



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:50 AM GMT

PDB ID : 3JUA  
Title : Structural basis of YAP recognition by TEAD4 in the Hippo pathway  
Authors : Chen, L.; Song, H.  
Deposited on : 2009-09-15  
Resolution : 3.00 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

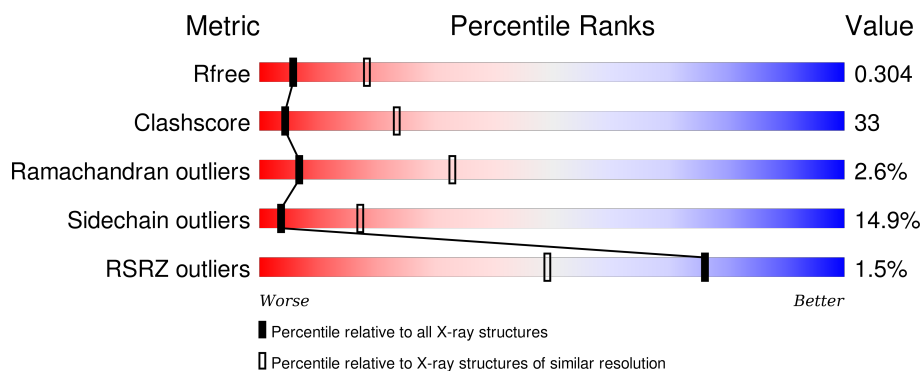
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	220	
1	C	220	
1	E	220	
1	G	220	
2	B	39	

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Mol	Chain	Length	Quality of chain
2	D	39	<div><div></div><div>51%26%13%10%</div></div>
2	F	39	<div><div>3%</div><div></div><div>41%38%13%8%</div></div>
2	H	39	<div><div>5%</div><div></div><div>21%15%13%51%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8055 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 Transcriptional enhancer factor TEF-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1692	1092	281	309	10			
1	C	213	Total	C	N	O	S	0	0	0
			1762	1131	293	328	10			
1	E	216	Total	C	N	O	S	0	0	0
			1782	1144	294	334	10			
1	G	190	Total	C	N	O	S	0	0	0
			1586	1021	263	292	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	SER	-	EXPRESSION TAG	UNP Q62296
A	209	MET	-	EXPRESSION TAG	UNP Q62296
C	208	SER	-	EXPRESSION TAG	UNP Q62296
C	209	MET	-	EXPRESSION TAG	UNP Q62296
E	208	SER	-	EXPRESSION TAG	UNP Q62296
E	209	MET	-	EXPRESSION TAG	UNP Q62296
G	208	SER	-	EXPRESSION TAG	UNP Q62296
G	209	MET	-	EXPRESSION TAG	UNP Q62296

- Molecule 2 is a protein called 65 kDa Yes-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	S	0	0	0
			311	200	52	57	2			
2	D	35	Total	C	N	O	S	0	0	0
			279	180	48	49	2			
2	F	36	Total	C	N	O	S	0	0	0
			286	185	49	50	2			
2	H	19	Total	C	N	O	S	0	0	0
			158	105	28	24	1			

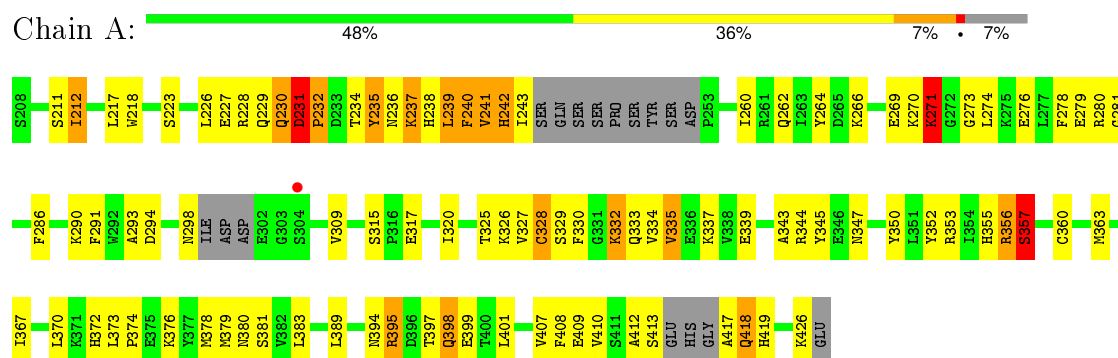
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	7	Total 7	O 7	0	0
3	C	45	Total 45	O 45	0	0
3	D	6	Total 6	O 6	0	0
3	E	51	Total 51	O 51	0	0
3	F	7	Total 7	O 7	0	0
3	G	42	Total 42	O 42	0	0

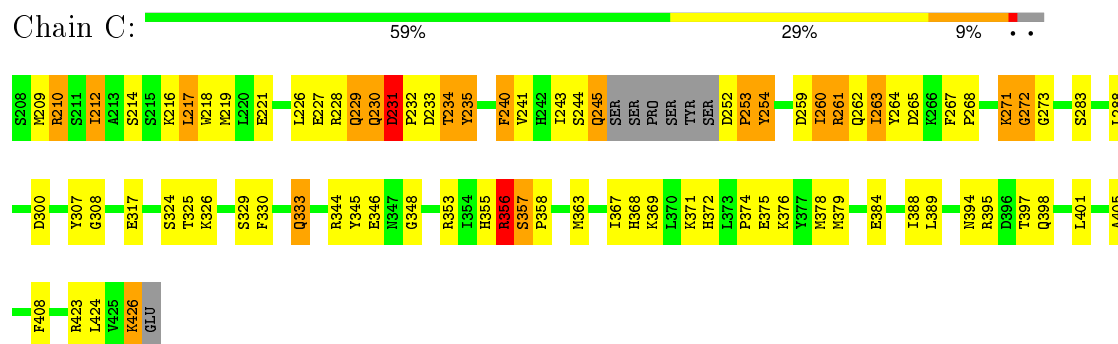
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

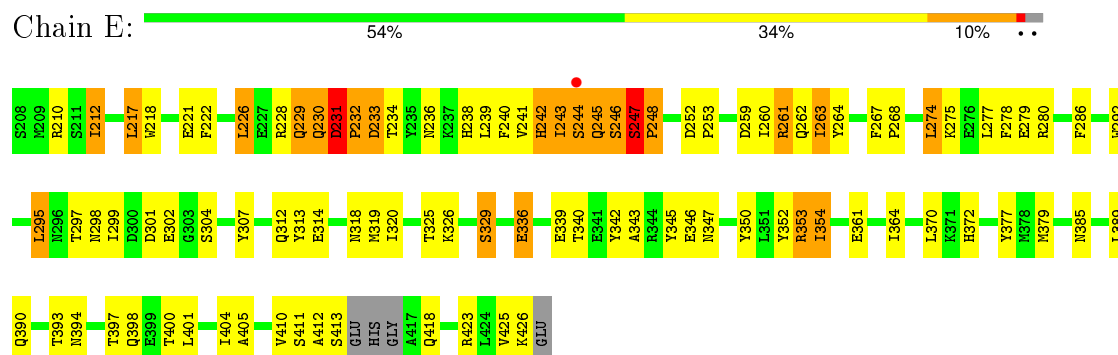
#### • Molecule 1: Transcriptional enhancer factor TEF-3



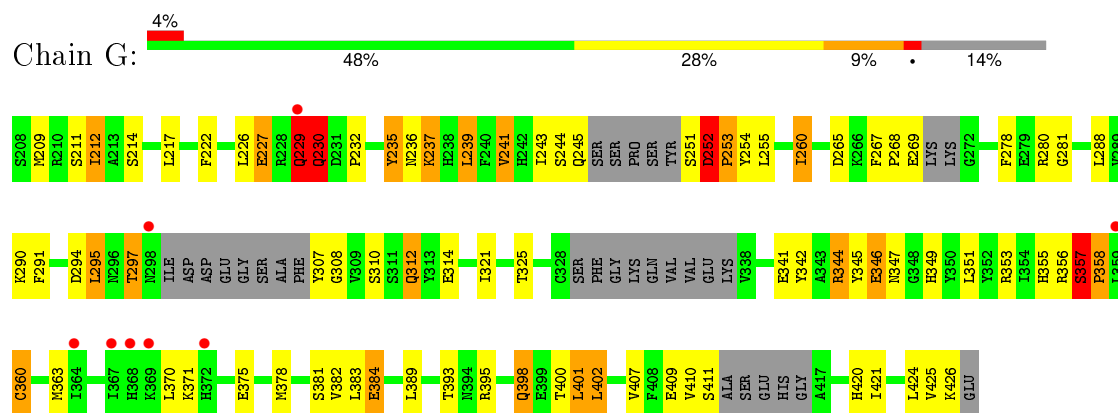
#### • Molecule 1: Transcriptional enhancer factor TEF-3



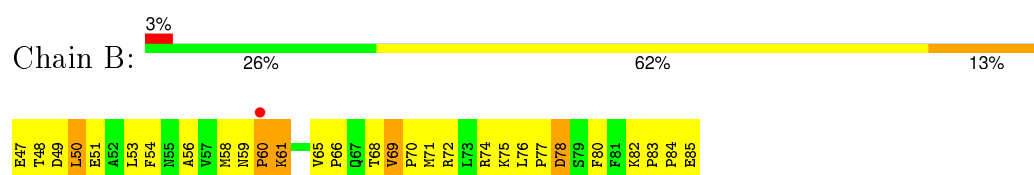
#### • Molecule 1: Transcriptional enhancer factor TEF-3



- Molecule 1: Transcriptional enhancer factor TEF-3



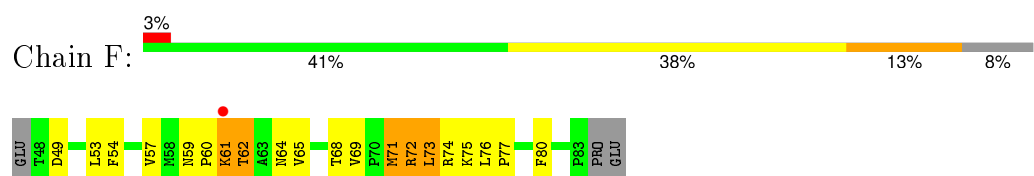
- Molecule 2: 65 kDa Yes-associated protein



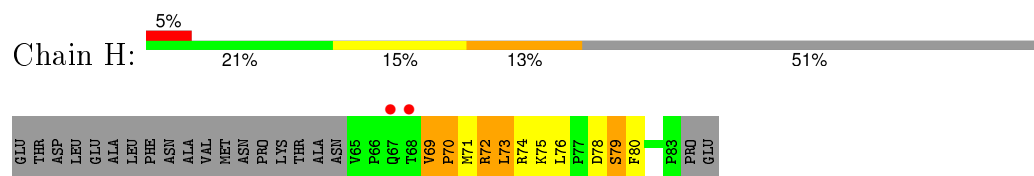
- Molecule 2: 65 kDa Yes-associated protein



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.98Å 146.91Å 165.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 74.35 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.00) 99.9 (74.35-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.236 , 0.288 0.253 , 0.304	Depositor DCC
$R_{free}$ test set	2517 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 61207 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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

### 5.1 Standard geometry

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	0.58	0/1733	0.69	1/2335 (0.0%)
1	C	0.61	0/1806	0.85	8/2438 (0.3%)
1	E	0.60	0/1827	0.83	4/2468 (0.2%)
1	G	0.49	0/1623	0.95	8/2189 (0.4%)
2	B	0.49	0/319	0.67	0/434
2	D	0.65	0/285	0.83	1/386 (0.3%)
2	F	0.61	0/293	0.98	2/398 (0.5%)
2	H	0.46	0/163	0.81	1/220 (0.5%)
All	All	0.57	0/8049	0.83	25/10868 (0.2%)

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	A	0	1
1	C	0	3
1	E	0	1
1	G	0	1
2	F	0	1
All	All	0	7

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	357	SER	C-N-CD	-19.15	78.46	120.60
1	G	252	ASP	C-N-CD	-16.01	85.37	120.60
1	G	230	GLN	N-CA-C	-10.08	83.78	111.00
1	G	358	PRO	N-CA-C	-9.87	86.45	112.10
1	C	272	GLY	N-CA-C	-9.60	89.10	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	346	GLU	N-CA-C	-8.98	86.74	111.00
1	E	247	SER	N-CA-C	-8.95	86.84	111.00
1	G	357	SER	N-CA-C	8.59	134.18	111.00
1	E	248	PRO	N-CA-C	-8.07	91.11	112.10
1	C	348	GLY	N-CA-C	-7.24	95.00	113.10
1	E	244	SER	N-CA-C	-7.03	92.02	111.00
1	C	253	PRO	N-CA-C	-6.93	94.09	112.10
1	A	239	LEU	CA-CB-CG	-6.79	99.69	115.30
1	C	230	GLN	N-CA-C	-6.69	92.95	111.00
1	G	252	ASP	N-CA-C	6.50	128.56	111.00
1	C	254	TYR	N-CA-C	-6.44	93.60	111.00
2	F	64	ASN	N-CA-C	-6.14	94.41	111.00
1	G	357	SER	C-N-CA	6.08	147.53	122.00
2	D	71	MET	CB-CA-C	-6.06	98.28	110.40
2	F	61	LYS	CB-CA-C	-5.96	98.47	110.40
2	H	72	ARG	N-CA-C	-5.72	95.56	111.00
1	C	273	GLY	N-CA-C	-5.65	98.98	113.10
1	C	231	ASP	C-N-CD	-5.56	108.37	120.60
1	E	231	ASP	C-N-CD	-5.55	108.39	120.60
1	C	231	ASP	N-CA-C	-5.25	96.82	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	SER	Peptide
1	C	229	GLN	Peptide
1	C	231	ASP	Peptide
1	C	357	SER	Peptide
1	E	229	GLN	Peptide
2	F	72	ARG	Peptide
1	G	229	GLN	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	1692	0	1657	121	0
1	C	1762	0	1710	100	0
1	E	1782	0	1730	111	0
1	G	1586	0	1537	95	0
2	B	311	0	315	23	0
2	D	279	0	289	31	0
2	F	286	0	296	26	0
2	H	158	0	170	29	0
3	A	41	0	0	3	0
3	B	7	0	0	2	0
3	C	45	0	0	10	0
3	D	6	0	0	3	0
3	E	51	0	0	6	0
3	F	7	0	0	1	0
3	G	42	0	0	9	0
All	All	8055	0	7704	511	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 33.

All (511) 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:69:VAL:HG12	2:H:70:PRO:CD	1.54	1.38
1:G:252:ASP:CB	1:G:253:PRO:HD3	1.30	1.37
2:H:75:LYS:O	2:H:76:LEU:HD23	1.18	1.32
1:C:210:ARG:HD3	1:C:252:ASP:OD1	1.27	1.25
1:C:271:LYS:O	1:C:271:LYS:CD	1.87	1.23
1:C:210:ARG:CD	1:C:252:ASP:OD1	1.86	1.22
2:H:75:LYS:C	2:H:76:LEU:HD23	1.62	1.19
1:C:271:LYS:HD2	1:C:271:LYS:C	1.33	1.19
1:E:246:SER:C	1:E:248:PRO:HD3	1.62	1.19
1:C:271:LYS:HD2	1:C:271:LYS:O	0.99	1.16
1:C:261:ARG:HG3	1:C:261:ARG:HH11	1.04	1.15
1:G:308:GLY:HA2	1:G:358:PRO:HG3	1.22	1.13
1:G:252:ASP:CB	1:G:253:PRO:CD	2.26	1.12
1:G:252:ASP:HB3	1:G:253:PRO:HD3	1.26	1.11
2:H:72:ARG:C	2:H:73:LEU:HD23	1.69	1.11
1:C:235:TYR:N	1:E:232:PRO:HG2	1.65	1.11
1:E:243:ILE:O	1:E:245:GLN:N	1.85	1.10
1:E:230:GLN:O	1:E:232:PRO:HA	1.51	1.09
1:A:237:LYS:HZ2	1:A:237:LYS:CA	1.62	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:LEU:O	2:F:73:LEU:HD23	1.52	1.08
2:H:73:LEU:CD2	2:H:73:LEU:N	2.15	1.07
2:H:73:LEU:HD23	2:H:73:LEU:N	1.68	1.06
2:F:61:LYS:CG	2:F:61:LYS:O	1.98	1.06
1:C:232:PRO:HG3	3:C:168:HOH:O	1.54	1.06
2:H:75:LYS:O	2:H:76:LEU:CD2	2.04	1.05
1:G:280:ARG:O	1:G:280:ARG:HD3	1.56	1.05
2:F:73:LEU:HD22	2:F:73:LEU:N	1.62	1.04
1:G:229:GLN:HB3	1:G:230:GLN:O	1.57	1.04
1:C:245:GLN:HA	1:C:245:GLN:OE1	1.50	1.04
1:G:345:TYR:OH	1:G:347:ASN:O	1.73	1.03
2:F:73:LEU:H	2:F:73:LEU:HD22	0.87	1.03
1:G:358:PRO:HB2	3:G:177:HOH:O	1.57	1.03
1:C:271:LYS:C	1:C:271:LYS:CD	2.04	1.03
1:C:227:GLU:HB3	1:C:235:TYR:HB2	1.04	1.03
1:C:235:TYR:H	1:E:232:PRO:HG2	0.87	1.02
1:G:252:ASP:HB2	1:G:253:PRO:HD3	1.40	1.02
1:C:210:ARG:HD3	1:C:252:ASP:CG	1.79	1.02
1:G:237:LYS:NZ	1:G:237:LYS:HB3	1.74	1.01
1:A:230:GLN:O	1:A:232:PRO:HD2	1.60	1.00
2:H:69:VAL:CG1	2:H:70:PRO:CD	2.38	1.00
1:E:231:ASP:HB2	3:E:26:HOH:O	1.59	1.00
1:C:235:TYR:H	1:E:232:PRO:CG	1.73	1.00
1:A:237:LYS:CA	1:A:237:LYS:NZ	2.23	0.99
1:C:227:GLU:HB3	1:C:235:TYR:CB	1.91	0.99
2:H:69:VAL:CG1	2:H:70:PRO:HD2	1.92	0.99
1:A:270:LYS:O	1:A:271:LYS:HB2	1.64	0.98
1:A:237:LYS:HA	1:A:237:LYS:NZ	1.79	0.98
1:C:261:ARG:CG	1:C:261:ARG:HH11	1.76	0.98
1:A:426:LYS:HA	3:A:14:HOH:O	1.64	0.97
1:G:398:GLN:HA	1:G:398:GLN:NE2	1.79	0.97
2:F:73:LEU:H	2:F:73:LEU:CD2	1.75	0.96
1:G:345:TYR:CZ	1:G:347:ASN:O	2.18	0.95
1:C:227:GLU:CB	1:C:235:TYR:HB2	1.95	0.95
1:G:226:LEU:O	1:G:235:TYR:HB2	1.67	0.95
1:A:270:LYS:C	1:A:271:LYS:HD2	1.88	0.94
2:H:69:VAL:HG12	2:H:70:PRO:HD2	0.96	0.93
2:F:73:LEU:HD23	2:F:73:LEU:C	1.87	0.93
2:F:73:LEU:CD2	2:F:73:LEU:C	2.38	0.92
1:E:246:SER:OG	1:E:248:PRO:HD3	1.70	0.91
2:F:61:LYS:O	2:F:61:LYS:HG2	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:61:LYS:O	2:F:61:LYS:CD	2.19	0.91
1:G:260:ILE:HD11	1:G:426:LYS:HA	1.50	0.90
1:A:229:GLN:O	1:A:230:GLN:HG2	1.72	0.89
1:C:218:TRP:HE1	1:C:243:ILE:HG21	1.37	0.89
1:E:232:PRO:CB	1:E:233:ASP:HB2	2.02	0.89
2:F:61:LYS:HD3	2:F:61:LYS:O	1.71	0.88
1:G:310:SER:HB3	1:G:355:HIS:O	1.74	0.88
2:D:71:MET:CE	2:D:74:ARG:CZ	2.52	0.88
1:C:229:GLN:HB3	1:C:233:ASP:HB3	1.56	0.88
1:A:237:LYS:HZ2	1:A:237:LYS:N	1.71	0.88
1:C:261:ARG:HG3	1:C:261:ARG:NH1	1.84	0.87
1:E:240:PHE:HZ	1:E:243:ILE:HG23	1.39	0.87
1:G:345:TYR:CD1	1:G:346:GLU:O	2.27	0.87
2:H:72:ARG:HB2	2:H:73:LEU:HD23	1.55	0.87
1:E:246:SER:C	1:E:248:PRO:CD	2.44	0.86
1:A:329:SER:O	1:A:330:PHE:HB2	1.74	0.85
1:E:261:ARG:HG3	1:E:261:ARG:HH11	1.40	0.85
1:A:380:ASN:HD21	1:A:410:VAL:H	1.24	0.85
1:E:320:ILE:HD13	1:E:342:TYR:CE1	2.11	0.85
1:G:307:TYR:O	1:G:358:PRO:HG2	1.76	0.85
1:C:426:LYS:HB2	1:C:426:LYS:NZ	1.91	0.85
1:G:252:ASP:HB3	1:G:253:PRO:CD	1.98	0.84
1:G:237:LYS:HZ3	1:G:237:LYS:HB3	1.39	0.84
1:A:230:GLN:O	1:A:232:PRO:CD	2.26	0.84
1:E:240:PHE:HZ	1:E:243:ILE:CG2	1.90	0.84
1:A:229:GLN:O	1:A:230:GLN:CG	2.26	0.84
1:A:231:ASP:HB2	1:A:232:PRO:HD3	1.60	0.83
1:A:238:HIS:O	1:A:239:LEU:HG	1.77	0.83
1:C:210:ARG:CG	1:C:252:ASP:OD1	2.26	0.83
1:G:308:GLY:CA	1:G:358:PRO:HG3	2.08	0.83
1:E:261:ARG:CG	1:E:261:ARG:HH11	1.92	0.82
1:A:212:ILE:HG22	1:A:243:ILE:HD11	1.62	0.82
1:G:229:GLN:CB	1:G:230:GLN:O	2.27	0.81
1:C:245:GLN:OE1	1:C:245:GLN:CA	2.29	0.81
1:C:212:ILE:HG23	1:C:243:ILE:HD11	1.62	0.80
2:F:73:LEU:CD2	2:F:73:LEU:O	2.30	0.80
1:G:280:ARG:C	1:G:280:ARG:HD3	2.00	0.80
1:A:229:GLN:HG3	1:A:230:GLN:H	1.47	0.80
1:C:214:SER:OG	1:C:217:LEU:N	2.15	0.79
1:E:354:ILE:HG22	1:E:354:ILE:O	1.83	0.79
2:B:59:ASN:H	2:B:60:PRO:HA	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:80:PHE:O	2:H:80:PHE:CD1	2.36	0.78
2:H:72:ARG:CB	2:H:73:LEU:HD23	2.12	0.78
1:A:229:GLN:CG	1:A:230:GLN:H	1.97	0.78
1:A:237:LYS:N	1:A:237:LYS:NZ	2.32	0.78
1:E:246:SER:OG	1:E:248:PRO:HG3	1.83	0.77
1:E:325:THR:HG22	1:E:390:GLN:HG3	1.66	0.77
1:E:221:GLU:OE2	1:E:243:ILE:HG22	1.84	0.77
1:A:227:GLU:HB2	1:A:235:TYR:HB3	1.66	0.77
1:A:238:HIS:O	1:A:239:LEU:CD2	2.33	0.77
2:H:72:ARG:HB2	2:H:73:LEU:CD2	2.14	0.76
1:A:270:LYS:O	1:A:271:LYS:CB	2.33	0.76
2:H:69:VAL:CG1	2:H:70:PRO:HD3	2.16	0.76
1:E:246:SER:OG	1:E:248:PRO:CD	2.32	0.76
1:E:240:PHE:CZ	1:E:243:ILE:HG23	2.21	0.76
1:A:229:GLN:CG	1:A:230:GLN:N	2.48	0.76
1:G:229:GLN:C	1:G:230:GLN:O	2.18	0.76
1:C:426:LYS:HZ2	1:C:426:LYS:HB2	1.50	0.76
1:C:271:LYS:CG	1:C:272:GLY:N	2.49	0.75
1:G:346:GLU:HG2	1:G:349:HIS:CE1	2.20	0.75
1:C:271:LYS:HG3	1:C:272:GLY:N	2.02	0.75
1:G:307:TYR:O	1:G:358:PRO:CG	2.35	0.75
2:D:71:MET:HE1	2:D:74:ARG:NE	2.01	0.75
1:A:227:GLU:CB	1:A:235:TYR:HB3	2.16	0.75
2:D:71:MET:HA	2:D:74:ARG:HD3	1.69	0.75
1:G:212:ILE:HG22	1:G:243:ILE:HG13	1.69	0.75
1:A:380:ASN:ND2	1:A:410:VAL:H	1.83	0.74
1:A:238:HIS:O	1:A:239:LEU:CG	2.35	0.74
1:E:243:ILE:C	1:E:245:GLN:N	2.41	0.73
1:A:237:LYS:HA	1:A:237:LYS:HZ1	1.49	0.73
2:H:70:PRO:O	2:H:72:ARG:O	2.06	0.73
1:C:271:LYS:HD2	1:C:272:GLY:N	2.01	0.73
1:E:247:SER:C	1:E:248:PRO:O	2.16	0.73
1:E:232:PRO:HB3	1:E:233:ASP:HB2	1.70	0.73
1:A:355:HIS:O	1:A:356:ARG:C	2.26	0.72
1:A:334:VAL:HG23	1:A:335:VAL:HG12	1.70	0.72
1:E:246:SER:OG	1:E:248:PRO:CG	2.36	0.72
1:A:230:GLN:C	1:A:231:ASP:OD2	2.28	0.72
2:H:73:LEU:HD22	2:H:73:LEU:N	2.04	0.72
1:G:237:LYS:HZ2	1:G:237:LYS:HB3	1.55	0.71
1:G:400:THR:HG21	3:G:154:HOH:O	1.88	0.71
1:E:347:ASN:N	1:E:347:ASN:OD1	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:HIS:C	1:A:239:LEU:HG	2.10	0.71
2:D:71:MET:CE	2:D:74:ARG:NE	2.54	0.70
1:E:260:ILE:HD11	1:E:274:LEU:HD22	1.74	0.70
1:A:226:LEU:O	1:A:235:TYR:HB2	1.92	0.70
1:G:370:LEU:HD11	1:G:383:LEU:HD21	1.74	0.70
1:A:229:GLN:O	1:A:230:GLN:CB	2.39	0.70
1:E:246:SER:O	1:E:248:PRO:HD3	1.91	0.70
1:G:260:ILE:HG23	1:G:424:LEU:HB3	1.74	0.70
2:D:69:VAL:O	2:D:74:ARG:NH1	2.25	0.70
1:C:356:ARG:HD3	3:C:158:HOH:O	1.91	0.69
1:C:230:GLN:O	1:C:232:PRO:O	2.10	0.69
2:F:77:PRO:HD2	2:F:80:PHE:HB2	1.74	0.69
1:C:376:LYS:HA	1:C:379:MET:HE3	1.75	0.69
1:A:271:LYS:O	1:A:276:GLU:CD	2.30	0.69
1:A:230:GLN:O	1:A:231:ASP:CG	2.31	0.68
2:D:71:MET:HE3	2:D:74:ARG:CZ	2.23	0.68
1:E:261:ARG:NH1	1:E:261:ARG:HG3	2.07	0.68
1:A:337:LYS:HD3	3:A:144:HOH:O	1.94	0.68
1:C:212:ILE:CG2	1:C:243:ILE:HD11	2.25	0.68
2:B:78:ASP:N	2:B:78:ASP:OD2	2.26	0.67
1:C:210:ARG:HB3	1:C:252:ASP:OD1	1.95	0.67
1:A:231:ASP:CB	1:A:232:PRO:HD3	2.23	0.67
1:A:355:HIS:O	1:A:357:SER:N	2.28	0.66
1:C:234:THR:HA	1:E:232:PRO:HB2	1.78	0.66
2:D:71:MET:O	2:D:81:PHE:HZ	1.78	0.66
1:A:317:GLU:HG3	1:C:317:GLU:OE2	1.95	0.66
1:E:297:THR:O	1:E:297:THR:HG23	1.95	0.66
1:G:360:CYS:SG	1:G:363:MET:HG2	2.36	0.66
2:H:69:VAL:HG12	2:H:70:PRO:HD3	1.64	0.65
2:H:72:ARG:CA	2:H:73:LEU:HD23	2.26	0.65
2:B:59:ASN:N	2:B:60:PRO:HA	2.06	0.65
1:G:243:ILE:HG22	1:G:244:SER:N	2.11	0.65
1:C:267:PHE:HB3	1:C:268:PRO:HD2	1.78	0.65
2:F:73:LEU:CD2	2:F:73:LEU:N	2.34	0.65
2:D:72:ARG:HA	2:D:81:PHE:CZ	2.32	0.64
1:A:266:LYS:HE3	2:B:71:MET:SD	2.37	0.64
1:C:356:ARG:HG3	1:C:356:ARG:O	1.97	0.64
1:A:376:LYS:O	1:A:379:MET:HB2	1.98	0.64
1:C:252:ASP:C	1:C:253:PRO:O	2.30	0.64
1:G:357:SER:N	1:G:358:PRO:HD3	2.03	0.63
1:G:398:GLN:HA	1:G:398:GLN:HE21	1.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLN:HG2	1:A:230:GLN:N	2.14	0.63
1:A:356:ARG:C	1:A:357:SER:O	2.31	0.63
1:G:252:ASP:HB3	1:G:253:PRO:CG	2.29	0.63
1:C:229:GLN:HB3	1:C:233:ASP:CB	2.26	0.63
1:C:356:ARG:CD	3:C:158:HOH:O	2.46	0.63
1:E:246:SER:CB	1:E:248:PRO:HD3	2.29	0.63
1:A:270:LYS:C	1:A:271:LYS:CD	2.66	0.63
2:F:76:LEU:HB3	2:F:77:PRO:CD	2.28	0.63
1:E:320:ILE:HD13	1:E:342:TYR:HE1	1.60	0.63
1:C:210:ARG:CB	1:C:252:ASP:OD1	2.47	0.62
1:C:212:ILE:O	1:C:212:ILE:HG12	1.97	0.62
1:G:229:GLN:CA	1:G:230:GLN:O	2.46	0.62
1:A:239:LEU:HD21	1:A:293:ALA:HA	1.81	0.62
1:C:214:SER:HB3	1:C:401:LEU:O	2.00	0.62
1:E:412:ALA:O	1:E:413:SER:C	2.37	0.62
1:A:344:ARG:HD2	1:G:342:TYR:O	1.99	0.62
1:C:271:LYS:CD	1:C:272:GLY:N	2.61	0.62
1:G:346:GLU:HG3	1:G:347:ASN:H	1.65	0.62
1:C:267:PHE:HB3	1:C:268:PRO:CD	2.28	0.62
1:E:262:GLN:NE2	2:F:75:LYS:H	1.97	0.62
1:A:212:ILE:C	1:A:212:ILE:HD13	2.20	0.62
1:G:212:ILE:CG2	1:G:243:ILE:HG13	2.29	0.62
1:A:223:SER:HB3	1:A:240:PHE:CD1	2.35	0.61
1:E:394:ASN:O	1:E:397:THR:O	2.18	0.61
1:C:394:ASN:O	1:C:397:THR:O	2.17	0.61
1:A:397:THR:O	1:A:399:GLU:N	2.33	0.61
1:G:222:PHE:HB3	1:G:241:VAL:HG13	1.82	0.61
2:D:81:PHE:O	2:D:82:LYS:O	2.18	0.61
1:G:398:GLN:CA	1:G:398:GLN:NE2	2.60	0.61
1:C:355:HIS:CG	1:C:356:ARG:H	2.18	0.61
1:G:290:LYS:HE3	1:G:409:GLU:HB2	1.81	0.61
1:C:374:PRO:HD2	1:C:378:MET:CE	2.30	0.61
1:G:314:GLU:HG3	1:G:351:LEU:HD23	1.82	0.61
2:H:72:ARG:C	2:H:73:LEU:CD2	2.54	0.61
1:A:238:HIS:O	1:A:239:LEU:HD23	2.00	0.61
1:E:261:ARG:HB2	1:E:261:ARG:HH11	1.66	0.60
1:E:246:SER:HG	1:E:248:PRO:HG3	1.66	0.60
1:E:232:PRO:CA	1:E:233:ASP:HB2	2.32	0.60
1:C:329:SER:O	1:C:330:PHE:HB2	2.00	0.60
1:E:246:SER:CA	1:E:248:PRO:HD3	2.31	0.60
1:G:211:SER:OG	1:G:243:ILE:HG21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:ASP:OD2	2:D:78:ASP:N	2.32	0.59
1:A:397:THR:C	1:A:399:GLU:H	2.06	0.59
1:C:230:GLN:O	1:C:231:ASP:C	2.41	0.59
1:C:260:ILE:HD12	1:C:424:LEU:HD13	1.84	0.59
1:E:261:ARG:CB	1:E:261:ARG:HH11	2.15	0.59
1:A:345:TYR:CZ	1:A:347:ASN:O	2.56	0.59
1:C:261:ARG:NH1	1:C:261:ARG:CG	2.49	0.58
1:E:275:LYS:HE3	1:E:279:GLU:OE1	2.03	0.58
1:C:259:ASP:OD2	1:C:261:ARG:NH1	2.34	0.58
1:A:270:LYS:HB3	1:A:271:LYS:HD2	1.85	0.58
2:B:48:THR:C	2:B:50:LEU:H	2.07	0.58
1:A:294:ASP:OD1	1:A:294:ASP:C	2.41	0.58
2:H:73:LEU:O	2:H:74:ARG:HG3	2.03	0.57
2:D:81:PHE:O	2:D:82:LYS:C	2.42	0.57
1:C:374:PRO:HD2	1:C:378:MET:HE1	1.85	0.57
1:A:239:LEU:HD13	1:A:291:PHE:CD1	2.39	0.57
1:G:356:ARG:NH1	3:G:185:HOH:O	2.36	0.57
1:E:325:THR:HG21	3:E:90:HOH:O	2.04	0.57
1:A:281:GLY:HA3	3:A:48:HOH:O	2.04	0.57
1:G:288:LEU:HD11	1:G:407:VAL:HG23	1.85	0.57
2:H:71:MET:C	2:H:72:ARG:O	2.39	0.57
2:H:80:PHE:HD1	2:H:80:PHE:O	1.85	0.57
1:A:231:ASP:OD2	1:A:231:ASP:N	2.37	0.57
1:C:214:SER:OG	1:C:216:LYS:N	2.36	0.57
1:A:241:VAL:HG23	1:A:242:HIS:N	2.19	0.56
1:C:212:ILE:HG23	1:C:243:ILE:CD1	2.34	0.56
1:G:312:GLN:HE21	1:G:353:ARG:HB3	1.69	0.56
2:B:60:PRO:HD2	2:B:61:LYS:H	1.69	0.56
1:E:262:GLN:HE21	2:F:74:ARG:HB3	1.70	0.56
1:E:347:ASN:OD1	1:E:347:ASN:O	2.24	0.56
1:E:242:HIS:C	1:E:243:ILE:O	2.40	0.56
2:D:72:ARG:HA	2:D:81:PHE:CE2	2.41	0.55
1:A:276:GLU:O	1:A:279:GLU:HG3	2.06	0.55
1:A:223:SER:HB3	1:A:240:PHE:HD1	1.71	0.55
1:C:240:PHE:HD1	1:C:241:VAL:N	2.04	0.55
1:A:238:HIS:C	1:A:239:LEU:CG	2.75	0.55
1:C:218:TRP:HE1	1:C:243:ILE:CG2	2.16	0.55
1:A:212:ILE:HD13	1:A:212:ILE:O	2.06	0.55
1:A:363:MET:O	1:A:367:ILE:HG13	2.07	0.55
1:A:231:ASP:HB2	1:A:232:PRO:CD	2.35	0.55
2:F:76:LEU:HB3	2:F:77:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:HG2	1:A:281:GLY:N	2.21	0.55
1:E:385:ASN:HB2	2:F:53:LEU:HD21	1.89	0.55
2:D:55:ASN:C	3:D:130:HOH:O	2.44	0.55
1:A:236:ASN:C	1:A:237:LYS:NZ	2.60	0.55
1:C:344:ARG:HG3	1:C:345:TYR:N	2.22	0.55
1:A:394:ASN:HB3	1:A:397:THR:O	2.08	0.54
1:E:240:PHE:HZ	1:E:243:ILE:HG22	1.72	0.54
1:E:345:TYR:CZ	1:E:346:GLU:O	2.60	0.54
1:E:295:LEU:H	1:E:295:LEU:HD23	1.71	0.54
1:A:229:GLN:C	1:A:230:GLN:CG	2.72	0.54
1:G:255:LEU:HD12	1:G:421:ILE:HG22	1.88	0.54
1:A:231:ASP:CB	1:A:232:PRO:CD	2.86	0.54
1:A:270:LYS:O	1:A:271:LYS:CD	2.55	0.54
1:E:280:ARG:HG2	1:E:280:ARG:O	2.08	0.54
1:G:232:PRO:HD3	3:G:73:HOH:O	2.08	0.54
1:C:262:GLN:NE2	2:D:74:ARG:HB2	2.23	0.54
1:E:292:TRP:HB3	1:E:411:SER:HB3	1.89	0.54
2:D:78:ASP:C	2:D:80:PHE:H	2.10	0.54
1:G:371:LYS:HB2	1:G:371:LYS:NZ	2.23	0.53
1:A:356:ARG:O	1:A:357:SER:C	2.47	0.53
1:A:343:ALA:HB1	1:A:350:TYR:HB3	1.90	0.53
1:A:397:THR:OG1	1:A:397:THR:O	2.27	0.53
1:E:247:SER:N	1:E:248:PRO:CD	2.65	0.53
1:C:244:SER:OG	1:C:245:GLN:N	2.42	0.53
1:G:260:ILE:HG13	1:G:425:VAL:O	2.09	0.53
1:C:265:ASP:OD1	3:C:431:HOH:O	2.19	0.53
1:A:230:GLN:C	1:A:231:ASP:CG	2.67	0.53
1:E:345:TYR:CE1	1:E:346:GLU:O	2.62	0.53
1:C:355:HIS:C	3:C:174:HOH:O	2.47	0.53
2:D:78:ASP:C	2:D:80:PHE:N	2.60	0.53
1:A:229:GLN:O	1:A:230:GLN:HB3	2.08	0.52
1:G:209:MET:HG2	1:G:254:TYR:CD2	2.44	0.52
1:A:353:ARG:HB3	1:G:344:ARG:HH22	1.73	0.52
1:E:217:LEU:HD23	1:E:314:GLU:O	2.10	0.52
1:C:226:LEU:HD13	1:C:307:TYR:CZ	2.44	0.52
1:E:318:ASN:C	1:E:318:ASN:OD1	2.47	0.52
1:E:260:ILE:HG12	1:E:264:TYR:CE1	2.45	0.52
1:E:329:SER:O	1:E:385:ASN:O	2.28	0.52
1:A:372:HIS:O	1:A:373:LEU:HD23	2.10	0.52
1:A:372:HIS:CD2	1:A:372:HIS:O	2.63	0.51
1:G:227:GLU:CD	1:G:307:TYR:N	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:MET:O	1:C:243:ILE:HD12	2.11	0.51
2:B:54:PHE:O	2:B:58:MET:HB2	2.11	0.51
1:G:321:ILE:HG22	1:G:341:GLU:HB2	1.92	0.51
1:C:262:GLN:HE22	2:D:74:ARG:HB2	1.75	0.51
1:A:343:ALA:HB2	1:A:352:TYR:CE1	2.44	0.51
1:C:209:MET:HG2	1:C:423:ARG:HD3	1.91	0.51
1:G:345:TYR:CG	1:G:346:GLU:O	2.63	0.51
1:A:270:LYS:HB3	1:A:271:LYS:CD	2.41	0.51
1:A:374:PRO:HG2	1:A:378:MET:SD	2.50	0.51
1:A:270:LYS:CB	1:A:271:LYS:HD2	2.41	0.51
1:C:214:SER:HG	1:C:217:LEU:N	2.09	0.51
2:B:82:LYS:O	2:B:83:PRO:C	2.49	0.51
1:G:268:PRO:HD3	3:G:44:HOH:O	2.10	0.51
1:A:239:LEU:CD1	1:A:408:PHE:HE2	2.24	0.51
2:B:60:PRO:CD	2:B:61:LYS:H	2.24	0.51
2:B:47:GLU:HB3	3:B:171:HOH:O	2.11	0.51
1:C:271:LYS:HG3	1:C:272:GLY:H	1.75	0.50
1:E:260:ILE:HD11	1:E:274:LEU:CD2	2.39	0.50
1:E:393:THR:HG22	1:E:400:THR:HA	1.93	0.50
1:G:357:SER:CB	1:G:358:PRO:CA	2.89	0.50
1:A:212:ILE:HG22	1:A:243:ILE:CD1	2.37	0.50
1:G:410:VAL:HG12	1:G:411:SER:N	2.25	0.50
1:G:239:LEU:HD22	1:G:291:PHE:CG	2.47	0.50
2:H:78:ASP:C	2:H:80:PHE:H	2.15	0.50
1:C:252:ASP:N	1:C:253:PRO:CD	2.74	0.50
1:E:275:LYS:HE3	1:E:279:GLU:CD	2.32	0.50
1:E:240:PHE:CZ	1:E:243:ILE:CG2	2.82	0.50
1:G:278:PHE:HE1	1:G:426:LYS:HB2	1.77	0.49
1:G:239:LEU:HD22	1:G:291:PHE:CD1	2.48	0.49
1:G:295:LEU:O	1:G:371:LYS:HE3	2.13	0.49
1:A:370:LEU:HD11	1:A:383:LEU:HD21	1.95	0.49
1:G:381:SER:O	1:G:384:GLU:HB2	2.13	0.49
1:E:410:VAL:HG12	1:E:411:SER:N	2.28	0.49
1:G:378:MET:O	1:G:382:VAL:HG23	2.13	0.49
2:D:72:ARG:HB2	2:D:81:PHE:CZ	2.46	0.49
1:A:271:LYS:O	1:A:276:GLU:OE2	2.30	0.49
2:B:48:THR:C	2:B:50:LEU:N	2.65	0.49
1:E:259:ASP:OD1	1:E:261:ARG:NH1	2.42	0.48
1:E:297:THR:O	1:E:297:THR:CG2	2.60	0.48
1:E:245:GLN:O	1:E:245:GLN:CD	2.52	0.48
1:C:252:ASP:N	1:C:253:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:LEU:HD23	1:C:288:LEU:C	2.34	0.48
1:E:377:TYR:C	1:E:377:TYR:CD2	2.86	0.48
1:A:418:GLN:HG2	2:B:84:PRO:HG2	1.95	0.48
2:D:71:MET:HE2	2:D:74:ARG:CZ	2.42	0.48
1:E:326:LYS:HG2	1:E:336:GLU:HB2	1.96	0.48
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.54	0.48
1:E:301:ASP:O	1:E:302:GLU:HB2	2.13	0.48
1:G:398:GLN:CA	1:G:398:GLN:HE21	2.23	0.48
1:A:326:LYS:HE2	1:A:333:GLN:NE2	2.29	0.48
1:C:217:LEU:HD12	1:C:401:LEU:HB3	1.96	0.47
2:H:78:ASP:O	2:H:80:PHE:N	2.47	0.47
1:E:425:VAL:O	1:E:426:LYS:HB2	2.12	0.47
1:G:307:TYR:O	1:G:358:PRO:HG3	2.12	0.47
2:D:49:ASP:HA	3:D:142:HOH:O	2.14	0.47
1:A:394:ASN:O	1:A:397:THR:O	2.32	0.47
2:H:78:ASP:C	2:H:80:PHE:N	2.68	0.47
1:A:290:LYS:O	1:A:419:HIS:HA	2.15	0.47
1:A:412:ALA:O	1:A:413:SER:C	2.53	0.47
1:A:212:ILE:HG23	1:A:212:ILE:O	2.15	0.47
1:G:209:MET:HG2	1:G:254:TYR:CE2	2.50	0.47
1:G:325:THR:HG22	3:G:62:HOH:O	2.15	0.47
1:C:252:ASP:HB2	3:C:22:HOH:O	2.13	0.47
2:D:72:ARG:HG3	2:D:72:ARG:O	2.13	0.47
2:D:49:ASP:HB2	3:D:24:HOH:O	2.14	0.47
1:A:262:GLN:O	2:B:74:ARG:NH1	2.42	0.47
1:A:262:GLN:NE2	2:B:75:LYS:HG3	2.30	0.47
1:C:259:ASP:OD1	1:C:259:ASP:C	2.53	0.47
1:C:375:GLU:HB2	1:C:378:MET:HG3	1.97	0.47
1:E:295:LEU:N	1:E:295:LEU:HD23	2.28	0.47
1:C:263:ILE:HD12	1:C:263:ILE:HA	1.75	0.47
1:G:281:GLY:HA3	1:G:400:THR:CG2	2.45	0.47
1:E:301:ASP:O	1:E:302:GLU:CB	2.63	0.47
1:A:271:LYS:HD2	1:A:271:LYS:N	2.29	0.47
1:E:217:LEU:CD2	1:E:313:TYR:HB3	2.45	0.47
1:A:373:LEU:HD22	1:A:374:PRO:HD2	1.97	0.47
1:A:260:ILE:HG13	1:A:264:TYR:CE1	2.50	0.47
2:D:72:ARG:CB	2:D:81:PHE:CZ	2.98	0.46
1:C:355:HIS:HB3	3:C:174:HOH:O	2.15	0.46
2:D:71:MET:HE1	2:D:74:ARG:CD	2.46	0.46
1:A:356:ARG:O	1:A:357:SER:O	2.32	0.46
1:C:267:PHE:CZ	1:C:405:ALA:HB1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH2	1:G:353:ARG:HG3	2.30	0.46
1:E:385:ASN:HD21	2:F:68:THR:HG21	1.79	0.46
1:E:353:ARG:O	1:E:353:ARG:HD2	2.14	0.46
1:C:363:MET:O	1:C:367:ILE:HG12	2.15	0.46
1:C:374:PRO:HD2	1:C:378:MET:HE3	1.98	0.46
1:A:294:ASP:HB2	1:A:417:ALA:HB2	1.98	0.46
2:F:49:ASP:HA	3:F:179:HOH:O	2.15	0.46
1:A:211:SER:OG	1:A:243:ILE:HG21	2.15	0.46
1:A:232:PRO:HB3	1:G:236:ASN:HA	1.97	0.46
1:C:326:LYS:HD3	1:C:333:GLN:NE2	2.30	0.46
1:E:226:LEU:HG	1:E:299:ILE:HD11	1.97	0.46
1:C:232:PRO:HG2	1:E:234:THR:HG23	1.98	0.46
2:D:71:MET:HE3	2:D:74:ARG:NH2	2.30	0.46
1:E:295:LEU:HD21	1:E:410:VAL:HG22	1.98	0.46
1:C:357:SER:C	3:C:428:HOH:O	2.55	0.46
2:B:56:ALA:HB2	2:B:65:VAL:HG21	1.98	0.46
1:E:218:TRP:HZ2	1:E:246:SER:OG	2.00	0.45
1:A:328:CYS:HB3	1:A:332:LYS:O	2.15	0.45
2:B:59:ASN:N	2:B:60:PRO:CA	2.77	0.45
2:D:78:ASP:O	2:D:80:PHE:N	2.49	0.45
1:E:212:ILE:O	1:E:212:ILE:HG23	2.16	0.45
1:G:251:SER:N	3:G:17:HOH:O	2.49	0.45
1:E:236:ASN:ND2	3:E:148:HOH:O	2.38	0.45
1:E:394:ASN:C	1:E:394:ASN:OD1	2.54	0.45
1:G:268:PRO:HD2	3:G:205:HOH:O	2.16	0.45
1:C:368:HIS:O	1:C:372:HIS:HD2	1.99	0.45
1:A:407:VAL:HG11	2:B:80:PHE:HZ	1.82	0.45
1:C:228:ARG:HA	1:C:228:ARG:HD2	1.51	0.45
1:E:263:ILE:HD11	2:F:71:MET:CE	2.47	0.45
1:E:245:GLN:O	1:E:245:GLN:OE1	2.34	0.45
1:G:252:ASP:HB3	1:G:253:PRO:HG3	1.97	0.45
1:C:355:HIS:CG	1:C:356:ARG:N	2.80	0.45
1:E:418:GLN:HA	3:E:167:HOH:O	2.17	0.45
1:A:218:TRP:C	1:A:218:TRP:CD1	2.89	0.45
1:E:252:ASP:HB3	1:E:253:PRO:HD2	1.97	0.45
2:D:72:ARG:CA	2:D:81:PHE:CZ	2.99	0.45
2:D:77:PRO:O	2:D:80:PHE:HB2	2.16	0.45
2:F:72:ARG:HG2	2:F:72:ARG:H	1.35	0.45
1:A:320:ILE:O	1:A:395:ARG:HB2	2.17	0.45
1:E:370:LEU:HD12	2:F:54:PHE:CZ	2.52	0.45
2:D:78:ASP:O	2:D:79:SER:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:PRO:CD	3:G:73:HOH:O	2.63	0.44
1:G:381:SER:HA	1:G:384:GLU:HG3	2.00	0.44
1:E:241:VAL:CG1	1:E:242:HIS:N	2.81	0.44
1:G:393:THR:HG22	1:G:400:THR:HA	2.00	0.44
1:A:315:SER:HB3	1:A:352:TYR:HE2	1.82	0.44
1:G:357:SER:H	1:G:358:PRO:HD3	1.79	0.44
2:F:59:ASN:HB3	2:F:62:THR:HG23	1.99	0.44
2:B:76:LEU:HB3	2:B:77:PRO:HD2	1.97	0.44
1:E:361:GLU:HA	1:E:364:ILE:HD12	2.00	0.44
1:G:355:HIS:C	1:G:356:ARG:HG3	2.36	0.44
1:C:426:LYS:CB	1:C:426:LYS:NZ	2.72	0.43
1:G:226:LEU:O	1:G:235:TYR:CB	2.53	0.43
1:G:211:SER:OG	1:G:212:ILE:N	2.51	0.43
2:H:72:ARG:O	2:H:73:LEU:HB2	2.19	0.43
1:E:278:PHE:HA	1:E:286:PHE:CZ	2.53	0.43
1:G:243:ILE:CG2	1:G:244:SER:N	2.79	0.43
1:C:355:HIS:CD2	1:C:356:ARG:H	2.36	0.43
1:G:410:VAL:HG12	1:G:411:SER:H	1.84	0.43
1:A:243:ILE:HG22	1:A:243:ILE:O	2.18	0.43
1:C:240:PHE:C	1:C:240:PHE:CD1	2.91	0.43
1:C:308:GLY:HA2	3:C:428:HOH:O	2.18	0.43
1:G:345:TYR:CE1	1:G:346:GLU:O	2.72	0.43
2:B:65:VAL:HB	2:B:66:PRO:HD2	2.00	0.43
1:E:267:PHE:CZ	1:E:405:ALA:HB1	2.54	0.43
1:E:228:ARG:HH12	1:E:304:SER:HB3	1.84	0.43
1:E:231:ASP:N	3:E:186:HOH:O	2.48	0.42
1:G:267:PHE:HA	1:G:268:PRO:HA	1.76	0.42
1:C:260:ILE:HG23	1:C:261:ARG:N	2.35	0.42
1:E:261:ARG:CG	1:E:261:ARG:NH1	2.62	0.42
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.91	0.42
2:B:85:GLU:HG3	3:B:35:HOH:O	2.19	0.42
1:A:269:GLU:O	1:A:273:GLY:HA3	2.19	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD2	1.83	0.42
1:G:243:ILE:HG22	1:G:244:SER:H	1.84	0.42
1:E:346:GLU:HG2	1:E:347:ASN:OD1	2.19	0.42
1:C:259:ASP:O	1:C:260:ILE:C	2.57	0.42
2:D:82:LYS:HB2	2:D:82:LYS:HE3	1.67	0.42
1:A:380:ASN:ND2	1:A:409:GLU:HG2	2.35	0.42
1:C:300:ASP:OD1	1:C:368:HIS:HE1	2.03	0.42
1:A:397:THR:C	1:A:399:GLU:N	2.69	0.41
1:G:209:MET:CG	1:G:254:TYR:HD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:HA	1:A:286:PHE:CZ	2.55	0.41
1:E:217:LEU:HD22	1:E:313:TYR:HB3	2.01	0.41
1:E:343:ALA:HB2	1:E:352:TYR:CE1	2.55	0.41
1:G:237:LYS:NZ	1:G:237:LYS:CB	2.58	0.41
1:E:231:ASP:CB	3:E:26:HOH:O	2.36	0.41
1:C:426:LYS:HZ3	1:C:426:LYS:HB2	1.82	0.41
1:E:267:PHE:HB3	1:E:268:PRO:HD2	2.03	0.41
1:E:222:PHE:C	1:E:222:PHE:CD2	2.93	0.41
1:A:239:LEU:HD11	1:A:408:PHE:HE2	1.84	0.41
1:A:355:HIS:C	1:A:357:SER:N	2.74	0.41
1:E:275:LYS:HE3	1:E:279:GLU:OE2	2.21	0.41
1:E:352:TYR:N	1:E:352:TYR:CD2	2.87	0.41
1:C:260:ILE:HG12	1:C:264:TYR:CE1	2.55	0.41
1:A:239:LEU:HA	1:A:239:LEU:HD23	1.35	0.41
1:E:263:ILE:HD11	2:F:71:MET:HE1	2.03	0.41
1:C:388:ILE:HD12	1:C:408:PHE:CZ	2.56	0.41
2:B:53:LEU:HA	2:B:53:LEU:HD23	1.82	0.41
1:G:265:ASP:OD1	2:H:74:ARG:NH2	2.53	0.41
1:A:212:ILE:O	1:A:212:ILE:CD1	2.69	0.41
1:G:314:GLU:HG3	1:G:351:LEU:CD2	2.48	0.41
1:E:212:ILE:HD11	1:E:404:ILE:HG12	2.03	0.41
2:H:72:ARG:O	2:H:73:LEU:CB	2.69	0.41
2:F:73:LEU:CG	2:F:73:LEU:O	2.66	0.41
1:C:356:ARG:NE	3:C:158:HOH:O	2.54	0.41
1:E:353:ARG:HD2	1:E:353:ARG:C	2.41	0.41
1:E:263:ILE:HD12	1:E:263:ILE:HA	1.85	0.41
1:G:214:SER:HB3	1:G:401:LEU:O	2.21	0.41
1:A:230:GLN:O	1:A:232:PRO:N	2.54	0.41
1:E:236:ASN:ND2	1:E:297:THR:HB	2.36	0.40
1:G:280:ARG:C	1:G:280:ARG:CD	2.69	0.40
1:G:226:LEU:HD23	1:G:297:THR:HG21	2.04	0.40
1:A:327:VAL:HB	1:A:335:VAL:HG13	2.03	0.40
2:B:80:PHE:O	2:B:80:PHE:CD2	2.75	0.40
2:D:69:VAL:HA	2:D:70:PRO:HD2	1.85	0.40
1:C:226:LEU:HD13	1:C:307:TYR:CE2	2.57	0.40
1:E:226:LEU:HD13	1:E:307:TYR:CZ	2.56	0.40
1:G:402:LEU:HA	1:G:402:LEU:HD22	1.95	0.40
1:E:232:PRO:CB	1:E:233:ASP:CB	2.88	0.40
1:A:394:ASN:HB3	1:A:397:THR:HG1	1.86	0.40
1:E:343:ALA:HB1	1:E:350:TYR:HB3	2.04	0.40
1:E:238:HIS:O	1:E:239:LEU:HD13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	196/220 (89%)	173 (88%)	16 (8%)	7 (4%)	4	24
1	C	209/220 (95%)	189 (90%)	18 (9%)	2 (1%)	19	61
1	E	212/220 (96%)	189 (89%)	16 (8%)	7 (3%)	5	26
1	G	178/220 (81%)	164 (92%)	10 (6%)	4 (2%)	8	38
2	B	37/39 (95%)	32 (86%)	4 (11%)	1 (3%)	6	32
2	D	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
2	F	34/39 (87%)	25 (74%)	8 (24%)	1 (3%)	6	29
2	H	17/39 (44%)	10 (59%)	5 (29%)	2 (12%)	0	2
All	All	916/1036 (88%)	812 (89%)	80 (9%)	24 (3%)	7	33

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	231	ASP
1	A	271	LYS
1	C	358	PRO
1	E	244	SER
1	G	253	PRO
1	G	357	SER
1	A	356	ARG
1	A	357	SER
2	F	60	PRO
2	H	79	SER
1	A	398	GLN
1	E	242	HIS
1	C	356	ARG

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Mol	Chain	Res	Type
1	E	233	ASP
1	E	231	ASP
1	G	252	ASP
2	H	70	PRO
1	E	232	PRO
1	A	232	PRO
1	E	243	ILE
2	B	60	PRO
1	G	212	ILE
1	E	212	ILE

### 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	188/203 (93%)	162 (86%)	26 (14%)	4	20
1	C	196/203 (97%)	169 (86%)	27 (14%)	4	20
1	E	200/203 (98%)	171 (86%)	29 (14%)	4	18
1	G	178/203 (88%)	152 (85%)	26 (15%)	4	18
2	B	36/36 (100%)	28 (78%)	8 (22%)	1	5
2	D	32/36 (89%)	26 (81%)	6 (19%)	2	10
2	F	33/36 (92%)	27 (82%)	6 (18%)	2	11
2	H	19/36 (53%)	16 (84%)	3 (16%)	3	15
All	All	882/956 (92%)	751 (85%)	131 (15%)	4	17

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ILE
1	A	217	LEU
1	A	228	ARG
1	A	231	ASP
1	A	234	THR

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Mol	Chain	Res	Type
1	A	235	TYR
1	A	237	LYS
1	A	240	PHE
1	A	241	VAL
1	A	242	HIS
1	A	271	LYS
1	A	274	LEU
1	A	298	ASN
1	A	309	VAL
1	A	325	THR
1	A	328	CYS
1	A	332	LYS
1	A	335	VAL
1	A	339	GLU
1	A	360	CYS
1	A	381	SER
1	A	389	LEU
1	A	395	ARG
1	A	398	GLN
1	A	401	LEU
1	A	418	GLN
2	B	49	ASP
2	B	50	LEU
2	B	51	GLU
2	B	61	LYS
2	B	68	THR
2	B	69	VAL
2	B	72	ARG
2	B	78	ASP
1	C	210	ARG
1	C	212	ILE
1	C	217	LEU
1	C	221	GLU
1	C	234	THR
1	C	235	TYR
1	C	240	PHE
1	C	245	GLN
1	C	254	TYR
1	C	260	ILE
1	C	261	ARG
1	C	263	ILE
1	C	271	LYS

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Mol	Chain	Res	Type
1	C	283	SER
1	C	324	SER
1	C	325	THR
1	C	333	GLN
1	C	346	GLU
1	C	353	ARG
1	C	356	ARG
1	C	369	LYS
1	C	371	LYS
1	C	384	GLU
1	C	389	LEU
1	C	395	ARG
1	C	398	GLN
1	C	426	LYS
2	D	50	LEU
2	D	72	ARG
2	D	73	LEU
2	D	74	ARG
2	D	78	ASP
2	D	79	SER
1	E	210	ARG
1	E	217	LEU
1	E	226	LEU
1	E	229	GLN
1	E	230	GLN
1	E	231	ASP
1	E	245	GLN
1	E	246	SER
1	E	247	SER
1	E	261	ARG
1	E	263	ILE
1	E	274	LEU
1	E	277	LEU
1	E	295	LEU
1	E	298	ASN
1	E	312	GLN
1	E	319	MET
1	E	329	SER
1	E	336	GLU
1	E	339	GLU
1	E	340	THR
1	E	353	ARG

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Mol	Chain	Res	Type
1	E	354	ILE
1	E	372	HIS
1	E	379	MET
1	E	389	LEU
1	E	398	GLN
1	E	401	LEU
1	E	423	ARG
2	F	57	VAL
2	F	62	THR
2	F	65	VAL
2	F	69	VAL
2	F	71	MET
2	F	73	LEU
1	G	217	LEU
1	G	227	GLU
1	G	229	GLN
1	G	230	GLN
1	G	235	TYR
1	G	237	LYS
1	G	239	LEU
1	G	241	VAL
1	G	245	GLN
1	G	252	ASP
1	G	260	ILE
1	G	269	GLU
1	G	294	ASP
1	G	295	LEU
1	G	297	THR
1	G	312	GLN
1	G	344	ARG
1	G	360	CYS
1	G	375	GLU
1	G	384	GLU
1	G	389	LEU
1	G	395	ARG
1	G	398	GLN
1	G	401	LEU
1	G	402	LEU
1	G	420	HIS
2	H	69	VAL
2	H	73	LEU
2	H	79	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	GLN
1	A	333	GLN
1	A	365	ASN
1	A	372	HIS
1	A	380	ASN
1	A	385	ASN
1	A	390	GLN
2	B	55	ASN
1	C	229	GLN
1	C	242	HIS
1	C	262	GLN
1	C	333	GLN
1	C	368	HIS
1	C	372	HIS
1	C	385	ASN
1	E	236	ASN
1	E	262	GLN
1	E	333	GLN
1	E	365	ASN
1	E	385	ASN
1	E	398	GLN
1	G	230	GLN
1	G	312	GLN
1	G	349	HIS
1	G	368	HIS
1	G	398	GLN
1	G	419	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	204/220 (92%)	-0.03	1 (0%) 91 76	15, 25, 35, 43	0
1	C	213/220 (96%)	-0.10	0 100 100	18, 28, 39, 53	0
1	E	216/220 (98%)	0.02	1 (0%) 91 76	19, 28, 40, 60	0
1	G	190/220 (86%)	0.35	8 (4%) 40 16	14, 28, 39, 43	0
2	B	39/39 (100%)	0.09	1 (2%) 59 29	21, 25, 36, 36	0
2	D	35/39 (89%)	-0.16	0 100 100	25, 28, 37, 39	0
2	F	36/39 (92%)	0.21	1 (2%) 56 27	26, 32, 39, 39	0
2	H	19/39 (48%)	0.42	2 (10%) 8 3	21, 27, 34, 34	0
All	All	952/1036 (91%)	0.06	14 (1%) 76 49	14, 28, 39, 60	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	229	GLN	4.0
2	F	61	LYS	3.5
2	H	67	GLN	3.1
1	G	367	ILE	3.1
1	G	359	LEU	2.9
1	G	372	HIS	2.7
1	G	368	HIS	2.6
2	B	60	PRO	2.5
2	H	68	THR	2.3
1	G	364	ILE	2.2
1	G	369	LYS	2.1
1	G	298	ASN	2.1
1	A	304	SER	2.1
1	E	244	SER	2.1

## 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.