



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:34 AM GMT

PDB ID : 3P45  
Title : Crystal structure of apo-caspase-6 at physiological pH  
Authors : Mueller, I.; Lamers, M.B.A.C.; Ritchie, A.J.; Dominguez, C.; Munoz, I.; Mail-  
lard, M.; Kiselyov, A.  
Deposited on : 2010-10-06  
Resolution : 2.53 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

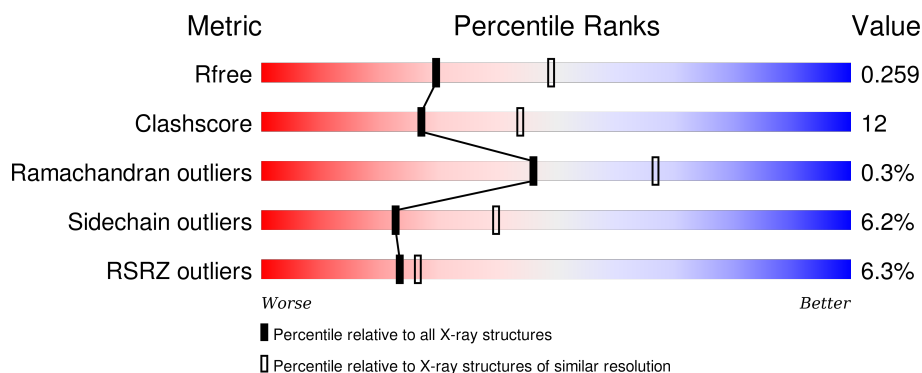
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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))
$R_{free}$	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	179	<div> <div>3%</div> <div>58% 13% 26%</div> </div>
1	C	179	<div> <div>6%</div> <div>54% 18% 26%</div> </div>
1	E	179	<div> <div>2%</div> <div>55% 16% 26%</div> </div>
1	G	179	<div> <div>6%</div> <div>60% 12% 27%</div> </div>
1	I	179	<div> <div>0%</div> <div>58% 13% 26%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	179	
1	M	179	
1	O	179	
2	B	108	
2	D	108	
2	F	108	
2	H	108	
2	J	108	
2	L	108	
2	N	108	
2	P	108	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12955 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 caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1058	678	183	190	7			
1	C	132	Total	C	N	O	S	0	0	0
			1054	676	184	188	6			
1	E	132	Total	C	N	O	S	0	0	0
			1058	679	186	187	6			
1	G	131	Total	C	N	O	S	0	0	0
			1040	666	180	188	6			
1	I	133	Total	C	N	O	S	0	0	0
			1063	681	185	190	7			
1	K	133	Total	C	N	O	S	0	0	0
			1037	665	181	184	7			
1	M	133	Total	C	N	O	S	0	0	0
			1055	677	183	188	7			
1	O	132	Total	C	N	O	S	0	0	0
			1043	670	179	188	6			

- Molecule 2 is a protein called caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	S	0	0	0
			579	377	94	102	6			
2	D	70	Total	C	N	O	S	0	0	0
			554	361	89	98	6			
2	F	68	Total	C	N	O	S	0	0	0
			535	348	86	95	6			
2	H	68	Total	C	N	O	S	0	0	0
			545	356	89	94	6			
2	J	70	Total	C	N	O	S	0	0	0
			543	353	87	97	6			
2	L	66	Total	C	N	O	S	0	0	0
			521	339	84	92	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	67	Total	C	N	O	S	0	0	0
			531	345	85	95	6			
2	P	68	Total	C	N	O	S	0	0	0
			538	349	87	96	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	ARG	-	EXPRESSION TAG	UNP P55212
B	295	HIS	-	EXPRESSION TAG	UNP P55212
B	296	HIS	-	EXPRESSION TAG	UNP P55212
B	297	HIS	-	EXPRESSION TAG	UNP P55212
B	298	HIS	-	EXPRESSION TAG	UNP P55212
B	299	HIS	-	EXPRESSION TAG	UNP P55212
B	300	HIS	-	EXPRESSION TAG	UNP P55212
D	294	ARG	-	EXPRESSION TAG	UNP P55212
D	295	HIS	-	EXPRESSION TAG	UNP P55212
D	296	HIS	-	EXPRESSION TAG	UNP P55212
D	297	HIS	-	EXPRESSION TAG	UNP P55212
D	298	HIS	-	EXPRESSION TAG	UNP P55212
D	299	HIS	-	EXPRESSION TAG	UNP P55212
D	300	HIS	-	EXPRESSION TAG	UNP P55212
F	294	ARG	-	EXPRESSION TAG	UNP P55212
F	295	HIS	-	EXPRESSION TAG	UNP P55212
F	296	HIS	-	EXPRESSION TAG	UNP P55212
F	297	HIS	-	EXPRESSION TAG	UNP P55212
F	298	HIS	-	EXPRESSION TAG	UNP P55212
F	299	HIS	-	EXPRESSION TAG	UNP P55212
F	300	HIS	-	EXPRESSION TAG	UNP P55212
H	294	ARG	-	EXPRESSION TAG	UNP P55212
H	295	HIS	-	EXPRESSION TAG	UNP P55212
H	296	HIS	-	EXPRESSION TAG	UNP P55212
H	297	HIS	-	EXPRESSION TAG	UNP P55212
H	298	HIS	-	EXPRESSION TAG	UNP P55212
H	299	HIS	-	EXPRESSION TAG	UNP P55212
H	300	HIS	-	EXPRESSION TAG	UNP P55212
J	294	ARG	-	EXPRESSION TAG	UNP P55212
J	295	HIS	-	EXPRESSION TAG	UNP P55212
J	296	HIS	-	EXPRESSION TAG	UNP P55212
J	297	HIS	-	EXPRESSION TAG	UNP P55212
J	298	HIS	-	EXPRESSION TAG	UNP P55212
J	299	HIS	-	EXPRESSION TAG	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
J	300	HIS	-	EXPRESSION TAG	UNP P55212
L	294	ARG	-	EXPRESSION TAG	UNP P55212
L	295	HIS	-	EXPRESSION TAG	UNP P55212
L	296	HIS	-	EXPRESSION TAG	UNP P55212
L	297	HIS	-	EXPRESSION TAG	UNP P55212
L	298	HIS	-	EXPRESSION TAG	UNP P55212
L	299	HIS	-	EXPRESSION TAG	UNP P55212
L	300	HIS	-	EXPRESSION TAG	UNP P55212
N	294	ARG	-	EXPRESSION TAG	UNP P55212
N	295	HIS	-	EXPRESSION TAG	UNP P55212
N	296	HIS	-	EXPRESSION TAG	UNP P55212
N	297	HIS	-	EXPRESSION TAG	UNP P55212
N	298	HIS	-	EXPRESSION TAG	UNP P55212
N	299	HIS	-	EXPRESSION TAG	UNP P55212
N	300	HIS	-	EXPRESSION TAG	UNP P55212
P	294	ARG	-	EXPRESSION TAG	UNP P55212
P	295	HIS	-	EXPRESSION TAG	UNP P55212
P	296	HIS	-	EXPRESSION TAG	UNP P55212
P	297	HIS	-	EXPRESSION TAG	UNP P55212
P	298	HIS	-	EXPRESSION TAG	UNP P55212
P	299	HIS	-	EXPRESSION TAG	UNP P55212
P	300	HIS	-	EXPRESSION TAG	UNP P55212

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	7	Total O 7 7	0	0
3	C	8	Total O 8 8	0	0
3	D	8	Total O 8 8	0	0
3	E	30	Total O 30 30	0	0
3	F	11	Total O 11 11	0	0
3	G	8	Total O 8 8	0	0
3	H	7	Total O 7 7	0	0

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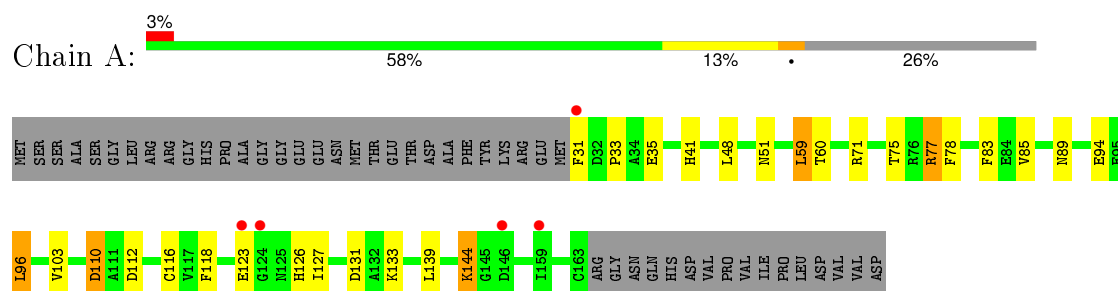
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	21	Total 21	O 21	0	0
3	J	10	Total 10	O 10	0	0
3	K	14	Total 14	O 14	0	0
3	L	6	Total 6	O 6	0	0
3	M	29	Total 29	O 29	0	0
3	N	4	Total 4	O 4	0	0
3	O	8	Total 8	O 8	0	0
3	P	6	Total 6	O 6	0	0

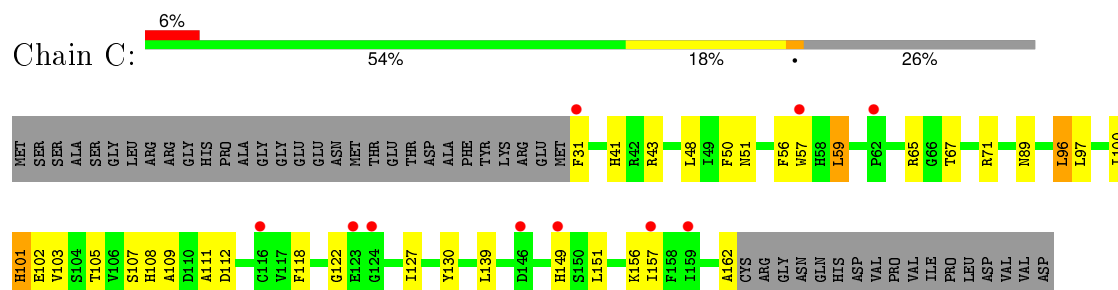
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

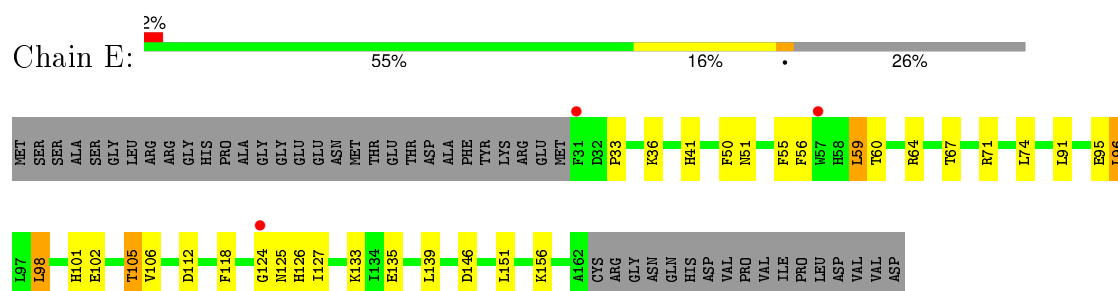
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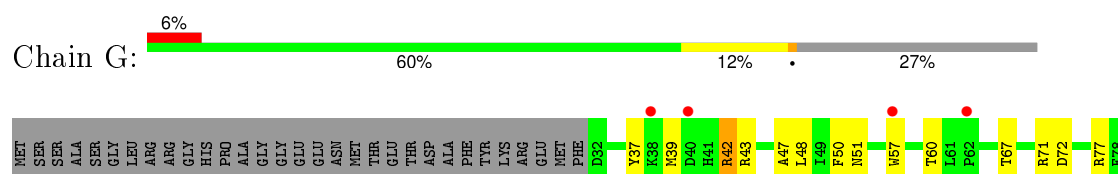
- Molecule 1: caspase-6



- Molecule 1: caspase-6



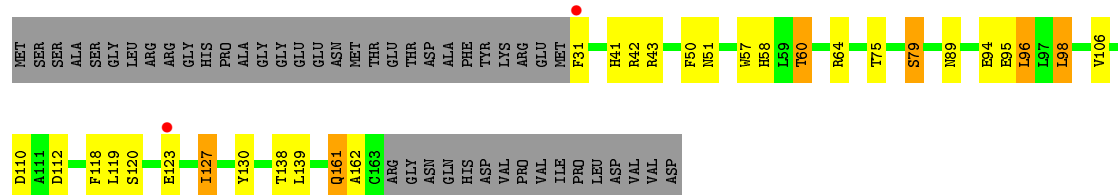
- Molecule 1: caspase-6



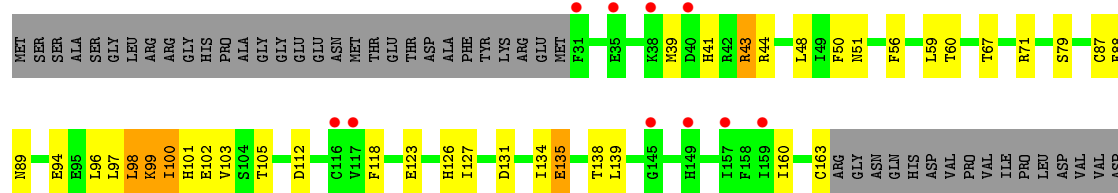




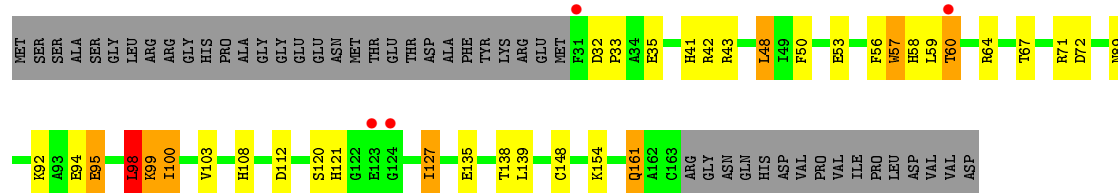
- Molecule 1: caspase-6



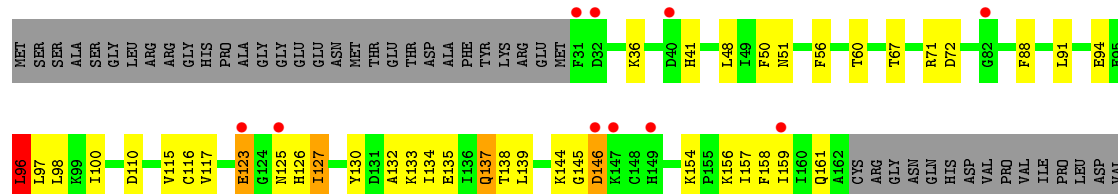
- Molecule 1: caspase-6



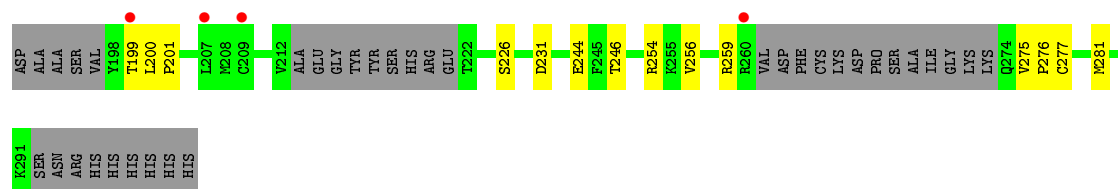
- Molecule 1: caspase-6



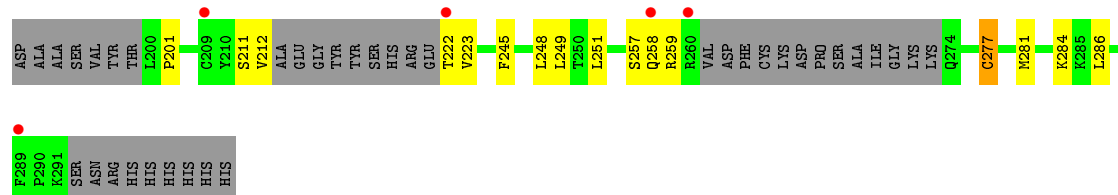
- Molecule 1: caspase-6



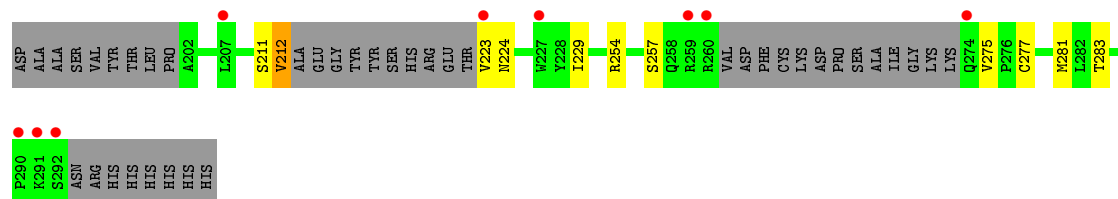
- Molecule 2: caspase-6



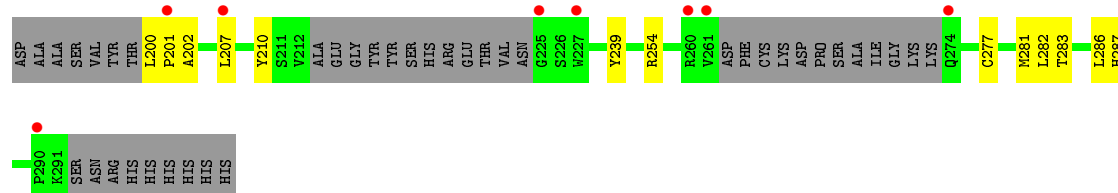
• Molecule 2: caspase-6



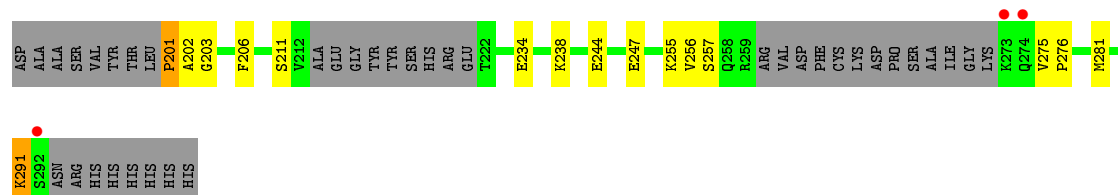
• Molecule 2: caspase-6



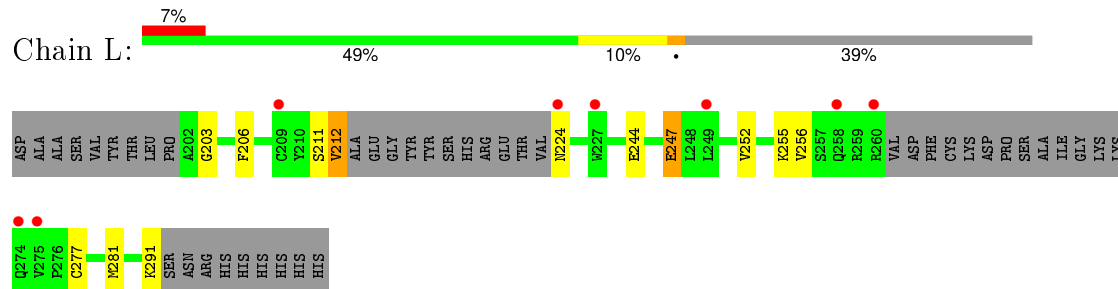
• Molecule 2: caspase-6



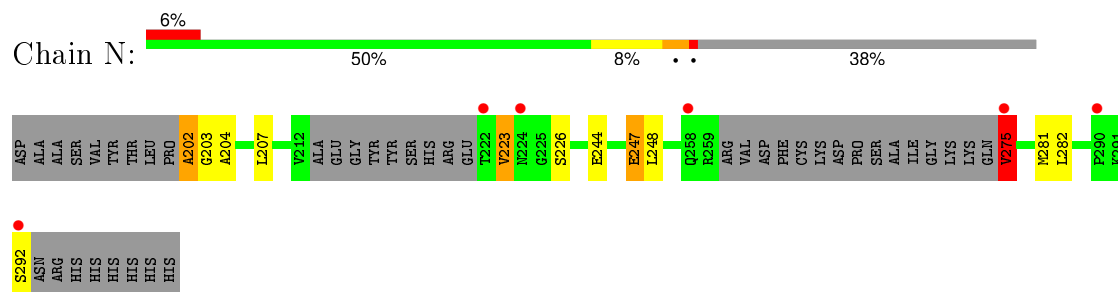
• Molecule 2: caspase-6



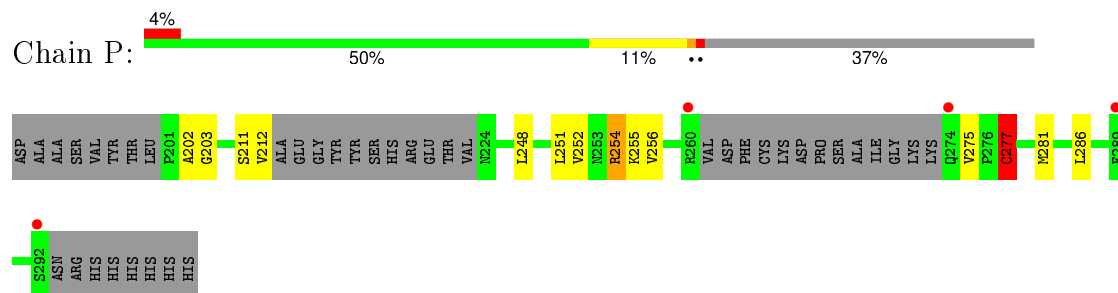
- Molecule 2: caspase-6



- Molecule 2: caspase-6



- Molecule 2: caspase-6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.23Å 161.24Å 88.92Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	29.96 – 2.53 29.96 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.96-2.53) 99.9 (29.96-2.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.207 , 0.264 0.207 , 0.259	Depositor DCC
$R_{free}$ test set	3815 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 75784 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.00	1/1083 (0.1%)	0.99	4/1460 (0.3%)
1	C	0.88	0/1080	0.87	0/1457
1	E	0.95	0/1083	0.92	0/1458
1	G	0.82	0/1065	0.82	0/1437
1	I	0.97	1/1089 (0.1%)	0.90	1/1468 (0.1%)
1	K	0.77	0/1061	0.84	0/1431
1	M	0.96	2/1080 (0.2%)	0.93	1/1456 (0.1%)
1	O	0.79	0/1068	0.88	1/1442 (0.1%)
2	B	0.90	1/591 (0.2%)	0.85	0/794
2	D	0.91	0/565	0.83	1/759 (0.1%)
2	F	1.00	1/545 (0.2%)	0.85	0/730
2	H	0.86	1/556 (0.2%)	0.85	0/745
2	J	0.99	1/554 (0.2%)	0.88	0/743
2	L	0.91	2/531 (0.4%)	0.81	0/711
2	N	0.95	1/541 (0.2%)	0.94	2/725 (0.3%)
2	P	0.92	1/549 (0.2%)	0.82	1/735 (0.1%)
All	All	0.91	12/13041 (0.1%)	0.88	11/17551 (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	C	0	2
1	I	0	1
1	O	0	1
2	J	0	1
2	N	0	2
All	All	0	7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	277	CYS	CB-SG	-8.36	1.68	1.82
2	P	277	CYS	CB-SG	-7.90	1.68	1.82
1	I	95	GLU	CG-CD	6.80	1.62	1.51
2	L	247	GLU	CG-CD	6.73	1.62	1.51
2	N	247	GLU	CG-CD	6.47	1.61	1.51
2	L	277	CYS	CB-SG	-5.98	1.72	1.81
1	M	95	GLU	CG-CD	5.77	1.60	1.51
1	A	116	CYS	CB-SG	-5.76	1.72	1.81
2	J	291	LYS	CE-NZ	5.76	1.63	1.49
2	B	277	CYS	CB-SG	-5.54	1.72	1.81
2	H	277	CYS	CB-SG	-5.43	1.73	1.81
1	M	148	CYS	CB-SG	-5.01	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	98	LEU	CB-CG-CD1	-7.32	98.56	111.00
1	O	96	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	110	ASP	CB-CA-C	-6.67	97.06	110.40
2	N	203	GLY	N-CA-C	-5.91	98.33	113.10
2	P	254	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	A	110	ASP	CB-CG-OD2	-5.53	113.32	118.30
2	D	259	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	71	ARG	NE-CZ-NH1	-5.26	117.67	120.30
2	N	275	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	131	ASP	N-CA-CB	-5.21	101.21	110.60
1	I	64	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	130	TYR	Peptide
1	C	31	PHE	Peptide
1	I	130	TYR	Peptide
2	J	201	PRO	Peptide
2	N	202	ALA	Mainchain,Peptide
1	O	130	TYR	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	1058	0	1020	25	0
1	C	1054	0	1013	28	0
1	E	1058	0	1033	40	0
1	G	1040	0	1000	19	0
1	I	1063	0	1025	35	0
1	K	1037	0	996	32	0
1	M	1055	0	1018	37	0
1	O	1043	0	997	38	0
2	B	579	0	582	12	0
2	D	554	0	555	14	0
2	F	535	0	531	7	0
2	H	545	0	553	13	0
2	J	543	0	533	14	0
2	L	521	0	515	13	0
2	N	531	0	532	12	0
2	P	538	0	534	16	0
3	A	24	0	0	1	0
3	B	7	0	0	1	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
3	E	30	0	0	3	0
3	F	11	0	0	0	0
3	G	8	0	0	0	0
3	H	7	0	0	1	0
3	I	21	0	0	0	0
3	J	10	0	0	0	0
3	K	14	0	0	4	0
3	L	6	0	0	0	0
3	M	29	0	0	1	0
3	N	4	0	0	0	0
3	O	8	0	0	0	0
3	P	6	0	0	0	0
All	All	12955	0	12437	301	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 12.

All (301) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:PRO:HB2	2:H:281:MET:SD	1.77	1.24
1:O:88:PHE:HB3	1:O:91:LEU:HD21	1.34	1.09
1:I:161:GLN:HE21	1:I:161:GLN:HA	1.12	1.09
2:B:201:PRO:HB2	2:B:281:MET:SD	1.97	1.03
1:I:127:ILE:HD12	1:I:127:ILE:O	1.60	1.01
1:I:60:THR:O	1:I:60:THR:HG22	1.61	0.99
1:I:60:THR:CG2	1:I:60:THR:O	2.11	0.97
1:I:161:GLN:HE21	1:I:161:GLN:CA	1.80	0.94
2:D:201:PRO:HB2	2:D:281:MET:SD	2.10	0.90
1:M:98:LEU:H	1:M:98:LEU:HD12	1.36	0.90
1:M:59:LEU:O	1:M:60:THR:HG22	1.76	0.86
1:E:51:ASN:ND2	1:E:67:THR:CG2	2.42	0.83
1:G:51:ASN:HD21	1:G:67:THR:HG23	1.44	0.82
1:O:127:ILE:HD12	1:O:127:ILE:O	1.79	0.82
1:E:59:LEU:O	1:E:60:THR:HG22	1.81	0.80
2:B:275:VAL:HB	2:D:281:MET:HE3	1.64	0.80
1:E:51:ASN:ND2	1:E:67:THR:HG22	1.97	0.80
1:M:98:LEU:HD13	1:M:99:LYS:N	1.97	0.79
1:I:127:ILE:HD12	1:I:127:ILE:C	2.00	0.78
1:G:60:THR:HG22	1:G:60:THR:O	1.82	0.78
1:M:95:GLU:O	1:M:98:LEU:CD1	2.32	0.78
2:L:203:GLY:HA2	2:L:281:MET:HE1	1.66	0.77
1:I:127:ILE:C	1:I:127:ILE:CD1	2.54	0.77
1:M:60:THR:HG23	1:M:60:THR:O	1.84	0.76
1:O:88:PHE:HB3	1:O:91:LEU:CD2	2.16	0.75
1:E:118:PHE:CZ	1:E:139:LEU:HD13	2.22	0.75
1:K:97:LEU:HD23	1:K:100:ILE:HD11	1.69	0.74
1:A:110:ASP:HB2	3:A:194:HOH:O	1.86	0.74
1:I:161:GLN:NE2	1:I:161:GLN:HA	1.97	0.73
1:A:133:LYS:HZ3	1:E:126:HIS:HE1	1.36	0.73
2:N:204:ALA:HB2	2:P:275:VAL:HG21	1.70	0.73
1:A:51:ASN:HB3	1:A:89:ASN:ND2	2.04	0.73
1:G:144:LYS:HD3	2:H:202:ALA:HB1	1.70	0.71
2:J:275:VAL:HB	2:L:281:MET:HE3	1.72	0.71
1:C:101:HIS:O	1:C:105:THR:HG22	1.91	0.71
1:M:161:GLN:NE2	2:N:226:SER:OG	2.17	0.70
2:N:202:ALA:HA	2:N:281:MET:SD	2.32	0.70
1:M:98:LEU:HD13	1:M:98:LEU:C	2.10	0.70
1:M:98:LEU:CD1	1:M:98:LEU:N	2.55	0.70
1:I:50:PHE:CE1	1:I:96:LEU:HD13	2.27	0.69
2:J:275:VAL:HB	2:L:281:MET:CE	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:97:LEU:HA	1:O:100:ILE:HG22	1.75	0.69
1:G:51:ASN:HD21	1:G:67:THR:CG2	2.06	0.69
2:B:201:PRO:HG2	2:B:281:MET:HG3	1.75	0.68
1:A:75:THR:HG23	1:A:85:VAL:HG11	1.75	0.68
1:M:120:SER:HB3	1:M:127:ILE:HD11	1.76	0.68
2:D:211:SER:OG	2:D:212:VAL:HG23	1.93	0.68
2:F:275:VAL:HB	2:H:281:MET:HE3	1.76	0.67
1:I:161:GLN:NE2	1:I:161:GLN:CA	2.57	0.67
1:E:60:THR:HG23	1:E:60:THR:O	1.94	0.67
1:E:51:ASN:HD21	1:E:67:THR:CG2	2.05	0.67
2:B:254:ARG:NE	3:B:96:HOH:O	2.22	0.67
1:C:51:ASN:HD21	1:C:67:THR:HG23	1.58	0.67
1:C:56:PHE:HZ	1:G:98:LEU:HD22	1.59	0.67
1:A:133:LYS:NZ	1:E:126:HIS:HE1	1.93	0.66
1:A:126:HIS:HE1	1:E:133:LYS:NZ	1.94	0.65
1:M:120:SER:HB3	1:M:127:ILE:CD1	2.26	0.65
2:F:275:VAL:HB	2:H:281:MET:CE	2.27	0.65
1:E:74:LEU:HD11	2:F:229:ILE:HD12	1.79	0.65
1:O:145:GLY:O	1:O:146:ASP:CB	2.44	0.65
1:I:127:ILE:O	1:I:127:ILE:CD1	2.43	0.64
2:B:275:VAL:HB	2:D:281:MET:CE	2.27	0.64
1:M:95:GLU:O	1:M:98:LEU:HD11	1.96	0.64
1:K:97:LEU:HA	1:K:100:ILE:HD11	1.78	0.64
1:K:48:LEU:HD12	1:K:103:VAL:HG21	1.77	0.64
1:K:118:PHE:CD2	1:K:127:ILE:HD13	2.33	0.64
1:M:98:LEU:HD12	1:M:98:LEU:N	2.03	0.64
2:L:203:GLY:HA2	2:L:281:MET:CE	2.28	0.64
1:M:48:LEU:HD13	1:M:50:PHE:CE2	2.33	0.63
1:A:51:ASN:HB3	1:A:89:ASN:HD22	1.63	0.63
2:H:207:LEU:HD22	2:H:282:LEU:HD11	1.78	0.63
2:D:248:LEU:O	2:D:248:LEU:HD23	1.99	0.62
1:K:59:LEU:O	1:K:60:THR:HG22	1.99	0.62
1:G:47:ALA:HB3	1:G:85:VAL:HG22	1.81	0.61
2:J:256:VAL:HG11	2:J:276:PRO:HD3	1.83	0.61
1:O:144:LYS:CE	2:P:202:ALA:HB1	2.31	0.61
1:A:127:ILE:O	1:A:127:ILE:HD12	2.00	0.61
1:G:48:LEU:HD13	1:G:50:PHE:CE2	2.35	0.61
1:G:48:LEU:HD13	1:G:50:PHE:CZ	2.35	0.60
1:C:118:PHE:CZ	1:C:139:LEU:HD13	2.36	0.60
1:C:48:LEU:HD11	1:C:103:VAL:HG11	1.83	0.60
1:A:118:PHE:CZ	1:A:139:LEU:HD13	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:MET:O	2:L:291:LYS:NZ	2.33	0.60
2:J:202:ALA:HB3	2:J:206:PHE:CD1	2.37	0.59
2:J:202:ALA:HB3	2:J:206:PHE:CG	2.37	0.59
1:A:133:LYS:NZ	1:E:135:GLU:OE1	2.34	0.59
1:I:118:PHE:CZ	1:I:139:LEU:HD13	2.38	0.58
2:D:248:LEU:C	2:D:248:LEU:HD23	2.24	0.58
1:O:127:ILE:C	1:O:127:ILE:HD12	2.24	0.57
1:C:100:ILE:O	1:C:103:VAL:HG22	2.04	0.57
1:O:96:LEU:HD12	1:O:134:ILE:CD1	2.34	0.57
2:F:283:THR:O	2:H:254:ARG:HD3	2.04	0.57
2:F:223:VAL:HG12	2:F:224:ASN:N	2.20	0.56
1:O:134:ILE:HG21	1:O:139:LEU:HD21	1.87	0.56
1:K:126:HIS:HE1	1:O:133:LYS:NZ	2.05	0.55
1:E:51:ASN:ND2	1:E:67:THR:HG21	2.20	0.55
1:O:127:ILE:C	1:O:127:ILE:CD1	2.75	0.55
1:C:51:ASN:HD21	1:C:67:THR:CG2	2.19	0.55
1:G:71:ARG:NH2	1:G:72:ASP:OD1	2.40	0.55
1:I:98:LEU:HD22	1:M:56:PHE:HZ	1.71	0.55
1:O:41:HIS:HB3	1:O:110:ASP:O	2.07	0.54
1:M:42:ARG:HH11	1:M:43:ARG:HE	1.54	0.54
1:E:51:ASN:HD21	1:E:67:THR:HG22	1.64	0.54
2:P:252:VAL:O	2:P:256:VAL:HG23	2.08	0.54
1:C:127:ILE:O	1:C:127:ILE:HD12	2.08	0.54
1:I:75:THR:O	1:I:79:SER:HB2	2.07	0.54
1:I:161:GLN:NE2	2:J:211:SER:CB	2.71	0.53
1:K:96:LEU:O	1:K:100:ILE:HG13	2.08	0.53
1:O:50:PHE:CE1	1:O:96:LEU:HD22	2.44	0.53
2:N:275:VAL:HB	2:P:281:MET:HE3	1.90	0.53
1:C:100:ILE:HA	1:C:103:VAL:HG22	1.90	0.53
1:A:31:PHE:HE2	2:D:258:GLN:NE2	2.07	0.53
1:M:59:LEU:O	1:M:60:THR:CG2	2.55	0.53
1:C:48:LEU:HD21	1:C:103:VAL:HG11	1.91	0.53
1:O:71:ARG:HD2	1:O:72:ASP:OD1	2.07	0.53
1:O:51:ASN:HD21	1:O:67:THR:HG23	1.74	0.53
1:E:102:GLU:CD	3:E:185:HOH:O	2.47	0.53
1:A:94:GLU:HG2	1:E:56:PHE:CE1	2.44	0.52
1:E:96:LEU:HD13	1:E:96:LEU:C	2.30	0.52
1:A:133:LYS:NZ	1:E:126:HIS:CE1	2.77	0.52
1:I:41:HIS:O	2:J:291:LYS:HE3	2.10	0.52
1:K:48:LEU:CD1	1:K:103:VAL:HG21	2.40	0.51
2:N:275:VAL:HB	2:P:281:MET:CE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:211:SER:OG	2:L:212:VAL:HG12	2.11	0.51
1:K:48:LEU:HD22	1:K:50:PHE:CE2	2.45	0.51
2:D:245:PHE:CE2	2:D:249:LEU:HD11	2.45	0.51
1:M:60:THR:CG2	1:M:60:THR:O	2.55	0.51
2:P:248:LEU:O	2:P:248:LEU:HD23	2.11	0.51
1:M:41:HIS:HD2	1:M:112:ASP:OD1	1.93	0.51
1:A:59:LEU:O	1:A:60:THR:HG22	2.11	0.51
1:I:161:GLN:HE22	2:J:211:SER:CB	2.24	0.51
1:E:51:ASN:HD22	1:E:67:THR:CG2	2.21	0.51
1:O:144:LYS:HE2	2:P:202:ALA:HB1	1.92	0.50
2:H:254:ARG:NE	3:H:122:HOH:O	2.44	0.50
1:C:43:ARG:O	1:C:111:ALA:HA	2.12	0.50
1:K:131:ASP:OD1	1:O:94:GLU:HG3	2.12	0.50
1:G:42:ARG:HD2	1:G:43:ARG:HG3	1.94	0.50
2:F:254:ARG:NH1	2:H:283:THR:O	2.37	0.50
1:I:41:HIS:CD2	1:I:112:ASP:HA	2.46	0.50
1:E:98:LEU:HD12	3:E:186:HOH:O	2.11	0.50
2:B:201:PRO:HB2	2:B:281:MET:CG	2.41	0.49
2:B:244:GLU:OE1	2:B:246:THR:OG1	2.25	0.49
1:E:33:PRO:HG3	2:H:239:TYR:CZ	2.47	0.49
1:E:71:ARG:NH2	3:E:194:HOH:O	2.46	0.49
1:O:127:ILE:O	1:O:127:ILE:CD1	2.57	0.49
1:E:118:PHE:CE2	1:E:139:LEU:HD13	2.47	0.49
2:P:203:GLY:HA2	2:P:281:MET:HE1	1.94	0.49
1:M:95:GLU:HA	1:M:98:LEU:HD11	1.95	0.49
1:C:102:GLU:HA	1:C:105:THR:CG2	2.43	0.49
2:N:207:LEU:HD22	2:N:282:LEU:HD11	1.95	0.48
2:L:224:ASN:OD1	2:L:224:ASN:O	2.30	0.48
1:E:101:HIS:O	1:E:105:THR:HB	2.13	0.48
1:M:42:ARG:HH11	1:M:43:ARG:NE	2.11	0.48
1:C:122:GLY:HA3	1:C:162:ALA:HB1	1.96	0.48
1:C:71:ARG:HE	1:C:89:ASN:HD21	1.62	0.48
1:C:41:HIS:CD2	1:C:112:ASP:HA	2.48	0.48
2:H:201:PRO:HG2	2:H:281:MET:HG3	1.95	0.48
1:O:50:PHE:CD1	1:O:96:LEU:HD22	2.48	0.48
2:D:201:PRO:CB	2:D:281:MET:SD	2.96	0.48
1:M:64:ARG:O	1:M:67:THR:HG22	2.13	0.48
1:E:91:LEU:HB3	1:E:95:GLU:HG3	1.96	0.48
1:I:43:ARG:HH12	1:I:110:ASP:HB2	1.79	0.48
1:M:121:HIS:O	1:M:127:ILE:HD13	2.14	0.47
1:O:154:LYS:O	1:O:156:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:HIS:HB3	1:O:133:LYS:HB2	1.96	0.47
1:A:60:THR:HG23	1:A:60:THR:O	2.15	0.47
2:L:244:GLU:O	2:L:247:GLU:HB2	2.15	0.47
2:J:203:GLY:O	2:J:206:PHE:HD2	1.97	0.47
2:H:201:PRO:CB	2:H:281:MET:SD	2.73	0.47
2:N:281:MET:HG2	2:P:277:CYS:HB3	1.97	0.47
2:J:244:GLU:O	2:J:247:GLU:HB2	2.14	0.47
1:E:127:ILE:HD12	1:E:127:ILE:C	2.35	0.47
1:K:94:GLU:O	1:K:98:LEU:HG	2.14	0.47
1:A:31:PHE:CE2	2:D:258:GLN:NE2	2.83	0.47
2:N:223:VAL:CG1	2:N:223:VAL:O	2.64	0.46
1:E:64:ARG:NH1	1:E:67:THR:OG1	2.48	0.46
1:E:50:PHE:CE1	1:E:96:LEU:HD22	2.49	0.46
1:K:94:GLU:HG2	1:O:56:PHE:CE1	2.50	0.46
1:O:116:CYS:O	1:O:158:PHE:HA	2.16	0.46
1:A:33:PRO:HB3	2:D:251:LEU:HD11	1.96	0.46
1:O:135:GLU:O	1:O:138:THR:HB	2.15	0.46
1:K:98:LEU:CD1	3:K:188:HOH:O	2.62	0.46
1:I:60:THR:O	1:I:60:THR:HG23	2.07	0.46
1:K:98:LEU:HD12	3:K:188:HOH:O	2.16	0.46
2:H:286:LEU:HD12	2:H:287:HIS:N	2.30	0.46
1:M:135:GLU:O	1:M:138:THR:HB	2.15	0.46
2:L:252:VAL:O	2:L:256:VAL:HG23	2.16	0.46
1:O:115:VAL:HG22	1:O:157:ILE:HB	1.96	0.46
1:M:57:TRP:HE1	1:M:58:HIS:CE1	2.34	0.46
2:B:201:PRO:CG	2:B:281:MET:HG3	2.45	0.46
1:M:71:ARG:HD2	1:M:72:ASP:OD1	2.15	0.46
1:E:96:LEU:CD1	1:E:96:LEU:C	2.84	0.46
1:A:77:ARG:HD2	1:A:77:ARG:HA	1.68	0.46
1:G:108:HIS:HB2	1:G:150:SER:OG	2.16	0.46
1:E:151:LEU:O	1:E:156:LYS:NZ	2.49	0.46
1:C:56:PHE:CZ	1:G:98:LEU:HD22	2.46	0.45
1:K:134:ILE:CG2	1:K:139:LEU:HD21	2.46	0.45
1:C:157:ILE:HD11	2:D:286:LEU:HD21	1.97	0.45
1:O:125:ASN:HB3	1:O:137:GLN:HE22	1.81	0.45
1:I:50:PHE:CE1	1:I:96:LEU:CD1	2.99	0.45
2:F:211:SER:OG	2:F:212:VAL:N	2.50	0.45
2:B:201:PRO:CB	2:B:281:MET:SD	2.88	0.45
1:E:55:PHE:N	1:E:55:PHE:CD2	2.84	0.45
1:K:71:ARG:HE	1:K:89:ASN:HD21	1.64	0.45
1:M:94:GLU:O	1:M:98:LEU:HD12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:157:ILE:HD11	2:P:286:LEU:HD21	1.98	0.45
3:K:180:HOH:O	1:O:132:ALA:HB1	2.17	0.45
1:I:94:GLU:OE1	1:M:92:LYS:NZ	2.41	0.45
2:N:281:MET:HG2	2:P:277:CYS:CB	2.47	0.45
1:K:87:CYS:N	3:K:187:HOH:O	2.41	0.45
1:I:119:LEU:HD23	1:I:161:GLN:HB3	1.98	0.45
1:E:50:PHE:CD1	1:E:96:LEU:HD22	2.52	0.45
1:K:44:ARG:HA	1:K:112:ASP:OD2	2.17	0.44
2:N:244:GLU:O	2:N:247:GLU:HB2	2.17	0.44
1:M:98:LEU:H	1:M:98:LEU:CD1	2.11	0.44
1:I:98:LEU:HD22	1:M:56:PHE:CZ	2.52	0.44
1:C:102:GLU:HA	1:C:105:THR:HG22	2.00	0.44
1:C:127:ILE:HD11	1:C:139:LEU:HD11	2.00	0.43
1:C:100:ILE:O	1:C:103:VAL:CG2	2.66	0.43
1:K:39:MET:SD	1:K:112:ASP:HB3	2.58	0.43
1:G:77:ARG:HD3	1:G:77:ARG:HA	1.79	0.43
1:A:78:PHE:O	1:A:83:PHE:HB2	2.18	0.43
1:E:41:HIS:CD2	1:E:112:ASP:HA	2.53	0.43
1:I:51:ASN:HD22	1:I:119:LEU:HD12	1.84	0.43
1:K:101:HIS:O	1:K:105:THR:HG23	2.18	0.43
1:M:48:LEU:HD13	1:M:50:PHE:HE2	1.79	0.43
1:G:98:LEU:HD13	1:G:98:LEU:HA	1.70	0.43
1:K:48:LEU:CD2	1:K:50:PHE:CE2	3.00	0.43
1:M:33:PRO:HA	2:P:251:LEU:HD21	2.00	0.43
1:M:41:HIS:CD2	1:M:112:ASP:OD1	2.71	0.43
1:I:31:PHE:CZ	2:L:255:LYS:HD2	2.53	0.43
1:O:117:VAL:HG22	1:O:159:ILE:HB	2.01	0.43
1:G:51:ASN:ND2	1:G:67:THR:OG1	2.52	0.43
2:J:234:GLU:OE2	2:J:238:LYS:HE2	2.18	0.43
1:E:124:GLY:O	1:E:125:ASN:HB2	2.19	0.43
1:I:50:PHE:CD1	1:I:96:LEU:HD13	2.52	0.43
2:L:211:SER:OG	2:L:212:VAL:N	2.52	0.43
2:P:248:LEU:C	2:P:248:LEU:HD23	2.39	0.43
1:I:51:ASN:HB3	1:I:89:ASN:ND2	2.34	0.42
1:K:134:ILE:HG21	1:K:139:LEU:HD21	2.01	0.42
1:O:137:GLN:H	1:O:137:GLN:NE2	2.17	0.42
1:E:50:PHE:CD1	1:E:96:LEU:CD2	3.01	0.42
1:M:32:ASP:HA	1:M:33:PRO:HD2	1.94	0.42
1:C:50:PHE:CD1	1:C:96:LEU:HD22	2.54	0.42
1:I:50:PHE:CZ	1:I:96:LEU:CD1	3.01	0.42
1:O:96:LEU:O	1:O:100:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:97:LEU:HA	1:O:100:ILE:CG2	2.48	0.42
1:C:41:HIS:HD2	1:C:112:ASP:OD1	2.02	0.42
2:B:200:LEU:HD12	2:D:277:CYS:SG	2.59	0.42
1:G:60:THR:O	1:G:60:THR:CG2	2.53	0.42
1:O:123:GLU:O	1:O:126:HIS:HD2	2.02	0.42
2:P:203:GLY:CA	2:P:281:MET:HE1	2.49	0.42
2:B:256:VAL:HG11	2:B:276:PRO:HD3	2.01	0.42
2:H:200:LEU:N	2:H:210:TYR:HH	2.18	0.42
1:A:127:ILE:C	1:A:127:ILE:HD12	2.40	0.42
1:M:71:ARG:HE	1:M:89:ASN:HD21	1.66	0.42
1:E:124:GLY:O	1:E:125:ASN:CB	2.68	0.42
1:O:97:LEU:CA	1:O:100:ILE:HG22	2.48	0.41
2:J:256:VAL:CG1	2:J:276:PRO:HD3	2.50	0.41
1:K:59:LEU:O	1:K:60:THR:CG2	2.65	0.41
1:I:118:PHE:CE2	1:I:139:LEU:HD13	2.55	0.41
1:M:108:HIS:O	1:M:154:LYS:NZ	2.53	0.41
1:M:100:ILE:HG21	1:M:139:LEU:HD22	2.02	0.41
1:I:57:TRP:CD1	1:I:58:HIS:CE1	3.08	0.41
1:C:151:LEU:O	1:C:156:LYS:NZ	2.53	0.41
1:A:133:LYS:HZ3	1:E:126:HIS:CE1	2.26	0.41
1:G:48:LEU:HA	1:G:48:LEU:HD23	1.86	0.41
1:O:115:VAL:HA	1:O:157:ILE:O	2.20	0.41
1:K:135:GLU:HG2	1:O:133:LYS:HZ3	1.85	0.41
1:C:56:PHE:O	1:C:59:LEU:HB2	2.21	0.41
1:K:88:PHE:CE1	1:K:99:LYS:HE3	2.56	0.41
1:K:41:HIS:CD2	1:K:112:ASP:HA	2.56	0.41
1:K:51:ASN:ND2	1:K:67:THR:OG1	2.53	0.41
1:I:161:GLN:NE2	2:J:211:SER:HB3	2.35	0.41
2:N:204:ALA:CB	2:P:275:VAL:HG21	2.45	0.41
1:C:97:LEU:O	1:C:100:ILE:HG22	2.21	0.41
1:O:123:GLU:HG3	1:O:123:GLU:O	2.20	0.41
1:A:94:GLU:HG2	1:E:56:PHE:CZ	2.56	0.41
1:C:65:ARG:HH21	2:D:223:VAL:HG13	1.85	0.41
1:O:51:ASN:HD21	1:O:67:THR:CG2	2.33	0.41
1:C:108:HIS:O	1:C:109:ALA:C	2.59	0.41
1:I:120:SER:O	1:I:162:ALA:HA	2.21	0.41
1:I:138:THR:HG21	3:M:207:HOH:O	2.21	0.41
2:P:211:SER:OG	2:P:212:VAL:N	2.53	0.41
1:E:51:ASN:HD21	1:E:67:THR:CB	2.34	0.41
1:K:97:LEU:CD2	1:K:100:ILE:HD11	2.45	0.41
1:I:57:TRP:HD1	1:I:58:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:ASP:OD2	2:L:291:LYS:NZ	2.48	0.40
2:B:231:ASP:OD2	2:B:259:ARG:HD2	2.20	0.40
1:K:56:PHE:HD2	1:K:59:LEU:HD23	1.86	0.40
2:N:248:LEU:HD23	2:N:248:LEU:C	2.41	0.40
1:C:56:PHE:CZ	1:G:98:LEU:CD2	3.04	0.40
1:K:43:ARG:HE	1:K:43:ARG:HB2	1.66	0.40
2:J:201:PRO:HB2	2:J:281:MET:HE1	2.03	0.40
1:G:37:TYR:O	1:G:39:MET:HG2	2.21	0.40
1:A:41:HIS:HD2	1:A:112:ASP:OD1	2.03	0.40
1:M:41:HIS:CE1	1:M:154:LYS:HE2	2.57	0.40
1:A:96:LEU:C	1:A:96:LEU:CD1	2.90	0.40
1:E:59:LEU:O	1:E:60:THR:CG2	2.60	0.40
2:L:203:GLY:O	2:L:206:PHE:HD2	2.04	0.40
1:A:126:HIS:HE1	1:E:133:LYS:HZ1	1.68	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	131/179 (73%)	126 (96%)	4 (3%)	1 (1%)	24	40
1	C	130/179 (73%)	123 (95%)	6 (5%)	1 (1%)	24	40
1	E	130/179 (73%)	120 (92%)	9 (7%)	1 (1%)	24	40
1	G	129/179 (72%)	120 (93%)	9 (7%)	0	100	100
1	I	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	K	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	M	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	O	130/179 (73%)	122 (94%)	6 (5%)	2 (2%)	13	22
2	B	66/108 (61%)	62 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	64/108 (59%)	62 (97%)	2 (3%)	0	100	100
2	F	62/108 (57%)	57 (92%)	5 (8%)	0	100	100
2	H	62/108 (57%)	59 (95%)	3 (5%)	0	100	100
2	J	64/108 (59%)	61 (95%)	3 (5%)	0	100	100
2	L	60/108 (56%)	57 (95%)	3 (5%)	0	100	100
2	N	61/108 (56%)	57 (93%)	4 (7%)	0	100	100
2	P	62/108 (57%)	60 (97%)	2 (3%)	0	100	100
All	All	1544/2296 (67%)	1467 (95%)	72 (5%)	5 (0%)	46	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	123	GLU
1	E	146	ASP
1	O	146	ASP
1	A	144	LYS
1	C	149	HIS

### 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	111/154 (72%)	103 (93%)	8 (7%)	18	32
1	C	110/154 (71%)	105 (96%)	5 (4%)	34	57
1	E	111/154 (72%)	105 (95%)	6 (5%)	27	47
1	G	109/154 (71%)	101 (93%)	8 (7%)	17	31
1	I	112/154 (73%)	103 (92%)	9 (8%)	15	27
1	K	107/154 (70%)	96 (90%)	11 (10%)	9	16
1	M	110/154 (71%)	99 (90%)	11 (10%)	9	17
1	O	108/154 (70%)	100 (93%)	8 (7%)	17	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	65/95 (68%)	63 (97%)	2 (3%)	47	74
2	D	62/95 (65%)	58 (94%)	4 (6%)	21	37
2	F	59/95 (62%)	56 (95%)	3 (5%)	29	51
2	H	61/95 (64%)	61 (100%)	0	100	100
2	J	59/95 (62%)	57 (97%)	2 (3%)	44	70
2	L	57/95 (60%)	56 (98%)	1 (2%)	66	87
2	N	60/95 (63%)	57 (95%)	3 (5%)	30	52
2	P	60/95 (63%)	57 (95%)	3 (5%)	30	52
All	All	1361/1992 (68%)	1277 (94%)	84 (6%)	23	40

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	48	LEU
1	A	59	LEU
1	A	77	ARG
1	A	96	LEU
1	A	103	VAL
1	A	123	GLU
1	A	144	LYS
2	B	199	THR
2	B	226	SER
1	C	57	TRP
1	C	59	LEU
1	C	96	LEU
1	C	101	HIS
1	C	107	SER
2	D	222	THR
2	D	257	SER
2	D	277	CYS
2	D	284	LYS
1	E	36	LYS
1	E	59	LEU
1	E	96	LEU
1	E	98	LEU
1	E	105	THR
1	E	106	VAL
2	F	212	VAL

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Mol	Chain	Res	Type
2	F	257	SER
2	F	281	MET
1	G	42	ARG
1	G	57	TRP
1	G	92	LYS
1	G	98	LEU
1	G	106	VAL
1	G	125	ASN
1	G	135	GLU
1	G	146	ASP
1	I	42	ARG
1	I	60	THR
1	I	79	SER
1	I	96	LEU
1	I	98	LEU
1	I	106	VAL
1	I	123	GLU
1	I	127	ILE
1	I	161	GLN
2	J	255	LYS
2	J	257	SER
1	K	43	ARG
1	K	79	SER
1	K	98	LEU
1	K	99	LYS
1	K	100	ILE
1	K	102	GLU
1	K	123	GLU
1	K	135	GLU
1	K	138	THR
1	K	160	ILE
1	K	163	CYS
2	L	212	VAL
1	M	35	GLU
1	M	48	LEU
1	M	53	GLU
1	M	57	TRP
1	M	60	THR
1	M	98	LEU
1	M	99	LYS
1	M	100	ILE
1	M	103	VAL

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Mol	Chain	Res	Type
1	M	127	ILE
1	M	161	GLN
2	N	223	VAL
2	N	275	VAL
2	N	292	SER
1	O	36	LYS
1	O	48	LEU
1	O	60	THR
1	O	96	LEU
1	O	98	LEU
1	O	127	ILE
1	O	137	GLN
1	O	161	GLN
2	P	254	ARG
2	P	255	LYS
2	P	277	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	51	ASN
1	A	89	ASN
1	A	126	HIS
2	B	230	GLN
2	B	274	GLN
1	C	41	HIS
1	C	51	ASN
1	C	58	HIS
1	C	89	ASN
1	C	126	HIS
2	D	258	GLN
1	E	41	HIS
1	E	51	ASN
1	E	89	ASN
1	E	126	HIS
1	G	51	ASN
1	G	58	HIS
1	G	101	HIS
1	G	125	ASN
1	I	41	HIS
1	I	51	ASN

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Mol	Chain	Res	Type
1	I	58	HIS
1	I	89	ASN
1	I	161	GLN
2	J	230	GLN
2	J	274	GLN
1	K	41	HIS
1	K	51	ASN
1	K	52	HIS
1	K	89	ASN
1	K	126	HIS
2	L	224	ASN
1	M	41	HIS
1	M	51	ASN
1	M	89	ASN
1	M	161	GLN
1	O	41	HIS
1	O	51	ASN
1	O	58	HIS
1	O	89	ASN
1	O	126	HIS
1	O	137	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

## 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, 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	133/179 (74%)	0.04	5 (3%) 44 50	13, 22, 41, 55	0
1	C	132/179 (73%)	0.23	10 (7%) 17 18	17, 34, 58, 66	0
1	E	132/179 (73%)	-0.09	3 (2%) 64 68	12, 23, 40, 56	0
1	G	131/179 (73%)	0.23	10 (7%) 17 18	20, 35, 52, 67	0
1	I	133/179 (74%)	-0.03	2 (1%) 76 80	11, 20, 41, 61	0
1	K	133/179 (74%)	0.42	10 (7%) 17 19	23, 38, 53, 62	0
1	M	133/179 (74%)	-0.02	4 (3%) 54 59	12, 23, 44, 60	0
1	O	132/179 (73%)	0.33	10 (7%) 17 18	23, 37, 68, 77	0
2	B	72/108 (66%)	0.42	4 (5%) 28 32	17, 27, 48, 67	0
2	D	70/108 (64%)	0.38	5 (7%) 19 21	19, 33, 53, 62	0
2	F	68/108 (62%)	0.46	9 (13%) 4 4	13, 28, 56, 72	0
2	H	68/108 (62%)	0.70	8 (11%) 6 6	18, 34, 53, 74	0
2	J	70/108 (64%)	0.24	3 (4%) 39 45	14, 27, 44, 52	0
2	L	66/108 (61%)	0.44	8 (12%) 6 6	21, 36, 52, 64	0
2	N	67/108 (62%)	0.37	6 (8%) 12 13	16, 31, 51, 55	0
2	P	68/108 (62%)	0.42	4 (5%) 26 30	23, 35, 53, 78	0
All	All	1608/2296 (70%)	0.24	101 (6%) 23 26	11, 30, 54, 78	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	260	ARG	6.1
2	H	261	VAL	6.0
2	B	260	ARG	5.3
1	O	31	PHE	4.9
2	P	292	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	I	31	PHE	4.2
2	L	260	ARG	4.1
2	H	225	GLY	4.1
1	K	31	PHE	3.9
1	G	57	TRP	3.9
1	E	31	PHE	3.9
1	A	31	PHE	3.8
1	C	146	ASP	3.8
2	J	292	SER	3.7
2	F	223	VAL	3.7
2	P	260	ARG	3.5
2	L	224	ASN	3.3
1	C	123	GLU	3.2
2	F	227	TRP	3.2
1	C	31	PHE	3.2
1	K	159	ILE	3.2
2	J	273	LYS	3.1
2	F	292	SER	3.0
1	C	124	GLY	3.0
1	O	146	ASP	3.0
1	E	57	TRP	2.9
1	G	79	SER	2.9
2	N	290	PRO	2.9
1	G	40	ASP	2.8
1	K	149	HIS	2.8
2	F	274	GLN	2.7
1	C	57	TRP	2.7
1	G	146	ASP	2.7
1	C	149	HIS	2.7
2	N	292	SER	2.7
1	M	31	PHE	2.7
2	D	222	THR	2.6
1	C	159	ILE	2.6
2	D	289	PHE	2.6
1	O	147	LYS	2.5
1	C	157	ILE	2.5
1	O	159	ILE	2.5
2	L	227	TRP	2.5
2	P	274	GLN	2.5
1	G	62	PRO	2.5
1	A	123	GLU	2.5
2	L	209	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	149	HIS	2.4
2	D	258	GLN	2.4
2	D	260	ARG	2.4
1	M	124	GLY	2.4
1	O	40	ASP	2.4
2	H	227	TRP	2.4
2	H	274	GLN	2.4
2	J	274	GLN	2.4
2	N	222	THR	2.3
1	G	82	GLY	2.3
1	A	159	ILE	2.3
1	K	38	LYS	2.3
1	I	123	GLU	2.2
1	K	116	CYS	2.2
1	E	124	GLY	2.2
2	F	290	PRO	2.2
1	O	32	ASP	2.2
1	G	38	LYS	2.2
2	L	274	GLN	2.2
1	M	123	GLU	2.2
2	F	207	LEU	2.2
2	B	199	THR	2.2
2	F	259	ARG	2.2
2	N	224	ASN	2.2
1	A	146	ASP	2.2
1	C	116	CYS	2.2
2	N	275	VAL	2.1
1	G	159	ILE	2.1
2	B	209	CYS	2.1
2	N	258	GLN	2.1
1	K	117	VAL	2.1
1	K	35	GLU	2.1
1	O	82	GLY	2.1
2	L	275	VAL	2.1
2	F	291	LYS	2.1
1	A	124	GLY	2.1
1	M	60	THR	2.1
2	L	249	LEU	2.1
1	K	157	ILE	2.1
1	K	145	GLY	2.1
1	O	123	GLU	2.1
2	B	207	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	80	ASP	2.1
1	K	40	ASP	2.1
2	L	258	GLN	2.0
2	F	260	ARG	2.0
1	G	157	ILE	2.0
2	H	201	PRO	2.0
2	D	209	CYS	2.0
1	O	125	ASN	2.0
1	C	62	PRO	2.0
2	H	290	PRO	2.0
2	H	207	LEU	2.0
2	P	289	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.