.3
1	A	297	ILE	4.3
1	B	179	SER	4.3
1	E	426	ALA	4.3
1	F	205	TRP	4.3
1	E	321	ASP	4.3
1	F	185	ASN	4.3
1	A	407	LEU	4.3
1	B	367	LEU	4.3
1	E	104	VAL	4.3
1	D	67	PRO	4.3
1	D	231	LEU	4.3
1	D	398	ILE	4.3
1	D	74	ASP	4.2
1	E	402	TYR	4.2
1	B	137	ASP	4.2
1	E	260	LEU	4.2
1	D	379	ALA	4.2
1	B	190	ALA	4.2
1	B	398	ILE	4.2
1	E	379	ALA	4.2
1	A	351	VAL	4.2
1	E	90	GLN	4.2
1	A	108	VAL	4.2
1	D	387	LYS	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	213	ILE	4.2
1	E	427	PHE	4.2
1	C	399	SER	4.2
1	E	139	ALA	4.2
1	B	347	PHE	4.2
1	A	17	TYR	4.2
1	E	36	GLY	4.2
1	E	388	ARG	4.2
1	F	15	LEU	4.2
1	D	216	ILE	4.1
1	E	32	PHE	4.1
1	B	350	THR	4.1
1	D	207	THR	4.1
1	B	185	ASN	4.1
1	A	420	ALA	4.1
1	B	302	PRO	4.1
1	F	194	GLY	4.1
1	A	103	GLU	4.1
1	A	5	VAL	4.1
1	A	231	LEU	4.1
1	A	390	ILE	4.1
1	A	37	HIS	4.1
1	A	191	ALA	4.1
1	D	110	SER	4.1
1	C	193	GLY	4.1
1	E	118	ALA	4.1
1	D	80	LEU	4.1
1	C	14	ASP	4.1
1	C	256	PRO	4.1
1	B	157	TYR	4.1
1	C	170	LEU	4.1
1	A	222	ILE	4.1
1	C	17	TYR	4.0
1	A	396	LYS	4.0
1	E	64	SER	4.0
1	B	348	THR	4.0
1	E	226	THR	4.0
1	A	317	GLY	4.0
1	E	185	ASN	4.0
1	E	397	GLU	4.0
1	B	113	THR	4.0
1	F	77	ALA	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	258	GLY	4.0
1	F	3	ILE	4.0
1	B	297	ILE	4.0
1	C	396	LYS	4.0
1	E	425	VAL	4.0
1	E	94	LEU	4.0
1	D	116	ILE	4.0
1	D	202	PRO	4.0
1	D	373	PRO	4.0
1	C	383	TYR	4.0
1	C	420	ALA	4.0
1	F	137	ASP	4.0
1	F	382	LEU	4.0
1	C	3	ILE	4.0
1	E	254	GLY	4.0
1	A	342	ILE	3.9
1	B	411	MET	3.9
1	A	30	HIS	3.9
1	A	1	PRO	3.9
1	C	261	TRP	3.9
1	E	422	THR	3.9
1	A	314	VAL	3.9
1	D	97	PHE	3.9
1	A	325	LEU	3.9
1	C	262	THR	3.9
1	F	125	LEU	3.9
1	D	71	TYR	3.9
1	E	314	VAL	3.9
1	F	407	LEU	3.9
1	A	398	ILE	3.9
1	C	124	SER	3.9
1	C	164	PHE	3.9
1	D	259	LEU	3.9
1	F	207	THR	3.9
1	F	206	TYR	3.9
1	E	207	THR	3.9
1	E	376	MET	3.9
1	A	102	GLY	3.9
1	B	300	SER	3.9
1	E	103	GLU	3.9
1	D	187	TRP	3.8
1	D	252	VAL	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	344	GLY	3.8
1	F	402	TYR	3.8
1	D	233	ILE	3.8
1	A	76	PHE	3.8
1	B	129	LEU	3.8
1	A	432	ALA	3.8
1	A	326	MET	3.8
1	D	160	TYR	3.8
1	D	262	THR	3.8
1	B	395	ALA	3.8
1	A	104	VAL	3.8
1	B	351	VAL	3.8
1	A	199	ALA	3.8
1	E	345	PHE	3.8
1	F	186	SER	3.8
1	B	319	ASN	3.8
1	D	371	GLY	3.8
1	A	105	ALA	3.8
1	E	30	HIS	3.8
1	B	418	MET	3.8
1	E	424	GLU	3.8
1	E	188	ASN	3.8
1	A	405	GLY	3.8
1	A	249	TYR	3.8
1	B	36	GLY	3.8
1	F	230	THR	3.8
1	C	213	ILE	3.8
1	E	91	ASP	3.8
1	E	105	ALA	3.8
1	B	91	ASP	3.8
1	D	436	GLN	3.7
1	E	28	LEU	3.7
1	B	410	CYS	3.7
1	C	257	HIS	3.7
1	E	390	ILE	3.7
1	F	209	PHE	3.7
1	E	205	TRP	3.7
1	B	189	THR	3.7
1	A	260	LEU	3.7
1	C	125	LEU	3.7
1	F	252	VAL	3.7
1	B	404	ALA	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	188	ASN	3.7
1	A	178	ILE	3.7
1	B	116	ILE	3.7
1	D	298	ILE	3.7
1	B	89	LEU	3.7
1	E	355	ARG	3.7
1	E	407	LEU	3.7
1	A	239	VAL	3.7
1	A	121	PHE	3.7
1	B	52	ARG	3.7
1	F	17	TYR	3.7
1	C	216	ILE	3.7
1	F	199	ALA	3.7
1	F	411	MET	3.7
1	F	409	SER	3.7
1	E	414	ILE	3.7
1	F	367	LEU	3.7
1	E	92	ALA	3.6
1	B	21	GLY	3.6
1	C	156	ARG	3.6
1	D	178	ILE	3.6
1	A	434	CYS	3.6
1	B	60	GLY	3.6
1	B	236	THR	3.6
1	E	362	PHE	3.6
1	E	216	ILE	3.6
1	B	396	LYS	3.6
1	D	406	ALA	3.6
1	F	105	ALA	3.6
1	C	223	LEU	3.6
1	B	382	LEU	3.6
1	B	345	PHE	3.6
1	F	111	TYR	3.6
1	F	30	HIS	3.6
1	A	35	SER	3.6
1	C	319	ASN	3.6
1	B	187	TRP	3.6
1	B	192	SER	3.6
1	A	71	TYR	3.6
1	A	429	LEU	3.6
1	A	262	THR	3.6
1	B	394	GLY	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	128	PHE	3.6
1	F	260	LEU	3.6
1	E	261	TRP	3.6
1	E	129	LEU	3.5
1	E	256	PRO	3.5
1	A	400	LEU	3.5
1	E	19	ASP	3.5
1	A	94	LEU	3.5
1	E	221	LEU	3.5
1	A	347	PHE	3.5
1	D	129	LEU	3.5
1	B	371	GLY	3.5
1	B	399	SER	3.5
1	E	163	PHE	3.5
1	A	307	ILE	3.5
1	E	178	ILE	3.5
1	C	199	ALA	3.5
1	E	206	TYR	3.5
1	C	228	ASP	3.5
1	A	392	PHE	3.5
1	C	191	ALA	3.5
1	B	436	GLN	3.5
1	C	258	GLY	3.5
1	E	371	GLY	3.5
1	A	439	ASP	3.5
1	C	380	VAL	3.5
1	C	16	TYR	3.5
1	E	258	GLY	3.5
1	F	127	PRO	3.5
1	E	5	VAL	3.5
1	E	429	LEU	3.5
1	C	354	GLU	3.5
1	D	433	THR	3.5
1	E	220	ALA	3.5
1	E	315	PHE	3.5
1	F	294	VAL	3.5
1	A	81	ASN	3.5
1	E	26	VAL	3.5
1	F	251	GLU	3.5
1	F	215	ARG	3.5
1	C	252	VAL	3.5
1	D	90	GLN	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	1	PRO	3.4
1	B	342	ILE	3.4
1	D	115	ARG	3.4
1	D	222	ILE	3.4
1	D	28	LEU	3.4
1	A	80	LEU	3.4
1	A	3	ILE	3.4
1	D	122	LEU	3.4
1	D	407	LEU	3.4
1	B	164	PHE	3.4
1	E	411	MET	3.4
1	C	186	SER	3.4
1	C	188	ASN	3.4
1	D	378	LYS	3.4
1	C	190	ALA	3.4
1	D	186	SER	3.4
1	E	380	VAL	3.4
1	A	254	GLY	3.4
1	D	2	PHE	3.4
1	E	29	ILE	3.4
1	C	104	VAL	3.4
1	B	41	ARG	3.4
1	E	361	ARG	3.4
1	A	216	ILE	3.4
1	B	188	ASN	3.4
1	C	382	LEU	3.4
1	B	254	GLY	3.4
1	F	183	VAL	3.4
1	E	410	CYS	3.4
1	A	382	LEU	3.4
1	B	183	VAL	3.4
1	D	89	LEU	3.4
1	E	430	VAL	3.4
1	B	209	PHE	3.4
1	A	110	SER	3.4
1	A	388	ARG	3.4
1	A	430	VAL	3.4
1	A	410	CYS	3.4
1	A	250	VAL	3.4
1	E	229	ARG	3.4
1	C	417	ARG	3.3
1	B	352	PRO	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	381	LYS	3.3
1	C	233	ILE	3.3
1	D	300	SER	3.3
1	C	167	PHE	3.3
1	E	109	SER	3.3
1	D	314	VAL	3.3
1	F	180	GLU	3.3
1	C	376	MET	3.3
1	A	355	ARG	3.3
1	E	363	VAL	3.3
1	D	367	LEU	3.3
1	A	123	ALA	3.3
1	F	108	VAL	3.3
1	F	369	GLY	3.3
1	D	83	VAL	3.3
1	E	347	PHE	3.3
1	A	230	THR	3.3
1	A	311	LEU	3.3
1	C	108	VAL	3.3
1	F	74	ASP	3.3
1	B	321	ASP	3.3
1	F	234	GLU	3.3
1	C	181	GLU	3.3
1	D	232	PRO	3.3
1	C	64	SER	3.3
1	C	182	ALA	3.3
1	F	182	ALA	3.3
1	E	240	PHE	3.3
1	C	353	SER	3.3
1	E	353	SER	3.3
1	E	93	VAL	3.3
1	F	104	VAL	3.3
1	A	14	ASP	3.3
1	F	420	ALA	3.2
1	A	343	LEU	3.2
1	E	43	SER	3.2
1	B	32	PHE	3.2
1	B	400	LEU	3.2
1	A	209	PHE	3.2
1	A	257	HIS	3.2
1	B	262	THR	3.2
1	E	352	PRO	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	383	TYR	3.2
1	F	222	ILE	3.2
1	C	197	ALA	3.2
1	C	1	PRO	3.2
1	F	92	ALA	3.2
1	A	77	ALA	3.2
1	B	207	THR	3.2
1	E	199	ALA	3.2
1	C	174	LEU	3.2
1	F	145	PHE	3.2
1	A	82	THR	3.2
1	C	251	GLU	3.2
1	D	435	GLU	3.2
1	B	173	ASN	3.2
1	D	362	PHE	3.2
1	D	414	ILE	3.2
1	F	157	TYR	3.2
1	F	232	PRO	3.2
1	C	379	ALA	3.2
1	E	202	PRO	3.2
1	C	127	PRO	3.1
1	A	411	MET	3.1
1	B	393	HIS	3.1
1	D	91	ASP	3.1
1	D	101	THR	3.1
1	C	416	ASN	3.1
1	D	263	HIS	3.1
1	F	432	ALA	3.1
1	B	184	ARG	3.1
1	A	368	ASN	3.1
1	F	421	VAL	3.1
1	D	350	THR	3.1
1	A	83	VAL	3.1
1	B	16	TYR	3.1
1	E	233	ILE	3.1
1	C	184	ARG	3.1
1	A	36	GLY	3.1
1	D	395	ALA	3.1
1	A	253	GLU	3.1
1	A	339	THR	3.1
1	D	286	LEU	3.1
1	F	69	THR	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	431	CYS	3.1
1	C	192	SER	3.1
1	B	240	PHE	3.1
1	F	94	LEU	3.1
1	F	70	GLY	3.1
1	E	180	GLU	3.1
1	C	105	ALA	3.1
1	D	410	CYS	3.1
1	A	391	THR	3.1
1	B	115	ARG	3.1
1	F	392	PHE	3.1
1	A	232	PRO	3.1
1	B	413	LEU	3.1
1	F	202	PRO	3.1
1	D	84	LEU	3.1
1	C	386	LEU	3.1
1	E	323	GLU	3.1
1	F	126	GLU	3.1
1	B	186	SER	3.1
1	A	127	PRO	3.1
1	E	251	GLU	3.1
1	A	395	ALA	3.1
1	B	294	VAL	3.1
1	F	93	VAL	3.1
1	D	368	ASN	3.1
1	F	223	LEU	3.1
1	A	112	GLY	3.1
1	C	103	GLU	3.1
1	C	35	SER	3.1
1	E	186	SER	3.0
1	F	118	ALA	3.0
1	A	205	TRP	3.0
1	D	320	THR	3.0
1	D	399	SER	3.0
1	D	39	TRP	3.0
1	E	112	GLY	3.0
1	A	373	PRO	3.0
1	B	53	VAL	3.0
1	C	119	VAL	3.0
1	D	75	THR	3.0
1	B	256	PRO	3.0
1	C	217	ASP	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	80	LEU	3.0
1	D	413	LEU	3.0
1	E	255	ALA	3.0
1	C	352	PRO	3.0
1	E	311	LEU	3.0
1	C	187	TRP	3.0
1	A	421	VAL	3.0
1	C	79	ASP	3.0
1	E	325	LEU	3.0
1	E	400	LEU	3.0
1	A	196	PHE	3.0
1	B	353	SER	3.0
1	C	160	TYR	3.0
1	A	329	LEU	3.0
1	D	322	LEU	3.0
1	E	232	PRO	3.0
1	A	321	ASP	3.0
1	F	419	GLY	3.0
1	C	355	ARG	3.0
1	E	237	ALA	3.0
1	D	196	PHE	3.0
1	D	139	ALA	3.0
1	A	438	ALA	3.0
1	A	345	PHE	3.0
1	B	414	ILE	3.0
1	E	183	VAL	3.0
1	F	354	GLU	3.0
1	F	410	CYS	3.0
1	B	25	PRO	3.0
1	E	326	MET	3.0
1	D	315	PHE	3.0
1	A	140	ALA	3.0
1	A	365	ASN	3.0
1	B	253	GLU	3.0
1	F	39	TRP	2.9
1	C	113	THR	2.9
1	D	335	LEU	2.9
1	D	348	THR	2.9
1	F	42	GLN	2.9
1	C	392	PHE	2.9
1	F	231	LEU	2.9
1	A	310	ARG	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	234	GLU	2.9
1	B	181	GLU	2.9
1	E	259	LEU	2.9
1	E	184	ARG	2.9
1	B	379	ALA	2.9
1	B	234	GLU	2.9
1	A	361	ARG	2.9
1	A	383	TYR	2.9
1	D	290	VAL	2.9
1	E	230	THR	2.9
1	E	423	THR	2.9
1	E	349	LEU	2.9
1	F	168	TYR	2.9
1	F	181	GLU	2.9
1	C	402	TYR	2.9
1	F	429	LEU	2.9
1	D	109	SER	2.9
1	E	27	VAL	2.9
1	B	349	LEU	2.9
1	D	369	GLY	2.9
1	B	325	LEU	2.9
1	E	381	LYS	2.9
1	B	43	SER	2.9
1	E	52	ARG	2.9
1	C	183	VAL	2.9
1	B	73	TYR	2.9
1	F	257	HIS	2.9
1	B	167	PHE	2.9
1	D	98	SER	2.9
1	E	167	PHE	2.9
1	F	436	GLN	2.9
1	B	368	ASN	2.9
1	B	191	ALA	2.9
1	B	216	ILE	2.9
1	A	13	ILE	2.9
1	C	415	TYR	2.8
1	F	225	GLY	2.9
1	E	189	THR	2.8
1	A	160	TYR	2.8
1	C	298	ILE	2.8
1	F	210	ARG	2.8
1	E	378	LYS	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	353	SER	2.8
1	B	251	GLU	2.8
1	F	138	GLY	2.8
1	A	406	ALA	2.8
1	B	54	ILE	2.8
1	A	188	ASN	2.8
1	B	355	ARG	2.8
1	D	311	LEU	2.8
1	C	30	HIS	2.8
1	B	237	ALA	2.8
1	D	426	ALA	2.8
1	F	413	LEU	2.8
1	A	190	ALA	2.8
1	E	127	PRO	2.8
1	B	138	GLY	2.8
1	D	405	GLY	2.8
1	A	335	LEU	2.8
1	A	349	LEU	2.8
1	D	352	PRO	2.8
1	E	20	HIS	2.8
1	A	168	TYR	2.8
1	A	316	ALA	2.8
1	D	94	LEU	2.8
1	C	121	PHE	2.8
1	D	351	VAL	2.8
1	A	210	ARG	2.8
1	B	24	THR	2.8
1	F	184	ARG	2.8
1	A	376	MET	2.8
1	B	429	LEU	2.8
1	C	403	SER	2.8
1	F	71	TYR	2.8
1	B	326	MET	2.8
1	E	377	ASP	2.8
1	A	427	PHE	2.8
1	E	213	ILE	2.8
1	E	374	ASN	2.8
1	C	71	TYR	2.8
1	E	203	THR	2.8
1	A	84	LEU	2.8
1	E	80	LEU	2.8
1	B	42	GLN	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	252	VAL	2.8
1	C	205	TRP	2.8
1	D	21	GLY	2.8
1	B	365	ASN	2.8
1	D	152	VAL	2.8
1	F	187	TRP	2.8
1	A	40	GLU	2.8
1	E	236	THR	2.8
1	B	361	ARG	2.8
1	F	29	ILE	2.8
1	F	376	MET	2.8
1	A	177	ARG	2.8
1	B	47	LEU	2.8
1	A	235	ASN	2.7
1	E	76	PHE	2.7
1	F	2	PHE	2.7
1	C	54	ILE	2.7
1	F	83	VAL	2.7
1	C	166	ASP	2.7
1	C	237	ALA	2.7
1	C	351	VAL	2.7
1	B	233	ILE	2.7
1	B	425	VAL	2.7
1	D	234	GLU	2.7
1	E	111	TYR	2.7
1	A	379	ALA	2.7
1	B	306	GLU	2.7
1	B	346	VAL	2.7
1	F	99	MET	2.7
1	A	129	LEU	2.7
1	F	120	ALA	2.7
1	C	253	GLU	2.7
1	D	226	THR	2.7
1	F	226	THR	2.7
1	A	27	VAL	2.7
1	A	394	GLY	2.7
1	B	295	LEU	2.7
1	E	413	LEU	2.7
1	E	116	ILE	2.7
1	D	121	PHE	2.7
1	F	240	PHE	2.7
1	F	427	PHE	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	236	THR	2.7
1	B	65	SER	2.7
1	E	77	ALA	2.7
1	D	345	PHE	2.7
1	B	258	GLY	2.7
1	C	299	PRO	2.7
1	A	408	ALA	2.7
1	B	170	LEU	2.7
1	D	411	MET	2.7
1	B	182	ALA	2.7
1	B	92	ALA	2.7
1	B	177	ARG	2.7
1	F	387	LYS	2.7
1	B	296	SER	2.7
1	D	353	SER	2.7
1	E	155	ASP	2.7
1	F	43	SER	2.7
1	B	435	GLU	2.7
1	C	210	ARG	2.7
1	D	92	ALA	2.7
1	B	180	GLU	2.6
1	C	179	SER	2.6
1	A	187	TRP	2.6
1	D	377	ASP	2.6
1	F	91	ASP	2.6
1	C	28	LEU	2.6
1	D	81	ASN	2.6
1	F	75	THR	2.6
1	D	267	VAL	2.6
1	E	95	VAL	2.6
1	F	112	GLY	2.6
1	D	130	LEU	2.6
1	A	113	THR	2.6
1	E	219	PRO	2.6
1	D	200	ALA	2.6
1	C	107	TYR	2.6
1	F	390	ILE	2.6
1	D	427	PHE	2.6
1	E	117	ALA	2.6
1	A	393	HIS	2.6
1	F	259	LEU	2.6
1	C	400	LEU	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	89	LEU	2.6
1	A	441	GLN	2.6
1	D	212	ASP	2.6
1	A	10	SER	2.6
1	C	123	ALA	2.6
1	A	363	VAL	2.6
1	B	412	GLY	2.6
1	A	2	PHE	2.6
1	B	376	MET	2.6
1	C	76	PHE	2.6
1	F	160	TYR	2.6
1	F	371	GLY	2.6
1	D	209	PHE	2.6
1	C	357	LEU	2.6
1	C	350	THR	2.6
1	F	10	SER	2.6
1	B	87	LEU	2.6
1	D	429	LEU	2.6
1	E	137	ASP	2.6
1	D	349	LEU	2.6
1	F	156	ARG	2.6
1	B	407	LEU	2.6
1	C	230	THR	2.6
1	A	409	SER	2.5
1	D	10	SER	2.5
1	F	357	LEU	2.5
1	F	430	VAL	2.5
1	D	408	ALA	2.5
1	E	79	ASP	2.5
1	B	307	ILE	2.5
1	E	25	PRO	2.5
1	E	42	GLN	2.5
1	C	13	ILE	2.5
1	E	318	LYS	2.5
1	D	291	GLU	2.5
1	C	359	ARG	2.5
1	D	215	ARG	2.5
1	F	4	THR	2.5
1	A	119	VAL	2.5
1	A	346	VAL	2.5
1	A	367	LEU	2.5
1	B	323	GLU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	78	ALA	2.5
1	E	67	PRO	2.5
1	D	96	GLY	2.5
1	B	226	THR	2.5
1	F	416	ASN	2.5
1	A	19	ASP	2.5
1	B	255	ALA	2.5
1	E	404	ALA	2.5
1	B	213	ILE	2.5
1	C	231	LEU	2.5
1	E	234	GLU	2.5
1	A	385	LYS	2.5
1	B	259	LEU	2.5
1	F	25	PRO	2.5
1	F	391	THR	2.5
1	C	27	VAL	2.5
1	F	13	ILE	2.5
1	F	224	HIS	2.5
1	B	301	GLY	2.5
1	B	335	LEU	2.5
1	F	434	CYS	2.5
1	D	256	PRO	2.5
1	A	202	PRO	2.5
1	F	28	LEU	2.5
1	D	347	PHE	2.5
1	F	414	ILE	2.5
1	D	42	GLN	2.4
1	D	319	ASN	2.4
1	F	406	ALA	2.4
1	A	201	ALA	2.4
1	B	39	TRP	2.4
1	D	87	LEU	2.4
1	D	228	ASP	2.4
1	F	102	GLY	2.4
1	E	249	TYR	2.4
1	A	294	VAL	2.4
1	E	375	ASN	2.4
1	E	182	ALA	2.4
1	B	222	ILE	2.4
1	C	421	VAL	2.4
1	A	139	ALA	2.4
1	C	122	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	204	THR	2.4
1	B	304	LYS	2.4
1	E	102	GLY	2.4
1	F	82	THR	2.4
1	C	4	THR	2.4
1	D	201	ALA	2.4
1	B	397	GLU	2.4
1	B	343	LEU	2.4
1	D	5	VAL	2.4
1	E	228	ASP	2.4
1	E	172	GLU	2.4
1	F	208	ASP	2.4
1	D	69	THR	2.4
1	D	355	ARG	2.4
1	E	433	THR	2.4
1	D	25	PRO	2.4
1	C	348	THR	2.4
1	F	355	ARG	2.4
1	B	257	HIS	2.4
1	E	294	VAL	2.4
1	E	262	THR	2.4
1	A	387	LYS	2.4
1	B	156	ARG	2.4
1	B	205	TRP	2.4
1	B	102	GLY	2.4
1	C	94	LEU	2.3
1	C	157	TYR	2.3
1	A	122	LEU	2.3
1	D	167	PHE	2.3
1	A	93	VAL	2.3
1	A	366	ALA	2.3
1	D	27	VAL	2.3
1	F	54	ILE	2.3
1	F	300	SER	2.3
1	E	290	VAL	2.3
1	F	297	ILE	2.3
1	C	236	THR	2.3
1	A	217	ASP	2.3
1	C	322	LEU	2.3
1	F	8	GLU	2.3
1	C	38	SER	2.3
1	E	356	GLY	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	31	GLY	2.3
1	C	356	GLY	2.3
1	B	430	VAL	2.3
1	D	95	VAL	2.3
1	A	120	ALA	2.3
1	B	339	THR	2.3
1	C	315	PHE	2.3
1	F	167	PHE	2.3
1	C	69	THR	2.3
1	F	41	ARG	2.3
1	D	177	ARG	2.3
1	E	46	LEU	2.3
1	B	26	VAL	2.3
1	C	398	ILE	2.3
1	B	381	LYS	2.3
1	F	90	GLN	2.3
1	A	371	GLY	2.3
1	D	137	ASP	2.3
1	B	2	PHE	2.3
1	E	83	VAL	2.3
1	C	180	GLU	2.3
1	B	369	GLY	2.3
1	C	189	THR	2.3
1	D	326	MET	2.3
1	B	433	THR	2.3
1	E	365	ASN	2.3
1	F	135	ASN	2.3
1	F	78	ALA	2.2
1	D	361	ARG	2.2
1	F	431	CYS	2.2
1	C	391	THR	2.2
1	F	81	ASN	2.2
1	B	363	VAL	2.2
1	E	158	ALA	2.2
1	B	103	GLU	2.2
1	E	351	VAL	2.2
1	F	221	LEU	2.2
1	F	396	LYS	2.2
1	C	36	GLY	2.2
1	B	310	ARG	2.2
1	E	171	ASP	2.2
1	A	70	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	64	SER	2.2
1	E	169	ASN	2.2
1	E	346	VAL	2.2
1	F	109	SER	2.2
1	B	174	LEU	2.2
1	E	210	ARG	2.2
1	F	339	THR	2.2
1	B	401	SER	2.2
1	D	72	ASP	2.2
1	D	82	THR	2.2
1	F	11	THR	2.2
1	F	239	VAL	2.2
1	F	113	THR	2.2
1	B	341	GLY	2.2
1	C	116	ILE	2.2
1	C	68	THR	2.2
1	A	95	VAL	2.2
1	D	100	GLY	2.2
1	A	259	LEU	2.2
1	A	426	ALA	2.2
1	C	2	PHE	2.2
1	E	401	SER	2.2
1	F	385	LYS	2.2
1	C	177	ARG	2.2
1	E	173	ASN	2.2
1	F	220	ALA	2.2
1	E	179	SER	2.2
1	D	372	ASP	2.1
1	F	364	GLN	2.1
1	B	224	HIS	2.1
1	D	374	ASN	2.1
1	E	110	SER	2.1
1	B	424	GLU	2.1
1	D	307	ILE	2.1
1	B	195	PHE	2.1
1	A	4	THR	2.1
1	E	161	THR	2.1
1	F	298	ILE	2.1
1	D	409	SER	2.1
1	F	249	TYR	2.1
1	A	118	ALA	2.1
1	A	380	VAL	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	369	GLY	2.1
1	E	227	GLY	2.1
1	F	415	TYR	2.1
1	A	323	GLU	2.1
1	C	390	ILE	2.1
1	D	182	ALA	2.1
1	D	240	PHE	2.1
1	F	121	PHE	2.1
1	E	403	SER	2.1
1	A	287	LEU	2.1
1	D	43	SER	2.1
1	F	110	SER	2.1
1	C	363	VAL	2.1
1	E	159	PHE	2.1
1	C	393	HIS	2.1
1	F	345	PHE	2.1
1	A	298	ILE	2.1
1	B	303	LEU	2.1
1	F	322	LEU	2.1
1	C	384	ARG	2.1
1	A	328	TRP	2.1
1	E	372	ASP	2.1
1	A	78	ALA	2.1
1	E	409	SER	2.1
1	D	153	LYS	2.1
1	B	356	GLY	2.1
1	A	440	SER	2.1
1	E	406	ALA	2.1
1	D	68	THR	2.1
1	A	413	LEU	2.1
1	C	222	ILE	2.1
1	B	51	ALA	2.1
1	C	395	ALA	2.1
1	D	294	VAL	2.1
1	D	363	VAL	2.1
1	B	15	LEU	2.1
1	A	211	ALA	2.1
1	F	295	LEU	2.1
1	F	217	ASP	2.1
1	F	307	ILE	2.1
1	E	343	LEU	2.1
1	A	189	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	426	ALA	2.1
1	C	238	ARG	2.0
1	D	14	ASP	2.0
1	A	401	SER	2.0
1	C	83	VAL	2.0
1	D	52	ARG	2.0
1	D	70	GLY	2.0
1	D	431	CYS	2.0
1	D	289	GLU	2.0
1	B	206	TYR	2.0
1	B	93	VAL	2.0
1	B	169	ASN	2.0
1	C	347	PHE	2.0
1	E	99	MET	2.0
1	F	84	LEU	2.0
1	A	384	ARG	2.0
1	D	339	THR	2.0
1	A	255	ALA	2.0
1	C	11	THR	2.0
1	A	54	ILE	2.0
1	B	232	PRO	2.0
1	E	367	LEU	2.0
1	A	318	LYS	2.0
1	B	426	ALA	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.