



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:34 pm BST

PDB ID : 1Q4Q  
Title : Crystal structure of a DIAP1-Dronc complex  
Authors : Chai, J.; Yan, N.; Shi, Y.  
Deposited on : 2003-08-04  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

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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 : 2.11  
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) : 2.11

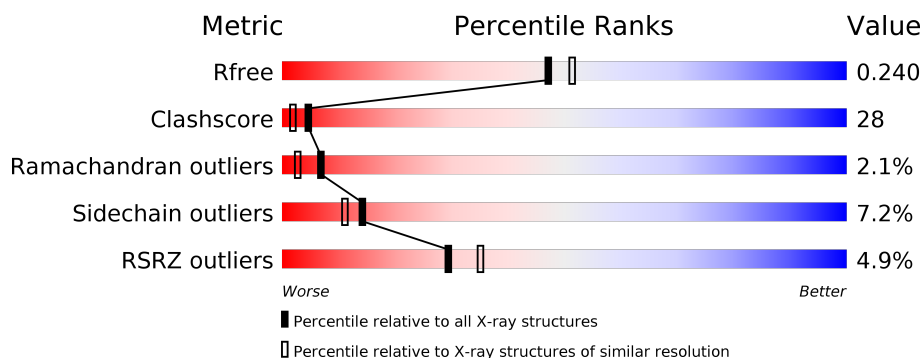
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	124	<div> <div>2%</div> <div>47% 26% 24%</div> </div>
1	B	124	<div> <div>58% 21% 19%</div> </div>
1	C	124	<div> <div>2%</div> <div>51% 20% 5% 24%</div> </div>
1	D	124	<div> <div>2%</div> <div>44% 27% 24%</div> </div>
1	E	124	<div> <div>11%</div> <div>35% 35% 10% 19%</div> </div>
1	F	124	<div> <div>2%</div> <div>47% 26% 24%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	124	
1	H	124	
1	I	124	
1	J	124	
2	K	12	
2	L	12	
2	M	12	
2	N	12	
2	O	12	
2	P	12	
2	Q	12	
2	R	12	
2	S	12	
2	T	12	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9166 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 Apoptosis 1 inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			777	502	134	136	5			
1	B	101	Total	C	N	O	S	0	0	0
			833	537	142	149	5			
1	C	94	Total	C	N	O	S	0	0	0
			777	502	134	136	5			
1	D	94	Total	C	N	O	S	0	0	0
			777	502	134	136	5			
1	E	101	Total	C	N	O	S	0	0	0
			833	537	142	149	5			
1	F	94	Total	C	N	O	S	0	0	0
			777	502	134	136	5			
1	G	101	Total	C	N	O	S	0	0	0
			833	537	142	149	5			
1	H	94	Total	C	N	O	S	0	0	0
			777	502	134	136	5			
1	I	94	Total	C	N	O	S	0	0	0
			777	502	134	136	5			
1	J	101	Total	C	N	O	S	0	0	0
			833	537	142	149	5			

- Molecule 2 is a protein called Nedd2-like caspase CG8091-PA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	8	Total	C	N	O	0	0	0
			66	44	12	10			
2	L	8	Total	C	N	O	0	0	0
			66	44	12	10			
2	M	7	Total	C	N	O	0	0	0
			55	38	8	9			
2	N	8	Total	C	N	O	0	0	0
			66	44	12	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	8	Total	C	N	O	0	0	0
			66	44	12	10			
2	P	8	Total	C	N	O	0	0	0
			66	44	12	10			
2	Q	7	Total	C	N	O	0	0	0
			55	38	8	9			
2	R	7	Total	C	N	O	0	0	0
			55	38	8	9			
2	S	7	Total	C	N	O	0	0	0
			55	38	8	9			
2	T	7	Total	C	N	O	0	0	0
			55	38	8	9			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		

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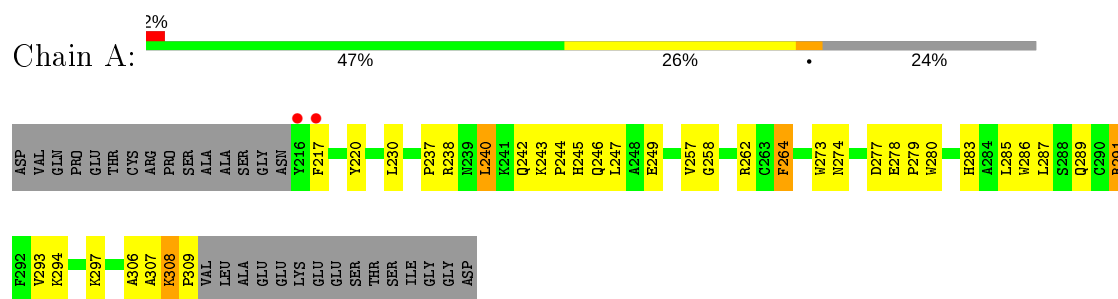
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	59	Total 59	O 59	0	0
4	C	57	Total 57	O 57	0	0
4	D	55	Total 55	O 55	0	0
4	E	35	Total 35	O 35	0	0
4	F	45	Total 45	O 45	0	0
4	G	69	Total 69	O 69	0	0
4	H	62	Total 62	O 62	0	0
4	I	42	Total 42	O 42	0	0
4	J	38	Total 38	O 38	0	0
4	K	3	Total 3	O 3	0	0
4	L	2	Total 2	O 2	0	0
4	M	1	Total 1	O 1	0	0
4	N	4	Total 4	O 4	0	0
4	O	9	Total 9	O 9	0	0
4	P	2	Total 2	O 2	0	0
4	Q	1	Total 1	O 1	0	0
4	R	7	Total 7	O 7	0	0
4	S	3	Total 3	O 3	0	0
4	T	6	Total 6	O 6	0	0

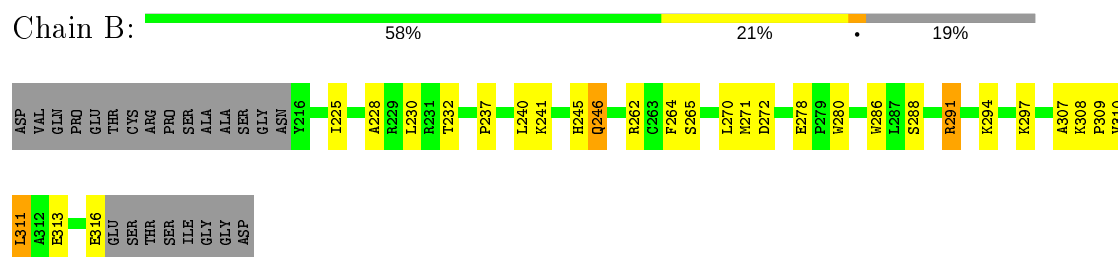
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

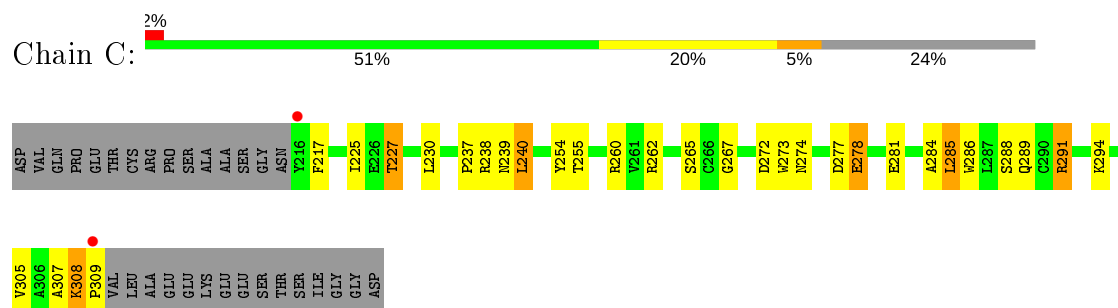
- Molecule 1: Apoptosis 1 inhibitor



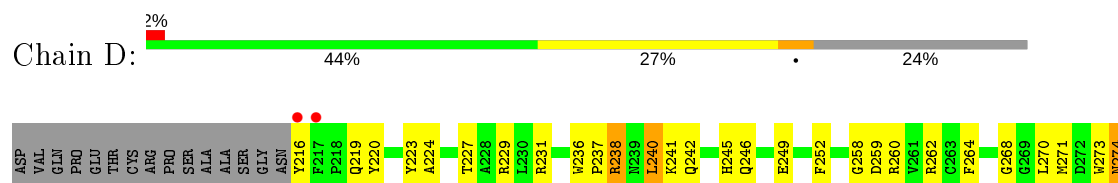
- Molecule 1: Apoptosis 1 inhibitor



- Molecule 1: Apoptosis 1 inhibitor



- Molecule 1: Apoptosis 1 inhibitor





- Molecule 1: Apoptosis 1 inhibitor



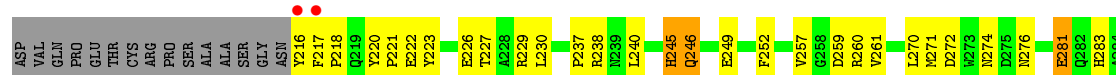
- Molecule 1: Apoptosis 1 inhibitor



- Molecule 1: Apoptosis 1 inhibitor



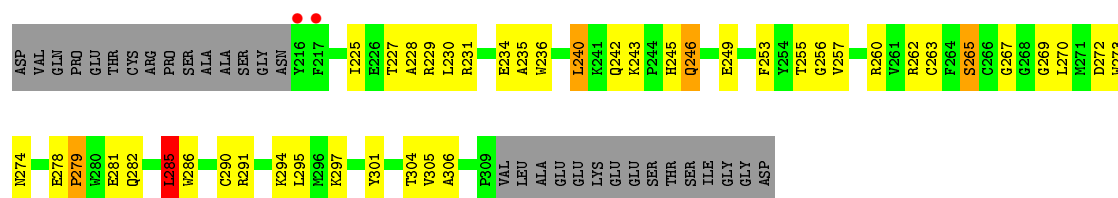
- Molecule 1: Apoptosis 1 inhibitor



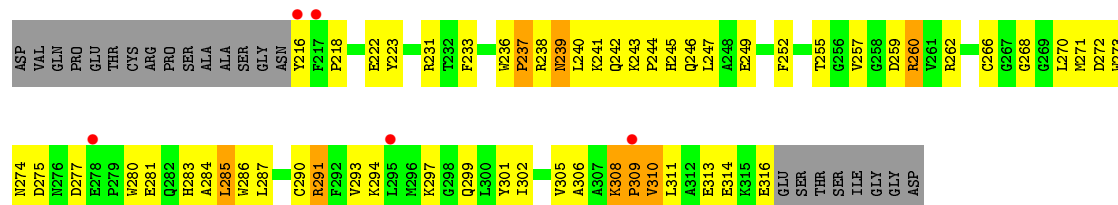
- Molecule 1: Apoptosis 1 inhibitor



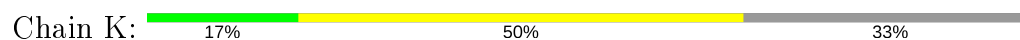




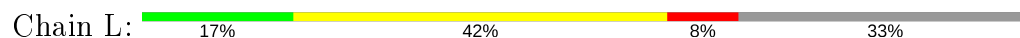
- Molecule 1: Apoptosis 1 inhibitor



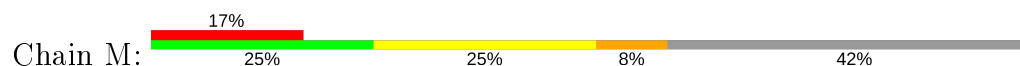
- Molecule 2: Nedd2-like caspase CG8091-PA



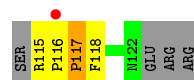
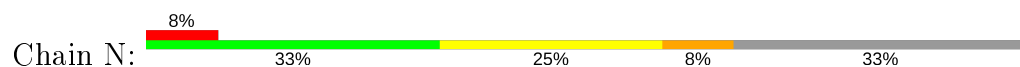
- Molecule 2: Nedd2-like caspase CG8091-PA



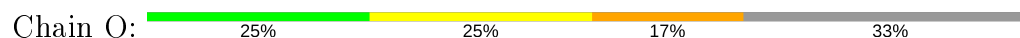
- Molecule 2: Nedd2-like caspase CG8091-PA



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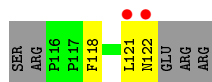
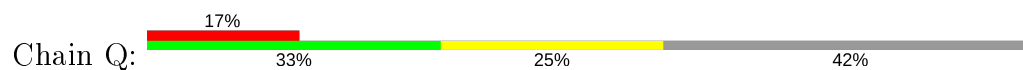




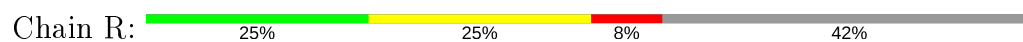
- Molecule 2: Nedd2-like caspase CG8091-PA



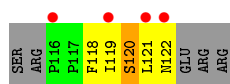
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- Molecule 2: Nedd2-like caspase CG8091-PA



- Molecule 2: Nedd2-like caspase CG8091-PA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.90Å 128.90Å 183.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10 29.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.10) 94.1 (29.53-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.39 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.199 , 0.246 0.197 , 0.240	Depositor DCC
$R_{free}$ test set	4404 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	0.40	0/803	0.62	0/1089
1	B	0.38	0/859	0.61	0/1164
1	C	0.37	0/803	0.62	0/1089
1	D	0.38	0/803	0.57	0/1089
1	E	0.35	0/859	0.70	2/1164 (0.2%)
1	F	0.38	0/803	0.61	0/1089
1	G	0.39	0/859	0.61	0/1164
1	H	0.36	0/803	0.59	0/1089
1	I	0.39	0/803	0.59	0/1089
1	J	0.37	0/859	0.58	0/1164
2	K	0.38	0/68	0.66	0/92
2	L	0.51	0/68	0.98	1/92 (1.1%)
2	M	0.34	0/57	0.60	0/77
2	N	0.70	0/68	1.19	2/92 (2.2%)
2	O	0.46	0/68	2.06	2/92 (2.2%)
2	P	0.48	0/68	0.77	0/92
2	Q	0.33	0/57	0.67	0/77
2	R	0.35	0/57	0.88	0/77
2	S	0.40	0/57	0.63	0/77
2	T	0.34	0/57	0.62	0/77
All	All	0.38	0/8879	0.65	7/12035 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	115	ARG	C-N-CD	-14.48	88.74	120.60
2	O	115	ARG	C-N-CA	8.86	159.21	122.00
1	E	308	LYS	C-N-CD	-7.67	103.73	120.60
2	N	115	ARG	NE-CZ-NH1	-7.03	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	309	PRO	N-CA-C	5.36	126.03	112.10
2	L	115	ARG	C-N-CD	5.09	139.09	128.40
2	N	115	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	777	0	734	35	0
1	B	833	0	790	21	0
1	C	777	0	734	40	0
1	D	777	0	734	39	0
1	E	833	0	790	90	0
1	F	777	0	734	42	0
1	G	833	0	790	56	1
1	H	777	0	734	30	0
1	I	777	0	734	46	0
1	J	833	0	790	82	0
2	K	66	0	68	10	0
2	L	66	0	68	12	0
2	M	55	0	56	9	0
2	N	66	0	68	2	0
2	O	66	0	68	10	0
2	P	66	0	68	8	1
2	Q	55	0	56	9	0
2	R	55	0	56	6	0
2	S	55	0	56	23	0
2	T	55	0	56	25	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	57	0	0	0	0
4	B	59	0	0	2	0
4	C	57	0	0	2	0
4	D	55	0	0	1	0
4	E	35	0	0	3	0
4	F	45	0	0	4	0
4	G	69	0	0	4	0
4	H	62	0	0	2	0
4	I	42	0	0	3	0
4	J	38	0	0	3	0
4	K	3	0	0	0	0
4	L	2	0	0	0	0
4	M	1	0	0	0	0
4	N	4	0	0	0	0
4	O	9	0	0	0	0
4	P	2	0	0	0	0
4	Q	1	0	0	0	0
4	R	7	0	0	1	0
4	S	3	0	0	0	0
4	T	6	0	0	1	0
All	All	9166	0	8184	473	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (473) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:LEU:HD23	2:S:121:LEU:HD21	1.28	1.11
1:E:274:ASN:HD21	2:S:122:ASN:ND2	1.56	1.03
2:K:115:ARG:HB3	2:K:116:PRO:HD2	1.46	0.96
1:G:237:PRO:HB2	1:G:240:LEU:HD22	1.48	0.95
1:E:274:ASN:HD21	2:S:122:ASN:HD22	1.12	0.94
1:A:243:LYS:HE2	1:A:243:LYS:HA	1.51	0.93
1:F:231:ARG:NH2	2:L:116:PRO:HB2	1.84	0.92
1:J:308:LYS:N	1:J:309:PRO:HD3	1.82	0.92
1:E:308:LYS:HA	1:E:310:VAL:H	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ARG:HH11	2:R:117:PRO:HD2	1.36	0.91
1:C:237:PRO:HB2	1:C:240:LEU:HD22	1.53	0.90
1:J:231:ARG:HE	2:N:117:PRO:HD2	1.34	0.90
1:C:308:LYS:HA	1:C:309:PRO:C	1.94	0.88
1:I:243:LYS:HE2	1:I:243:LYS:HA	1.56	0.87
1:E:260:ARG:HB3	2:S:118:PHE:CE2	2.09	0.87
1:F:308:LYS:CB	1:F:309:PRO:HD2	2.05	0.87
1:E:265:SER:HB3	1:E:292:PHE:HB2	1.56	0.86
1:C:278:GLU:H	1:C:278:GLU:CD	1.79	0.86
1:J:237:PRO:HB2	1:J:240:LEU:HD22	1.58	0.86
1:J:266:CYS:SG	1:J:287:LEU:HD13	2.16	0.86
1:E:237:PRO:HB2	1:E:240:LEU:HD13	1.58	0.85
1:G:308:LYS:O	1:G:311:LEU:HD22	1.76	0.85
1:D:231:ARG:NH1	2:R:117:PRO:HD2	1.92	0.85
2:L:115:ARG:HB2	2:L:116:PRO:HD2	1.57	0.84
1:D:237:PRO:HB2	1:D:240:LEU:HD22	1.58	0.84
1:J:242:GLN:HB3	1:J:247:LEU:HD21	1.62	0.81
1:D:270:LEU:HD13	2:Q:121:LEU:HD21	1.62	0.81
1:J:245:HIS:O	1:J:249:GLU:HG3	1.81	0.81
1:E:290:CYS:SG	1:E:292:PHE:HB3	2.20	0.81
1:F:308:LYS:HB2	1:F:309:PRO:HD2	1.61	0.80
1:J:260:ARG:HG2	1:J:260:ARG:HH11	1.47	0.79
1:E:227:THR:HA	1:E:230:LEU:HD12	1.63	0.79
1:E:291:ARG:O	1:E:295:LEU:HD13	1.82	0.78
1:J:283:HIS:HD2	1:J:287:LEU:HB2	1.49	0.78
1:H:291:ARG:O	1:H:295:LEU:HD13	1.85	0.76
1:D:291:ARG:O	1:D:295:LEU:HD13	1.86	0.76
1:A:246:GLN:HG2	1:A:279:PRO:HG2	1.68	0.75
1:A:243:LYS:H	1:A:246:GLN:NE2	1.84	0.75
1:F:237:PRO:HB2	1:F:240:LEU:HD22	1.69	0.75
1:J:310:VAL:O	1:J:314:GLU:HG3	1.87	0.74
1:F:231:ARG:HG2	2:L:119:ILE:HD11	1.70	0.73
1:C:238:ARG:HB3	1:C:238:ARG:HH11	1.53	0.73
1:I:243:LYS:HE2	1:I:243:LYS:CA	2.19	0.73
1:E:238:ARG:HH11	1:E:238:ARG:HG2	1.52	0.73
1:J:257:VAL:O	1:J:260:ARG:HD3	1.88	0.73
1:I:231:ARG:HD3	2:K:119:ILE:HD11	1.70	0.73
1:E:308:LYS:HG2	1:E:308:LYS:O	1.89	0.73
1:E:229:ARG:HD2	1:E:252:PHE:O	1.90	0.72
1:E:274:ASN:ND2	2:S:122:ASN:ND2	2.36	0.72
1:J:308:LYS:N	1:J:309:PRO:CD	2.52	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:ASN:ND2	2:S:122:ASN:HD22	1.85	0.71
1:E:274:ASN:ND2	2:S:122:ASN:HB2	2.06	0.70
1:G:228:ALA:O	1:G:231:ARG:HG2	1.92	0.70
1:J:260:ARG:HD2	1:J:260:ARG:N	2.07	0.70
1:J:272:ASP:O	2:T:121:LEU:HB2	1.92	0.69
1:E:238:ARG:CG	1:E:238:ARG:HH11	2.05	0.69
1:A:306:ALA:O	1:A:309:PRO:HD2	1.93	0.69
1:D:241:LYS:HG3	1:D:275:ASP:O	1.93	0.69
1:J:308:LYS:H	1:J:309:PRO:HD3	1.56	0.69
1:F:231:ARG:NH2	4:F:611:HOH:O	2.25	0.68
1:E:270:LEU:CD2	2:S:121:LEU:HD21	2.15	0.68
1:H:238:ARG:HD3	1:I:272:ASP:HB3	1.75	0.68
1:B:270:LEU:HD22	2:R:121:LEU:HD21	1.75	0.68
1:E:237:PRO:HA	4:J:620:HOH:O	1.93	0.68
1:I:242:GLN:NE2	1:I:273:TRP:HB3	2.09	0.68
1:E:238:ARG:HH21	2:T:122:ASN:N	1.91	0.68
1:E:240:LEU:HD11	1:J:240:LEU:HD11	1.76	0.68
1:F:219:GLN:HG2	1:F:267:GLY:HA3	1.75	0.68
1:A:220:TYR:OH	2:O:115:ARG:HD3	1.94	0.68
1:E:270:LEU:HD23	2:S:121:LEU:CD2	2.16	0.67
1:C:274:ASN:ND2	2:P:122:ASN:HB2	2.10	0.67
1:A:243:LYS:O	1:A:246:GLN:HB3	1.94	0.67
1:G:237:PRO:HB2	1:G:240:LEU:CD2	2.22	0.67
1:B:237:PRO:HB2	1:B:240:LEU:HD13	1.78	0.66
1:C:307:ALA:O	1:C:308:LYS:HB2	1.96	0.66
1:F:285:LEU:HD23	1:F:305:VAL:HG12	1.76	0.66
1:G:260:ARG:HB3	2:K:118:PHE:CE2	2.29	0.66
1:B:230:LEU:HB3	2:T:119:ILE:HD13	1.77	0.66
1:A:240:LEU:O	1:A:243:LYS:HE3	1.96	0.66
1:E:282:GLN:O	1:E:286:TRP:HD1	1.79	0.66
1:G:290:CYS:O	1:G:294:LYS:HG3	1.96	0.66
1:J:271:MET:SD	2:T:118:PHE:HB2	2.36	0.66
1:H:285:LEU:HG	1:H:305:VAL:HG12	1.79	0.65
1:E:233:PHE:HB2	1:E:244:PRO:HB3	1.78	0.65
1:J:290:CYS:HB3	1:J:293:VAL:HG23	1.78	0.65
2:K:115:ARG:CB	2:K:116:PRO:HD2	2.24	0.65
1:G:310:VAL:O	1:G:314:GLU:HG3	1.97	0.65
1:F:216:TYR:HD1	1:F:291:ARG:HD2	1.62	0.65
1:A:285:LEU:O	1:A:285:LEU:HD13	1.96	0.64
1:E:238:ARG:NH2	2:T:122:ASN:H	1.95	0.64
1:D:274:ASN:HB2	2:Q:122:ASN:ND2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ALA:HB1	1:J:257:VAL:HG12	1.80	0.64
1:J:272:ASP:OD2	2:T:120:SER:HA	1.98	0.63
1:E:282:GLN:CB	2:S:121:LEU:HD13	2.29	0.63
1:J:299:GLN:NE2	1:J:302:ILE:HB	2.13	0.63
4:E:608:HOH:O	1:J:237:PRO:HB3	1.98	0.63
1:D:245:HIS:HD2	1:D:249:GLU:OE2	1.81	0.63
1:J:309:PRO:HD2	1:J:310:VAL:HG12	1.81	0.63
2:T:118:PHE:H	2:T:118:PHE:HD1	1.45	0.63
1:D:291:ARG:NH2	1:D:294:LYS:HD2	2.14	0.63
1:E:243:LYS:HG2	1:E:245:HIS:H	1.64	0.63
1:E:274:ASN:HD21	2:S:122:ASN:CG	2.01	0.63
1:E:262:ARG:HH11	1:E:262:ARG:HG2	1.65	0.62
1:C:239:ASN:ND2	1:D:274:ASN:HA	2.14	0.62
1:F:308:LYS:CB	1:F:309:PRO:CD	2.77	0.62
1:E:286:TRP:CZ2	2:S:121:LEU:O	2.52	0.62
1:E:274:ASN:HD21	2:S:122:ASN:CB	2.12	0.62
2:T:118:PHE:CD1	2:T:118:PHE:N	2.68	0.62
1:E:291:ARG:HA	1:E:291:ARG:HE	1.65	0.61
1:C:289:GLN:HA	1:C:289:GLN:HE21	1.64	0.61
1:J:313:GLU:O	1:J:316:GLU:HG3	2.00	0.61
1:B:307:ALA:HA	1:B:310:VAL:CG1	2.31	0.61
1:E:309:PRO:HD2	4:E:606:HOH:O	2.00	0.61
1:G:308:LYS:HG3	1:G:311:LEU:HD13	1.83	0.61
1:J:260:ARG:HG2	1:J:260:ARG:NH1	2.16	0.61
1:J:291:ARG:HH21	1:J:294:LYS:HD2	1.66	0.61
1:I:234:GLU:O	1:I:235:ALA:HB3	2.00	0.61
1:I:274:ASN:HD21	2:M:122:ASN:HB2	1.66	0.60
1:C:281:GLU:O	1:C:285:LEU:HB2	2.01	0.60
1:E:272:ASP:OD1	1:J:238:ARG:HD3	2.01	0.60
1:C:291:ARG:HH21	1:C:294:LYS:CD	2.14	0.60
1:D:277:ASP:OD2	2:Q:122:ASN:ND2	2.33	0.60
1:G:278:GLU:OE2	1:G:281:GLU:HB2	2.02	0.60
1:A:308:LYS:H	1:A:309:PRO:CD	2.14	0.60
1:H:260:ARG:HH21	1:I:235:ALA:HA	1.66	0.60
1:D:216:TYR:CE1	1:D:295:LEU:HD21	2.37	0.59
1:J:285:LEU:HD13	1:J:286:TRP:NE1	2.17	0.59
1:A:262:ARG:NH2	2:O:115:ARG:HB2	2.17	0.59
1:J:268:GLY:HA3	1:J:287:LEU:CD2	2.33	0.59
1:C:238:ARG:HB3	1:C:238:ARG:NH1	2.18	0.59
1:A:280:TRP:CD2	1:A:297:LYS:HD2	2.38	0.59
1:D:216:TYR:HE1	1:D:295:LEU:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:GLY:HA2	1:J:237:PRO:HG3	1.84	0.59
1:E:291:ARG:O	1:E:295:LEU:HD22	2.02	0.59
1:G:311:LEU:HD23	1:G:312:ALA:N	2.18	0.59
1:D:242:GLN:CD	1:D:242:GLN:H	2.07	0.58
1:F:281:GLU:O	1:F:285:LEU:HB2	2.03	0.58
1:C:291:ARG:HH21	1:C:294:LYS:HD2	1.68	0.58
2:T:120:SER:HB2	4:T:322:HOH:O	2.03	0.58
1:J:247:LEU:HD23	1:J:247:LEU:N	2.17	0.58
1:E:238:ARG:HH21	2:T:122:ASN:CA	2.16	0.58
1:F:216:TYR:CD1	1:F:291:ARG:HD2	2.38	0.58
1:J:273:TRP:HE3	1:J:277:ASP:HB3	1.69	0.58
1:E:223:TYR:C	1:E:225:ILE:N	2.56	0.58
1:F:243:LYS:H	1:F:246:GLN:NE2	2.02	0.58
1:D:260:ARG:HB3	2:Q:118:PHE:CZ	2.39	0.57
1:G:308:LYS:HB3	1:G:309:PRO:HD3	1.86	0.57
1:J:283:HIS:CD2	1:J:287:LEU:HB2	2.36	0.57
1:H:245:HIS:CD2	1:H:246:GLN:HG3	2.39	0.57
1:G:285:LEU:HD22	1:I:245:HIS:NE2	2.19	0.57
1:J:311:LEU:HD23	1:J:311:LEU:O	2.04	0.57
1:J:274:ASN:HD21	2:T:121:LEU:HB3	1.70	0.57
1:A:280:TRP:CG	1:A:297:LYS:HD2	2.39	0.57
1:J:271:MET:CG	2:T:118:PHE:HB2	2.35	0.57
1:E:286:TRP:CZ3	1:G:245:HIS:HB2	2.39	0.57
1:G:227:THR:HA	1:G:230:LEU:HD12	1.87	0.57
2:L:115:ARG:HB2	2:L:116:PRO:CD	2.28	0.57
1:A:291:ARG:HH21	1:A:294:LYS:HE3	1.71	0.56
1:G:311:LEU:HA	1:G:314:GLU:OE2	2.05	0.56
2:K:115:ARG:HB3	2:K:116:PRO:CD	2.27	0.56
1:E:282:GLN:HB3	2:S:121:LEU:HD13	1.87	0.56
1:E:255:THR:HG21	1:E:262:ARG:HD3	1.87	0.56
1:C:291:ARG:NH2	1:C:294:LYS:HE3	2.21	0.56
1:F:285:LEU:HD12	1:F:286:TRP:CE2	2.41	0.56
1:I:274:ASN:HD21	2:M:122:ASN:CG	2.08	0.56
1:J:306:ALA:O	1:J:309:PRO:HD3	2.05	0.56
1:F:285:LEU:HD23	1:F:305:VAL:CG1	2.36	0.56
1:B:313:GLU:O	1:B:316:GLU:HG3	2.05	0.56
1:G:310:VAL:O	1:G:313:GLU:HB3	2.06	0.56
1:I:265:SER:HB3	4:I:622:HOH:O	2.06	0.56
1:I:305:VAL:O	1:I:305:VAL:HG12	2.05	0.56
1:C:285:LEU:HD12	1:C:305:VAL:CG1	2.36	0.55
1:I:260:ARG:HB3	2:M:118:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:TYR:HE1	4:E:609:HOH:O	1.88	0.55
1:H:257:VAL:HG22	1:I:256:GLY:O	2.07	0.55
1:A:308:LYS:H	1:A:309:PRO:HD2	1.72	0.55
1:H:281:GLU:O	1:H:285:LEU:HB2	2.07	0.55
1:I:278:GLU:OE1	1:I:279:PRO:HD2	2.06	0.55
1:J:273:TRP:CE3	1:J:277:ASP:HB3	2.42	0.55
1:I:245:HIS:O	1:I:249:GLU:HG3	2.06	0.55
2:P:119:ILE:HD12	2:P:119:ILE:N	2.21	0.55
2:R:117:PRO:HG2	4:R:77:HOH:O	2.07	0.55
1:A:243:LYS:HE2	1:A:243:LYS:CA	2.30	0.55
1:E:223:TYR:O	1:E:229:ARG:NH2	2.40	0.55
1:I:243:LYS:HA	1:I:243:LYS:CE	2.35	0.55
1:E:233:PHE:CB	1:E:244:PRO:HB3	2.36	0.55
1:E:238:ARG:NH2	2:T:122:ASN:N	2.53	0.55
1:G:238:ARG:HG3	1:G:239:ASN:N	2.21	0.55
1:G:313:GLU:HG3	4:I:623:HOH:O	2.07	0.55
1:J:301:TYR:O	1:J:305:VAL:HG23	2.07	0.55
1:E:241:LYS:HG3	1:E:275:ASP:HA	1.88	0.54
1:F:272:ASP:HA	1:G:238:ARG:HG2	1.90	0.54
1:J:297:LYS:HA	1:J:297:LYS:HE2	1.88	0.54
1:B:307:ALA:O	1:B:311:LEU:HD23	2.07	0.54
1:I:274:ASN:HD21	2:M:122:ASN:CB	2.20	0.54
1:J:241:LYS:HE3	1:J:275:ASP:OD1	2.08	0.54
1:E:274:ASN:ND2	2:S:122:ASN:CB	2.68	0.54
1:A:289:GLN:O	1:A:291:ARG:CZ	2.55	0.54
1:G:238:ARG:NH1	1:G:239:ASN:HB2	2.23	0.54
1:G:313:GLU:OE2	1:I:297:LYS:HE2	2.07	0.54
1:H:285:LEU:HB3	1:H:286:TRP:CD1	2.43	0.53
1:A:286:TRP:CE3	2:O:119:ILE:HG21	2.43	0.53
1:C:289:GLN:HA	1:C:289:GLN:NE2	2.24	0.53
1:E:281:GLU:HA	1:E:281:GLU:OE1	2.08	0.53
1:C:260:ARG:HB3	2:P:118:PHE:CE2	2.44	0.53
1:F:285:LEU:HD12	1:F:286:TRP:NE1	2.23	0.53
1:F:272:ASP:HB3	1:G:238:ARG:HD3	1.90	0.53
1:A:274:ASN:HB2	2:O:122:ASN:ND2	2.24	0.53
1:C:286:TRP:CE3	2:P:119:ILE:HG21	2.43	0.53
1:E:231:ARG:HD2	2:O:117:PRO:HG2	1.90	0.53
1:H:271:MET:HG2	2:L:118:PHE:HB3	1.90	0.53
1:J:274:ASN:OD1	2:T:122:ASN:HB2	2.09	0.53
1:F:308:LYS:O	1:F:309:PRO:O	2.27	0.53
1:D:223:TYR:HB3	1:D:229:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:HG2	1:A:273:TRP:CE3	2.44	0.52
1:C:285:LEU:HB3	1:C:286:TRP:CD1	2.44	0.52
1:C:278:GLU:OE2	1:C:278:GLU:N	2.38	0.52
1:D:260:ARG:HG2	1:D:271:MET:HB3	1.92	0.52
1:H:221:PRO:HD2	1:H:222:GLU:OE2	2.10	0.52
2:L:115:ARG:O	2:L:116:PRO:C	2.44	0.52
1:E:233:PHE:CD2	1:E:254:TYR:HB2	2.44	0.52
1:G:225:ILE:HG22	1:G:227:THR:H	1.75	0.52
1:J:310:VAL:HG23	4:J:637:HOH:O	2.10	0.52
1:E:238:ARG:HH21	2:T:122:ASN:H	1.54	0.52
1:C:255:THR:HG21	2:P:118:PHE:HZ	1.74	0.52
2:T:119:ILE:O	2:T:121:LEU:HD12	2.10	0.52
1:A:280:TRP:HZ3	1:A:293:VAL:HG22	1.75	0.51
1:J:262:ARG:HA	1:J:268:GLY:O	2.09	0.51
1:G:257:VAL:O	1:G:258:GLY:C	2.48	0.51
1:E:238:ARG:CG	1:E:238:ARG:NH1	2.65	0.51
1:J:243:LYS:H	1:J:246:GLN:NE2	2.08	0.51
1:E:252:PHE:HA	1:E:262:ARG:O	2.11	0.51
1:F:308:LYS:HB3	1:F:309:PRO:HD2	1.87	0.51
1:G:226:GLU:OE2	1:G:249:GLU:HA	2.11	0.51
1:J:271:MET:O	2:T:121:LEU:HD13	2.11	0.51
1:D:224:ALA:HA	1:D:264:PHE:CD1	2.46	0.50
1:F:282:GLN:O	1:F:286:TRP:HD1	1.93	0.50
1:E:254:TYR:HA	1:E:261:VAL:HG12	1.93	0.50
1:H:237:PRO:HB2	1:H:240:LEU:HD13	1.93	0.50
1:F:285:LEU:HD13	1:J:245:HIS:CE1	2.46	0.50
1:G:306:ALA:O	1:G:309:PRO:HD2	2.12	0.50
1:J:216:TYR:N	1:J:291:ARG:HG2	2.26	0.50
1:J:260:ARG:HB3	2:T:118:PHE:CE2	2.45	0.50
1:E:223:TYR:C	1:E:225:ILE:H	2.14	0.50
1:E:223:TYR:O	1:E:225:ILE:N	2.43	0.50
1:E:286:TRP:CD1	1:E:286:TRP:N	2.80	0.50
1:B:225:ILE:HG12	4:B:655:HOH:O	2.11	0.50
1:C:278:GLU:CD	1:C:278:GLU:N	2.56	0.50
1:G:274:ASN:HB2	2:K:122:ASN:ND2	2.26	0.50
1:B:278:GLU:OE2	1:B:280:TRP:N	2.45	0.50
1:G:231:ARG:HD2	4:G:659:HOH:O	2.12	0.50
2:P:115:ARG:HB3	2:P:116:PRO:HD2	1.93	0.50
1:D:278:GLU:OE1	1:D:281:GLU:N	2.35	0.50
1:C:262:ARG:HH12	2:P:116:PRO:HG2	1.76	0.49
1:G:311:LEU:HA	1:G:314:GLU:CD	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:GLU:CD	1:I:297:LYS:HE2	2.32	0.49
1:I:242:GLN:NE2	1:I:274:ASN:O	2.45	0.49
1:I:301:TYR:O	1:I:305:VAL:HG23	2.12	0.49
1:C:225:ILE:HG22	1:C:227:THR:H	1.76	0.49
1:D:246:GLN:HG3	4:D:634:HOH:O	2.12	0.49
1:J:268:GLY:HA3	1:J:287:LEU:HD22	1.93	0.49
1:J:299:GLN:HE22	1:J:302:ILE:HB	1.77	0.49
1:E:260:ARG:HB3	2:S:118:PHE:CZ	2.46	0.49
1:E:262:ARG:HG2	1:E:262:ARG:NH1	2.27	0.49
1:F:231:ARG:NH1	4:F:615:HOH:O	2.45	0.49
1:A:285:LEU:C	1:A:285:LEU:HD13	2.33	0.49
1:F:241:LYS:O	1:F:243:LYS:NZ	2.45	0.49
1:I:270:LEU:HD13	2:M:121:LEU:HD21	1.95	0.49
1:E:236:TRP:CZ3	1:E:259:ASP:HA	2.47	0.48
1:E:315:LYS:O	1:E:316:GLU:HB2	2.12	0.48
1:I:227:THR:O	1:I:231:ARG:HG2	2.13	0.48
1:D:291:ARG:HH21	1:D:294:LYS:HD2	1.78	0.48
1:E:237:PRO:HB2	1:E:240:LEU:CD1	2.39	0.48
1:E:243:LYS:CD	1:E:245:HIS:HB3	2.43	0.48
4:F:609:HOH:O	1:G:241:LYS:HG2	2.12	0.48
1:E:278:GLU:HB3	1:E:281:GLU:HB2	1.94	0.48
1:F:308:LYS:HB3	1:F:309:PRO:CD	2.42	0.48
1:C:291:ARG:HH21	1:C:294:LYS:HE3	1.78	0.48
1:E:222:GLU:O	1:E:223:TYR:HD2	1.96	0.48
1:I:290:CYS:O	1:I:294:LYS:HG3	2.14	0.48
1:H:301:TYR:O	1:H:305:VAL:HG23	2.13	0.48
2:S:122:ASN:OD1	2:S:122:ASN:C	2.52	0.48
1:E:289:GLN:HE21	1:G:225:ILE:HD12	1.79	0.48
1:E:240:LEU:CD1	1:J:240:LEU:HD11	2.43	0.48
1:J:311:LEU:HD23	1:J:311:LEU:C	2.34	0.48
1:I:229:ARG:HG2	1:I:253:PHE:HB3	1.96	0.47
2:T:121:LEU:N	2:T:121:LEU:HD12	2.27	0.47
1:H:270:LEU:HD22	2:L:121:LEU:HD21	1.97	0.47
1:J:233:PHE:CG	1:J:244:PRO:HB3	2.49	0.47
1:F:230:LEU:HD21	1:F:245:HIS:HA	1.96	0.47
1:E:270:LEU:HB3	2:S:121:LEU:HD21	1.97	0.47
1:C:254:TYR:OH	1:D:258:GLY:HA2	2.14	0.47
1:H:220:TYR:OH	2:L:115:ARG:NH1	2.45	0.47
1:J:280:TRP:CD2	1:J:297:LYS:HD2	2.50	0.47
1:G:285:LEU:HB3	1:G:286:TRP:CD1	2.50	0.47
1:H:216:TYR:CZ	1:H:218:PRO:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:260:ARG:CD	1:J:260:ARG:N	2.76	0.47
1:B:271:MET:O	1:B:272:ASP:HB2	2.15	0.47
1:B:291:ARG:HA	1:B:291:ARG:HE	1.80	0.47
1:F:308:LYS:O	1:F:309:PRO:C	2.52	0.47
1:J:241:LYS:HG3	1:J:275:ASP:HA	1.96	0.47
1:J:290:CYS:HB3	1:J:293:VAL:CG2	2.44	0.47
1:A:245:HIS:O	1:A:249:GLU:HG3	2.15	0.46
1:D:294:LYS:HG2	1:D:302:ILE:CD1	2.44	0.46
1:D:270:LEU:HB3	2:Q:121:LEU:HD21	1.97	0.46
1:E:278:GLU:O	1:E:282:GLN:HG2	2.15	0.46
1:J:252:PHE:CZ	1:J:270:LEU:HD12	2.51	0.46
1:F:231:ARG:CZ	2:L:116:PRO:HB2	2.44	0.46
1:E:218:PRO:HB3	1:E:264:PHE:CE1	2.50	0.46
1:E:308:LYS:HA	1:E:310:VAL:N	2.15	0.46
1:B:228:ALA:O	1:B:232:THR:HG23	2.14	0.46
1:C:289:GLN:O	1:C:291:ARG:CZ	2.63	0.46
1:H:216:TYR:OH	1:H:218:PRO:HG3	2.15	0.46
1:A:307:ALA:O	1:A:308:LYS:HG3	2.16	0.46
1:C:272:ASP:OD1	1:D:238:ARG:HD2	2.15	0.46
1:D:245:HIS:O	1:D:249:GLU:HG3	2.15	0.46
1:G:270:LEU:HD22	2:K:121:LEU:HD21	1.98	0.46
1:I:257:VAL:HG22	4:I:630:HOH:O	2.16	0.46
1:F:272:ASP:HB3	1:G:238:ARG:CD	2.46	0.46
1:B:286:TRP:CE3	2:R:119:ILE:HG21	2.51	0.46
1:F:274:ASN:HA	1:G:238:ARG:HH12	1.82	0.46
1:J:236:TRP:CZ3	1:J:259:ASP:HA	2.51	0.46
1:J:281:GLU:HG2	1:J:301:TYR:OH	2.15	0.46
1:J:309:PRO:CD	1:J:310:VAL:H	2.29	0.46
1:A:238:ARG:NH1	1:A:238:ARG:HB3	2.31	0.45
1:B:241:LYS:HA	1:B:241:LYS:HD3	1.82	0.45
1:F:219:GLN:HB2	1:F:265:SER:O	2.16	0.45
1:G:283:HIS:HD2	1:G:287:LEU:HB2	1.82	0.45
1:H:309:PRO:HD3	4:H:667:HOH:O	2.15	0.45
1:I:304:THR:C	1:I:306:ALA:H	2.20	0.45
1:J:231:ARG:HD3	4:J:623:HOH:O	2.16	0.45
1:F:235:ALA:HB1	1:G:257:VAL:HG12	1.99	0.45
1:H:283:HIS:HD2	1:H:287:LEU:HB2	1.81	0.45
1:A:262:ARG:NH2	2:O:116:PRO:O	2.34	0.45
1:A:283:HIS:HD2	1:A:287:LEU:HB2	1.82	0.45
1:D:262:ARG:HA	1:D:268:GLY:O	2.16	0.45
1:E:265:SER:CB	1:E:292:PHE:HB2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:ARG:HH11	2:K:116:PRO:HB3	1.81	0.45
1:E:260:ARG:HG2	1:E:271:MET:HB3	1.99	0.45
1:E:231:ARG:CD	2:O:117:PRO:HG2	2.47	0.45
1:B:280:TRP:CD2	1:B:297:LYS:HD3	2.51	0.45
1:C:291:ARG:HH21	1:C:294:LYS:CE	2.29	0.45
1:F:273:TRP:O	1:G:238:ARG:NH1	2.50	0.45
1:H:286:TRP:N	1:H:286:TRP:CD1	2.85	0.45
1:I:225:ILE:O	1:I:228:ALA:HB3	2.17	0.45
1:I:286:TRP:CD2	2:M:119:ILE:HG21	2.52	0.45
1:G:312:ALA:HB3	4:G:674:HOH:O	2.16	0.44
1:H:222:GLU:CD	1:H:222:GLU:H	2.20	0.44
1:J:260:ARG:NH1	1:J:260:ARG:CG	2.80	0.44
1:C:278:GLU:OE2	1:C:281:GLU:HB2	2.18	0.44
1:G:286:TRP:CZ3	1:I:230:LEU:HD22	2.52	0.44
1:E:270:LEU:HB3	2:S:121:LEU:HG	1.99	0.44
1:E:233:PHE:CE2	1:E:247:LEU:HD13	2.52	0.44
1:G:278:GLU:HB3	1:G:281:GLU:HB3	2.00	0.44
1:D:270:LEU:HD22	2:Q:121:LEU:HD21	1.99	0.44
1:C:285:LEU:HD12	1:C:305:VAL:HG13	1.99	0.44
1:F:222:GLU:HG2	1:F:223:TYR:CD1	2.53	0.44
1:H:223:TYR:HB3	1:H:229:ARG:HG2	1.98	0.44
1:J:222:GLU:HG2	1:J:223:TYR:CD1	2.52	0.44
1:F:233:PHE:CB	1:F:244:PRO:HB3	2.48	0.44
1:G:289:GLN:O	1:G:291:ARG:CZ	2.66	0.44
1:D:260:ARG:HB3	2:Q:118:PHE:CE2	2.53	0.44
1:A:297:LYS:HE2	1:A:297:LYS:HA	1.99	0.44
1:I:263:CYS:O	1:I:267:GLY:HA2	2.17	0.44
1:B:308:LYS:N	1:B:309:PRO:HD2	2.33	0.43
1:D:219:GLN:HB3	1:D:220:TYR:CD1	2.53	0.43
1:E:249:GLU:C	1:E:251:GLY:H	2.21	0.43
1:G:311:LEU:HA	1:G:314:GLU:CG	2.48	0.43
1:I:234:GLU:O	1:I:235:ALA:CB	2.64	0.43
1:D:252:PHE:HA	1:D:262:ARG:O	2.18	0.43
1:I:262:ARG:NH1	1:I:269:GLY:HA3	2.33	0.43
1:A:308:LYS:N	1:A:309:PRO:CD	2.80	0.43
1:C:308:LYS:CA	1:C:309:PRO:C	2.78	0.43
1:H:285:LEU:HG	1:H:305:VAL:CG1	2.46	0.43
2:T:116:PRO:HA	2:T:117:PRO:HA	1.85	0.43
1:A:220:TYR:OH	2:O:115:ARG:CD	2.63	0.43
1:C:239:ASN:HD22	1:D:274:ASN:HA	1.83	0.43
1:G:245:HIS:CD2	1:G:249:GLU:OE2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:LYS:HE2	4:G:612:HOH:O	2.18	0.43
1:I:282:GLN:HG3	2:M:121:LEU:HD13	2.00	0.43
1:J:281:GLU:O	1:J:285:LEU:HB2	2.18	0.43
1:G:257:VAL:HG12	1:G:258:GLY:N	2.33	0.43
1:J:272:ASP:CB	2:T:121:LEU:H	2.31	0.43
2:K:115:ARG:CB	2:K:116:PRO:CD	2.90	0.43
4:B:643:HOH:O	1:D:227:THR:HG21	2.18	0.43
1:E:309:PRO:C	1:E:311:LEU:N	2.71	0.43
1:F:255:THR:HG21	2:N:118:PHE:HZ	1.84	0.43
1:J:280:TRP:HA	1:J:280:TRP:CE3	2.53	0.43
1:A:257:VAL:O	1:A:258:GLY:C	2.56	0.43
1:B:245:HIS:NE2	1:J:286:TRP:HH2	2.16	0.43
1:J:216:TYR:CZ	1:J:218:PRO:HG3	2.54	0.43
1:D:283:HIS:HD2	1:D:287:LEU:HB2	1.83	0.43
1:E:218:PRO:HB3	1:E:264:PHE:HE1	1.83	0.43
1:E:243:LYS:HD2	1:E:245:HIS:HB3	1.99	0.43
1:E:270:LEU:HB3	2:S:121:LEU:CG	2.49	0.43
1:H:274:ASN:ND2	2:L:122:ASN:CG	2.72	0.43
1:H:276:ASN:HB3	4:H:636:HOH:O	2.17	0.43
1:G:308:LYS:C	1:G:310:VAL:H	2.21	0.43
1:G:230:LEU:HD21	1:G:245:HIS:ND1	2.34	0.43
1:G:279:PRO:O	1:G:283:HIS:HB2	2.19	0.43
1:I:297:LYS:HD2	1:I:297:LYS:HA	1.91	0.43
1:C:286:TRP:HE3	2:P:119:ILE:HG21	1.84	0.43
1:E:260:ARG:HE	1:E:271:MET:HE3	1.84	0.42
1:F:274:ASN:CG	1:F:275:ASP:H	2.21	0.42
1:H:260:ARG:HB3	2:L:118:PHE:CE2	2.54	0.42
1:I:240:LEU:O	1:I:243:LYS:HE3	2.18	0.42
1:I:255:THR:HG21	2:M:118:PHE:HZ	1.85	0.42
1:E:278:GLU:O	1:E:281:GLU:HB2	2.20	0.42
1:H:237:PRO:HB2	1:H:240:LEU:HD22	2.01	0.42
1:J:309:PRO:CG	1:J:310:VAL:H	2.32	0.42
1:A:237:PRO:HB2	1:A:240:LEU:HD22	2.02	0.42
1:A:247:LEU:HD23	1:A:279:PRO:HG3	2.02	0.42
1:C:284:ALA:O	1:C:288:SER:HB3	2.20	0.42
1:J:255:THR:O	1:J:257:VAL:HG23	2.18	0.42
1:F:223:TYR:HB3	1:F:229:ARG:HG2	2.00	0.42
1:I:281:GLU:O	1:I:285:LEU:HB2	2.20	0.42
1:J:293:VAL:O	1:J:297:LYS:HB2	2.19	0.42
1:I:270:LEU:CD2	2:M:119:ILE:HB	2.49	0.42
1:B:262:ARG:NH2	2:R:116:PRO:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:284:ALA:HA	1:J:293:VAL:HG11	2.00	0.42
1:A:264:PHE:CD1	1:A:264:PHE:C	2.93	0.42
1:B:246:GLN:HG3	1:B:246:GLN:H	1.67	0.42
1:C:281:GLU:HB3	4:C:604:HOH:O	2.20	0.42
4:C:617:HOH:O	1:D:238:ARG:HG2	2.20	0.42
1:E:269:GLY:O	2:S:119:ILE:HB	2.19	0.42
1:F:291:ARG:HG3	4:F:612:HOH:O	2.18	0.42
1:D:270:LEU:CD1	2:Q:121:LEU:HD21	2.40	0.42
1:B:264:PHE:CG	1:B:265:SER:N	2.87	0.42
1:J:236:TRP:HA	1:J:237:PRO:HD3	1.93	0.42
1:J:285:LEU:HD13	1:J:286:TRP:HE1	1.83	0.42
1:F:273:TRP:O	1:G:239:ASN:HB2	2.20	0.41
2:O:116:PRO:HA	2:O:117:PRO:HD3	1.60	0.41
1:J:272:ASP:O	2:T:121:LEU:HD22	2.20	0.41
2:T:121:LEU:CD1	2:T:121:LEU:N	2.83	0.41
1:G:255:THR:HG21	2:K:118:PHE:HZ	1.85	0.41
1:A:277:ASP:OD2	2:O:122:ASN:ND2	2.52	0.41
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.82	0.41
1:H:259:ASP:OD2	1:H:272:ASP:N	2.53	0.41
1:A:243:LYS:HA	1:A:244:PRO:HD3	1.95	0.41
1:D:236:TRP:CZ3	1:D:259:ASP:HA	2.55	0.41
1:G:231:ARG:NH2	4:G:646:HOH:O	2.53	0.41
1:H:226:GLU:OE2	1:H:249:GLU:HA	2.20	0.41
1:J:233:PHE:CB	1:J:244:PRO:HB3	2.50	0.41
2:S:119:ILE:O	2:S:120:SER:C	2.59	0.41
1:B:291:ARG:HH21	1:B:294:LYS:HD2	1.86	0.41
1:C:289:GLN:CA	1:C:289:GLN:NE2	2.82	0.41
1:J:272:ASP:HB2	2:T:121:LEU:H	1.84	0.41
1:H:226:GLU:HG3	1:H:227:THR:N	2.33	0.41
1:I:243:LYS:N	1:I:243:LYS:HE2	2.35	0.41
1:J:274:ASN:ND2	2:T:122:ASN:OD1	2.54	0.41
1:C:262:ARG:NH1	1:C:267:GLY:O	2.52	0.41
1:E:236:TRP:O	1:E:237:PRO:C	2.59	0.41
1:E:274:ASN:HD22	2:S:122:ASN:HB2	1.82	0.41
1:D:270:LEU:HD22	2:Q:121:LEU:CD2	2.51	0.41
1:C:238:ARG:CB	1:C:238:ARG:HH11	2.29	0.41
1:C:278:GLU:HG2	1:C:281:GLU:OE2	2.21	0.41
1:J:274:ASN:O	1:J:277:ASP:HB2	2.21	0.41
1:D:242:GLN:HG2	1:D:273:TRP:CE3	2.56	0.41
1:E:289:GLN:HA	1:E:294:LYS:HZ1	1.84	0.41
1:F:260:ARG:HG2	1:F:271:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ASN:CG	1:F:275:ASP:N	2.74	0.41
1:I:236:TRP:CZ2	1:I:240:LEU:HD23	2.56	0.40
1:I:278:GLU:CD	1:I:279:PRO:HD2	2.41	0.40
1:J:309:PRO:HD2	1:J:310:VAL:H	1.86	0.40
1:E:286:TRP:O	1:G:227:THR:HG23	2.21	0.40
1:G:245:HIS:O	1:G:249:GLU:HG3	2.22	0.40
1:I:243:LYS:H	1:I:246:GLN:CD	2.24	0.40
1:I:242:GLN:C	1:I:243:LYS:HE2	2.42	0.40
1:C:273:TRP:CE3	1:C:277:ASP:HB3	2.56	0.40
1:G:291:ARG:HH21	1:G:294:LYS:HD2	1.85	0.40
1:H:252:PHE:HB3	1:H:261:VAL:HB	2.03	0.40
1:E:273:TRP:O	1:J:239:ASN:HB2	2.21	0.40
2:L:115:ARG:CB	2:L:116:PRO:CD	2.99	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:GLU:OE2	2:P:115:ARG:NH1[3_665]	2.17	0.03

## 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	92/124 (74%)	83 (90%)	8 (9%)	1 (1%)	14	9
1	B	99/124 (80%)	91 (92%)	8 (8%)	0	100	100
1	C	92/124 (74%)	83 (90%)	8 (9%)	1 (1%)	14	9
1	D	92/124 (74%)	86 (94%)	6 (6%)	0	100	100
1	E	99/124 (80%)	78 (79%)	17 (17%)	4 (4%)	3	1
1	F	92/124 (74%)	87 (95%)	2 (2%)	3 (3%)	4	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	99/124 (80%)	91 (92%)	7 (7%)	1 (1%)	15	11
1	H	92/124 (74%)	88 (96%)	4 (4%)	0	100	100
1	I	92/124 (74%)	81 (88%)	9 (10%)	2 (2%)	6	2
1	J	99/124 (80%)	83 (84%)	13 (13%)	3 (3%)	4	1
2	K	6/12 (50%)	5 (83%)	1 (17%)	0	100	100
2	L	6/12 (50%)	6 (100%)	0	0	100	100
2	M	5/12 (42%)	5 (100%)	0	0	100	100
2	N	6/12 (50%)	4 (67%)	0	2 (33%)	0	0
2	O	6/12 (50%)	5 (83%)	0	1 (17%)	0	0
2	P	6/12 (50%)	6 (100%)	0	0	100	100
2	Q	5/12 (42%)	5 (100%)	0	0	100	100
2	R	5/12 (42%)	4 (80%)	0	1 (20%)	0	0
2	S	5/12 (42%)	3 (60%)	1 (20%)	1 (20%)	0	0
2	T	5/12 (42%)	3 (60%)	1 (20%)	1 (20%)	0	0
All	All	1003/1360 (74%)	897 (89%)	85 (8%)	21 (2%)	7	3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	LYS
1	E	309	PRO
1	F	308	LYS
1	J	309	PRO
2	N	116	PRO
2	O	116	PRO
1	E	272	ASP
1	F	307	ALA
1	G	258	GLY
1	I	285	LEU
2	T	121	LEU
1	C	308	LYS
1	E	275	ASP
1	F	217	PHE
1	E	266	CYS
2	R	117	PRO
2	S	120	SER
1	I	265	SER

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Mol	Chain	Res	Type
1	J	237	PRO
2	N	117	PRO
1	J	308	LYS

### 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	79/103 (77%)	73 (92%)	6 (8%)	13	10
1	B	85/103 (82%)	81 (95%)	4 (5%)	26	25
1	C	79/103 (77%)	71 (90%)	8 (10%)	7	4
1	D	79/103 (77%)	73 (92%)	6 (8%)	13	10
1	E	85/103 (82%)	74 (87%)	11 (13%)	4	2
1	F	79/103 (77%)	75 (95%)	4 (5%)	24	22
1	G	85/103 (82%)	81 (95%)	4 (5%)	26	25
1	H	79/103 (77%)	73 (92%)	6 (8%)	13	10
1	I	79/103 (77%)	73 (92%)	6 (8%)	13	10
1	J	85/103 (82%)	80 (94%)	5 (6%)	19	17
2	K	8/12 (67%)	8 (100%)	0	100	100
2	L	8/12 (67%)	7 (88%)	1 (12%)	4	2
2	M	7/12 (58%)	6 (86%)	1 (14%)	3	1
2	N	8/12 (67%)	8 (100%)	0	100	100
2	O	8/12 (67%)	8 (100%)	0	100	100
2	P	8/12 (67%)	8 (100%)	0	100	100
2	Q	7/12 (58%)	7 (100%)	0	100	100
2	R	7/12 (58%)	6 (86%)	1 (14%)	3	1
2	S	7/12 (58%)	7 (100%)	0	100	100
2	T	7/12 (58%)	6 (86%)	1 (14%)	3	1
All	All	889/1150 (77%)	825 (93%)	64 (7%)	14	11

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	PHE
1	A	230	LEU
1	A	240	LEU
1	A	264	PHE
1	A	278	GLU
1	A	291	ARG
1	B	246	GLN
1	B	288	SER
1	B	291	ARG
1	B	311	LEU
1	C	217	PHE
1	C	227	THR
1	C	230	LEU
1	C	240	LEU
1	C	265	SER
1	C	278	GLU
1	C	285	LEU
1	C	291	ARG
1	D	238	ARG
1	D	240	LEU
1	D	274	ASN
1	D	278	GLU
1	D	285	LEU
1	D	291	ARG
1	E	238	ARG
1	E	245	HIS
1	E	262	ARG
1	E	264	PHE
1	E	270	LEU
1	E	278	GLU
1	E	280	TRP
1	E	286	TRP
1	E	291	ARG
1	E	309	PRO
1	E	311	LEU
1	F	217	PHE
1	F	240	LEU
1	F	278	GLU
1	F	285	LEU
1	G	240	LEU
1	G	285	LEU
1	G	291	ARG

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Mol	Chain	Res	Type
1	G	311	LEU
1	H	217	PHE
1	H	230	LEU
1	H	245	HIS
1	H	246	GLN
1	H	281	GLU
1	H	285	LEU
1	I	240	LEU
1	I	246	GLN
1	I	279	PRO
1	I	285	LEU
1	I	291	ARG
1	I	295	LEU
1	J	239	ASN
1	J	260	ARG
1	J	285	LEU
1	J	291	ARG
1	J	310	VAL
2	L	115	ARG
2	M	122	ASN
2	R	117	PRO
2	T	118	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	245	HIS
1	A	246	GLN
1	A	289	GLN
1	B	274	ASN
1	C	239	ASN
1	C	246	GLN
1	C	274	ASN
1	C	289	GLN
1	D	245	HIS
1	D	246	GLN
1	D	274	ASN
1	D	289	GLN
1	D	299	GLN
1	E	246	GLN
1	E	274	ASN

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Mol	Chain	Res	Type
1	F	246	GLN
1	F	289	GLN
1	G	246	GLN
1	H	246	GLN
1	H	274	ASN
1	I	239	ASN
1	I	274	ASN
1	J	239	ASN
1	J	246	GLN
1	J	282	GLN
1	J	299	GLN
2	M	122	ASN
2	O	122	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	94/124 (75%)	-0.16	2 (2%) 63 68	11, 20, 47, 104	0
1	B	101/124 (81%)	-0.35	0 100 100	11, 20, 46, 57	0
1	C	94/124 (75%)	-0.16	2 (2%) 63 68	10, 21, 54, 95	0
1	D	94/124 (75%)	-0.07	2 (2%) 63 68	13, 27, 51, 123	0
1	E	101/124 (81%)	0.84	14 (13%) 2 3	24, 50, 83, 120	0
1	F	94/124 (75%)	-0.18	3 (3%) 47 54	11, 23, 51, 86	0
1	G	101/124 (81%)	-0.06	7 (6%) 16 21	10, 22, 69, 88	0
1	H	94/124 (75%)	-0.12	3 (3%) 47 54	12, 22, 61, 97	0
1	I	94/124 (75%)	-0.02	2 (2%) 63 68	13, 28, 65, 99	0
1	J	101/124 (81%)	0.42	5 (4%) 28 34	19, 38, 65, 111	0
2	K	8/12 (66%)	-0.18	0 100 100	24, 32, 49, 57	0
2	L	8/12 (66%)	-0.18	0 100 100	22, 29, 46, 48	0
2	M	7/12 (58%)	1.14	2 (28%) 0 0	42, 50, 64, 83	0
2	N	8/12 (66%)	0.32	1 (12%) 3 5	22, 31, 60, 65	0
2	O	8/12 (66%)	0.09	0 100 100	21, 32, 44, 55	0
2	P	8/12 (66%)	-0.14	0 100 100	25, 34, 41, 49	0
2	Q	7/12 (58%)	1.26	2 (28%) 0 0	36, 51, 74, 82	0
2	R	7/12 (58%)	-0.03	0 100 100	19, 26, 56, 59	0
2	S	7/12 (58%)	3.21	4 (57%) 0 0	46, 79, 91, 93	0
2	T	7/12 (58%)	1.61	2 (28%) 0 0	53, 61, 70, 78	0
All	All	1043/1360 (76%)	0.07	51 (4%) 29 35	10, 27, 71, 123	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	216	TYR	10.7
1	D	216	TYR	9.0
1	A	216	TYR	8.7
1	J	216	TYR	8.5
1	H	309	PRO	7.2
1	I	216	TYR	7.2
1	J	217	PHE	7.2
2	S	119	ILE	7.0
1	C	216	TYR	6.8
1	D	217	PHE	6.5
1	I	217	PHE	6.5
1	C	309	PRO	6.2
2	S	116	PRO	4.9
1	F	216	TYR	4.6
1	J	309	PRO	4.4
2	S	121	LEU	4.4
1	H	216	TYR	4.2
1	E	225	ILE	4.0
1	E	224	ALA	4.0
1	E	218	PRO	3.7
2	M	122	ASN	3.7
2	T	119	ILE	3.3
1	G	216	TYR	3.3
1	E	235	ALA	3.3
2	Q	121	LEU	3.1
1	G	311	LEU	3.1
1	A	217	PHE	3.1
2	Q	122	ASN	3.1
1	G	315	LYS	3.1
1	G	312	ALA	3.0
1	E	223	TYR	2.8
1	G	313	GLU	2.8
1	F	309	PRO	2.7
1	E	217	PHE	2.6
1	G	314	GLU	2.6
1	G	310	VAL	2.5
1	F	217	PHE	2.5
1	J	295	LEU	2.5
1	H	217	PHE	2.5
2	N	116	PRO	2.4
1	E	243	LYS	2.4
2	T	116	PRO	2.3
1	E	252	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	291	ARG	2.3
2	M	121	LEU	2.3
1	E	258	GLY	2.2
1	E	286	TRP	2.1
1	J	278	GLU	2.1
2	S	122	ASN	2.1
1	E	230	LEU	2.0
1	E	309	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	E	605	1/1	0.99	0.11	37,37,37,37	0
3	ZN	D	603	1/1	0.99	0.13	26,26,26,26	0
3	ZN	I	609	1/1	0.99	0.14	22,22,22,22	0
3	ZN	H	608	1/1	1.00	0.15	17,17,17,17	0
3	ZN	F	606	1/1	1.00	0.14	17,17,17,17	0
3	ZN	J	610	1/1	1.00	0.09	29,29,29,29	0
3	ZN	A	604	1/1	1.00	0.14	22,22,22,22	0
3	ZN	C	602	1/1	1.00	0.15	22,22,22,22	0
3	ZN	B	601	1/1	1.00	0.15	18,18,18,18	0
3	ZN	G	607	1/1	1.00	0.14	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.