



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:15 AM GMT

PDB ID : 3LA6
Title : Octameric kinase domain of the E. coli tyrosine kinase Wzc with bound ADP
Authors : Gruszczyk, J.; Nessler, S.; Gueguen-Chaignon, V.; Vigouroux, A.; Bechet, E.; Grangeasse, C.
Deposited on : 2010-01-06
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

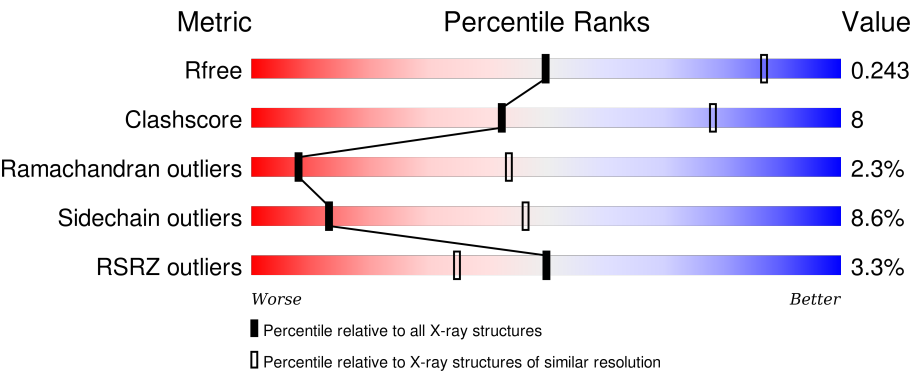
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 ≥ 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	286	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>64%23%•9%</div></div>
1	B	286	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>69%18%•9%</div></div>
1	C	286	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>67%21%•9%</div></div>
1	D	286	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>65%21%•10%</div></div>
1	E	286	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>69%18%•9%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	286	
1	G	286	
1	H	286	
1	I	286	
1	J	286	
1	K	286	
1	L	286	
1	M	286	
1	N	286	
1	O	286	
1	P	286	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	1001	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32420 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 Tyrosine-protein kinase wzc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1998	1262	343	383	10			
1	B	260	Total	C	N	O	S	0	0	0
			2004	1265	344	385	10			
1	C	260	Total	C	N	O	S	0	0	0
			2006	1266	345	385	10			
1	D	258	Total	C	N	O	S	0	0	0
			1993	1259	343	381	10			
1	E	260	Total	C	N	O	S	0	0	0
			2013	1272	345	386	10			
1	F	257	Total	C	N	O	S	0	0	0
			1982	1252	340	380	10			
1	G	259	Total	C	N	O	S	0	0	0
			2003	1266	343	384	10			
1	H	260	Total	C	N	O	S	0	0	0
			2004	1265	344	385	10			
1	I	260	Total	C	N	O	S	0	0	0
			2008	1268	345	385	10			
1	J	259	Total	C	N	O	S	0	0	0
			2000	1264	344	382	10			
1	K	258	Total	C	N	O	S	0	0	0
			1993	1259	343	381	10			
1	L	259	Total	C	N	O	S	0	0	0
			1999	1265	343	381	10			
1	M	256	Total	C	N	O	S	0	0	0
			1977	1249	339	379	10			
1	N	260	Total	C	N	O	S	0	0	0
			2008	1268	345	385	10			
1	O	260	Total	C	N	O	S	0	0	0
			2008	1269	344	385	10			
1	P	256	Total	C	N	O	S	0	0	0
			1976	1250	338	378	10			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	MET	-	EXPRESSION TAG	UNP P76387
A	436	ARG	-	EXPRESSION TAG	UNP P76387
A	437	GLY	-	EXPRESSION TAG	UNP P76387
A	438	SER	-	EXPRESSION TAG	UNP P76387
A	439	HIS	-	EXPRESSION TAG	UNP P76387
A	440	HIS	-	EXPRESSION TAG	UNP P76387
A	441	HIS	-	EXPRESSION TAG	UNP P76387
A	442	HIS	-	EXPRESSION TAG	UNP P76387
A	443	HIS	-	EXPRESSION TAG	UNP P76387
A	444	HIS	-	EXPRESSION TAG	UNP P76387
A	445	GLY	-	EXPRESSION TAG	UNP P76387
A	446	SER	-	EXPRESSION TAG	UNP P76387
A	540	MET	LYS	SEE REMARK 999	UNP P76387
B	435	MET	-	EXPRESSION TAG	UNP P76387
B	436	ARG	-	EXPRESSION TAG	UNP P76387
B	437	GLY	-	EXPRESSION TAG	UNP P76387
B	438	SER	-	EXPRESSION TAG	UNP P76387
B	439	HIS	-	EXPRESSION TAG	UNP P76387
B	440	HIS	-	EXPRESSION TAG	UNP P76387
B	441	HIS	-	EXPRESSION TAG	UNP P76387
B	442	HIS	-	EXPRESSION TAG	UNP P76387
B	443	HIS	-	EXPRESSION TAG	UNP P76387
B	444	HIS	-	EXPRESSION TAG	UNP P76387
B	445	GLY	-	EXPRESSION TAG	UNP P76387
B	446	SER	-	EXPRESSION TAG	UNP P76387
B	540	MET	LYS	SEE REMARK 999	UNP P76387
C	435	MET	-	EXPRESSION TAG	UNP P76387
C	436	ARG	-	EXPRESSION TAG	UNP P76387
C	437	GLY	-	EXPRESSION TAG	UNP P76387
C	438	SER	-	EXPRESSION TAG	UNP P76387
C	439	HIS	-	EXPRESSION TAG	UNP P76387
C	440	HIS	-	EXPRESSION TAG	UNP P76387
C	441	HIS	-	EXPRESSION TAG	UNP P76387
C	442	HIS	-	EXPRESSION TAG	UNP P76387
C	443	HIS	-	EXPRESSION TAG	UNP P76387
C	444	HIS	-	EXPRESSION TAG	UNP P76387
C	445	GLY	-	EXPRESSION TAG	UNP P76387
C	446	SER	-	EXPRESSION TAG	UNP P76387
C	540	MET	LYS	SEE REMARK 999	UNP P76387
D	435	MET	-	EXPRESSION TAG	UNP P76387
D	436	ARG	-	EXPRESSION TAG	UNP P76387
D	437	GLY	-	EXPRESSION TAG	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
D	438	SER	-	EXPRESSION TAG	UNP P76387
D	439	HIS	-	EXPRESSION TAG	UNP P76387
D	440	HIS	-	EXPRESSION TAG	UNP P76387
D	441	HIS	-	EXPRESSION TAG	UNP P76387
D	442	HIS	-	EXPRESSION TAG	UNP P76387
D	443	HIS	-	EXPRESSION TAG	UNP P76387
D	444	HIS	-	EXPRESSION TAG	UNP P76387
D	445	GLY	-	EXPRESSION TAG	UNP P76387
D	446	SER	-	EXPRESSION TAG	UNP P76387
D	540	MET	LYS	SEE REMARK 999	UNP P76387
E	435	MET	-	EXPRESSION TAG	UNP P76387
E	436	ARG	-	EXPRESSION TAG	UNP P76387
E	437	GLY	-	EXPRESSION TAG	UNP P76387
E	438	SER	-	EXPRESSION TAG	UNP P76387
E	439	HIS	-	EXPRESSION TAG	UNP P76387
E	440	HIS	-	EXPRESSION TAG	UNP P76387
E	441	HIS	-	EXPRESSION TAG	UNP P76387
E	442	HIS	-	EXPRESSION TAG	UNP P76387
E	443	HIS	-	EXPRESSION TAG	UNP P76387
E	444	HIS	-	EXPRESSION TAG	UNP P76387
E	445	GLY	-	EXPRESSION TAG	UNP P76387
E	446	SER	-	EXPRESSION TAG	UNP P76387
E	540	MET	LYS	SEE REMARK 999	UNP P76387
F	435	MET	-	EXPRESSION TAG	UNP P76387
F	436	ARG	-	EXPRESSION TAG	UNP P76387
F	437	GLY	-	EXPRESSION TAG	UNP P76387
F	438	SER	-	EXPRESSION TAG	UNP P76387
F	439	HIS	-	EXPRESSION TAG	UNP P76387
F	440	HIS	-	EXPRESSION TAG	UNP P76387
F	441	HIS	-	EXPRESSION TAG	UNP P76387
F	442	HIS	-	EXPRESSION TAG	UNP P76387
F	443	HIS	-	EXPRESSION TAG	UNP P76387
F	444	HIS	-	EXPRESSION TAG	UNP P76387
F	445	GLY	-	EXPRESSION TAG	UNP P76387
F	446	SER	-	EXPRESSION TAG	UNP P76387
F	540	MET	LYS	SEE REMARK 999	UNP P76387
G	435	MET	-	EXPRESSION TAG	UNP P76387
G	436	ARG	-	EXPRESSION TAG	UNP P76387
G	437	GLY	-	EXPRESSION TAG	UNP P76387
G	438	SER	-	EXPRESSION TAG	UNP P76387
G	439	HIS	-	EXPRESSION TAG	UNP P76387
G	440	HIS	-	EXPRESSION TAG	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
G	441	HIS	-	EXPRESSION TAG	UNP P76387
G	442	HIS	-	EXPRESSION TAG	UNP P76387
G	443	HIS	-	EXPRESSION TAG	UNP P76387
G	444	HIS	-	EXPRESSION TAG	UNP P76387
G	445	GLY	-	EXPRESSION TAG	UNP P76387
G	446	SER	-	EXPRESSION TAG	UNP P76387
G	540	MET	LYS	SEE REMARK 999	UNP P76387
H	435	MET	-	EXPRESSION TAG	UNP P76387
H	436	ARG	-	EXPRESSION TAG	UNP P76387
H	437	GLY	-	EXPRESSION TAG	UNP P76387
H	438	SER	-	EXPRESSION TAG	UNP P76387
H	439	HIS	-	EXPRESSION TAG	UNP P76387
H	440	HIS	-	EXPRESSION TAG	UNP P76387
H	441	HIS	-	EXPRESSION TAG	UNP P76387
H	442	HIS	-	EXPRESSION TAG	UNP P76387
H	443	HIS	-	EXPRESSION TAG	UNP P76387
H	444	HIS	-	EXPRESSION TAG	UNP P76387
H	445	GLY	-	EXPRESSION TAG	UNP P76387
H	446	SER	-	EXPRESSION TAG	UNP P76387
H	540	MET	LYS	SEE REMARK 999	UNP P76387
I	435	MET	-	EXPRESSION TAG	UNP P76387
I	436	ARG	-	EXPRESSION TAG	UNP P76387
I	437	GLY	-	EXPRESSION TAG	UNP P76387
I	438	SER	-	EXPRESSION TAG	UNP P76387
I	439	HIS	-	EXPRESSION TAG	UNP P76387
I	440	HIS	-	EXPRESSION TAG	UNP P76387
I	441	HIS	-	EXPRESSION TAG	UNP P76387
I	442	HIS	-	EXPRESSION TAG	UNP P76387
I	443	HIS	-	EXPRESSION TAG	UNP P76387
I	444	HIS	-	EXPRESSION TAG	UNP P76387
I	445	GLY	-	EXPRESSION TAG	UNP P76387
I	446	SER	-	EXPRESSION TAG	UNP P76387
I	540	MET	LYS	SEE REMARK 999	UNP P76387
J	435	MET	-	EXPRESSION TAG	UNP P76387
J	436	ARG	-	EXPRESSION TAG	UNP P76387
J	437	GLY	-	EXPRESSION TAG	UNP P76387
J	438	SER	-	EXPRESSION TAG	UNP P76387
J	439	HIS	-	EXPRESSION TAG	UNP P76387
J	440	HIS	-	EXPRESSION TAG	UNP P76387
J	441	HIS	-	EXPRESSION TAG	UNP P76387
J	442	HIS	-	EXPRESSION TAG	UNP P76387
J	443	HIS	-	EXPRESSION TAG	UNP P76387

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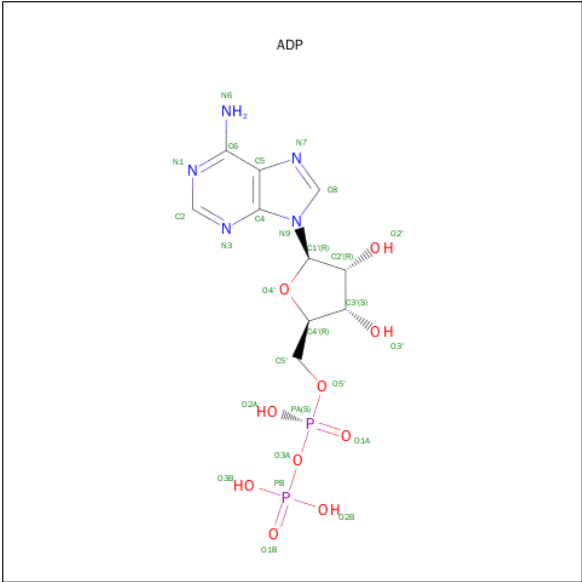
Chain	Residue	Modelled	Actual	Comment	Reference
J	444	HIS	-	EXPRESSION TAG	UNP P76387
J	445	GLY	-	EXPRESSION TAG	UNP P76387
J	446	SER	-	EXPRESSION TAG	UNP P76387
J	540	MET	LYS	SEE REMARK 999	UNP P76387
K	435	MET	-	EXPRESSION TAG	UNP P76387
K	436	ARG	-	EXPRESSION TAG	UNP P76387
K	437	GLY	-	EXPRESSION TAG	UNP P76387
K	438	SER	-	EXPRESSION TAG	UNP P76387
K	439	HIS	-	EXPRESSION TAG	UNP P76387
K	440	HIS	-	EXPRESSION TAG	UNP P76387
K	441	HIS	-	EXPRESSION TAG	UNP P76387
K	442	HIS	-	EXPRESSION TAG	UNP P76387
K	443	HIS	-	EXPRESSION TAG	UNP P76387
K	444	HIS	-	EXPRESSION TAG	UNP P76387
K	445	GLY	-	EXPRESSION TAG	UNP P76387
K	446	SER	-	EXPRESSION TAG	UNP P76387
K	540	MET	LYS	SEE REMARK 999	UNP P76387
L	435	MET	-	EXPRESSION TAG	UNP P76387
L	436	ARG	-	EXPRESSION TAG	UNP P76387
L	437	GLY	-	EXPRESSION TAG	UNP P76387
L	438	SER	-	EXPRESSION TAG	UNP P76387
L	439	HIS	-	EXPRESSION TAG	UNP P76387
L	440	HIS	-	EXPRESSION TAG	UNP P76387
L	441	HIS	-	EXPRESSION TAG	UNP P76387
L	442	HIS	-	EXPRESSION TAG	UNP P76387
L	443	HIS	-	EXPRESSION TAG	UNP P76387
L	444	HIS	-	EXPRESSION TAG	UNP P76387
L	445	GLY	-	EXPRESSION TAG	UNP P76387
L	446	SER	-	EXPRESSION TAG	UNP P76387
L	540	MET	LYS	SEE REMARK 999	UNP P76387
M	435	MET	-	EXPRESSION TAG	UNP P76387
M	436	ARG	-	EXPRESSION TAG	UNP P76387
M	437	GLY	-	EXPRESSION TAG	UNP P76387
M	438	SER	-	EXPRESSION TAG	UNP P76387
M	439	HIS	-	EXPRESSION TAG	UNP P76387
M	440	HIS	-	EXPRESSION TAG	UNP P76387
M	441	HIS	-	EXPRESSION TAG	UNP P76387
M	442	HIS	-	EXPRESSION TAG	UNP P76387
M	443	HIS	-	EXPRESSION TAG	UNP P76387
M	444	HIS	-	EXPRESSION TAG	UNP P76387
M	445	GLY	-	EXPRESSION TAG	UNP P76387
M	446	SER	-	EXPRESSION TAG	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
M	540	MET	LYS	SEE REMARK 999	UNP P76387
N	435	MET	-	EXPRESSION TAG	UNP P76387
N	436	ARG	-	EXPRESSION TAG	UNP P76387
N	437	GLY	-	EXPRESSION TAG	UNP P76387
N	438	SER	-	EXPRESSION TAG	UNP P76387
N	439	HIS	-	EXPRESSION TAG	UNP P76387
N	440	HIS	-	EXPRESSION TAG	UNP P76387
N	441	HIS	-	EXPRESSION TAG	UNP P76387
N	442	HIS	-	EXPRESSION TAG	UNP P76387
N	443	HIS	-	EXPRESSION TAG	UNP P76387
N	444	HIS	-	EXPRESSION TAG	UNP P76387
N	445	GLY	-	EXPRESSION TAG	UNP P76387
N	446	SER	-	EXPRESSION TAG	UNP P76387
N	540	MET	LYS	SEE REMARK 999	UNP P76387
O	435	MET	-	EXPRESSION TAG	UNP P76387
O	436	ARG	-	EXPRESSION TAG	UNP P76387
O	437	GLY	-	EXPRESSION TAG	UNP P76387
O	438	SER	-	EXPRESSION TAG	UNP P76387
O	439	HIS	-	EXPRESSION TAG	UNP P76387
O	440	HIS	-	EXPRESSION TAG	UNP P76387
O	441	HIS	-	EXPRESSION TAG	UNP P76387
O	442	HIS	-	EXPRESSION TAG	UNP P76387
O	443	HIS	-	EXPRESSION TAG	UNP P76387
O	444	HIS	-	EXPRESSION TAG	UNP P76387
O	445	GLY	-	EXPRESSION TAG	UNP P76387
O	446	SER	-	EXPRESSION TAG	UNP P76387
O	540	MET	LYS	SEE REMARK 999	UNP P76387
P	435	MET	-	EXPRESSION TAG	UNP P76387
P	436	ARG	-	EXPRESSION TAG	UNP P76387
P	437	GLY	-	EXPRESSION TAG	UNP P76387
P	438	SER	-	EXPRESSION TAG	UNP P76387
P	439	HIS	-	EXPRESSION TAG	UNP P76387
P	440	HIS	-	EXPRESSION TAG	UNP P76387
P	441	HIS	-	EXPRESSION TAG	UNP P76387
P	442	HIS	-	EXPRESSION TAG	UNP P76387
P	443	HIS	-	EXPRESSION TAG	UNP P76387
P	444	HIS	-	EXPRESSION TAG	UNP P76387
P	445	GLY	-	EXPRESSION TAG	UNP P76387
P	446	SER	-	EXPRESSION TAG	UNP P76387
P	540	MET	LYS	SEE REMARK 999	UNP P76387

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

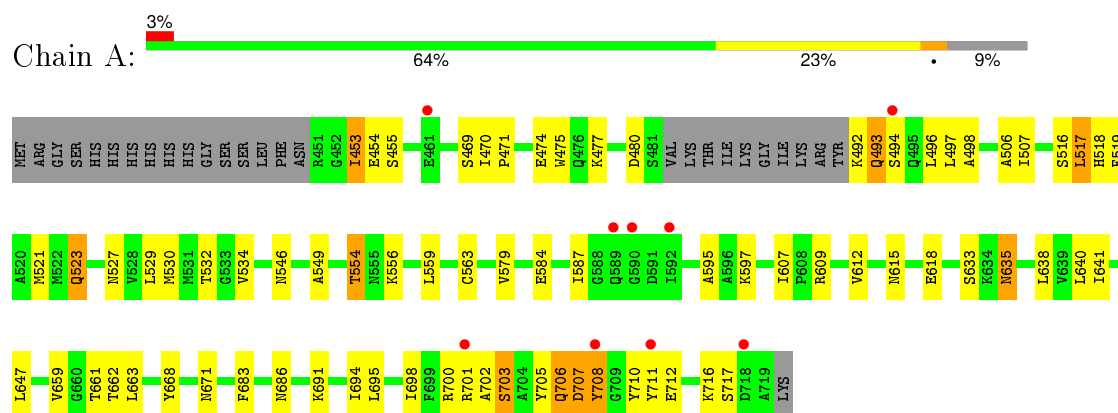
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	J	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	N	1	Total	Ca	0	0
			1	1		
3	O	1	Total	Ca	0	0
			1	1		
3	L	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		

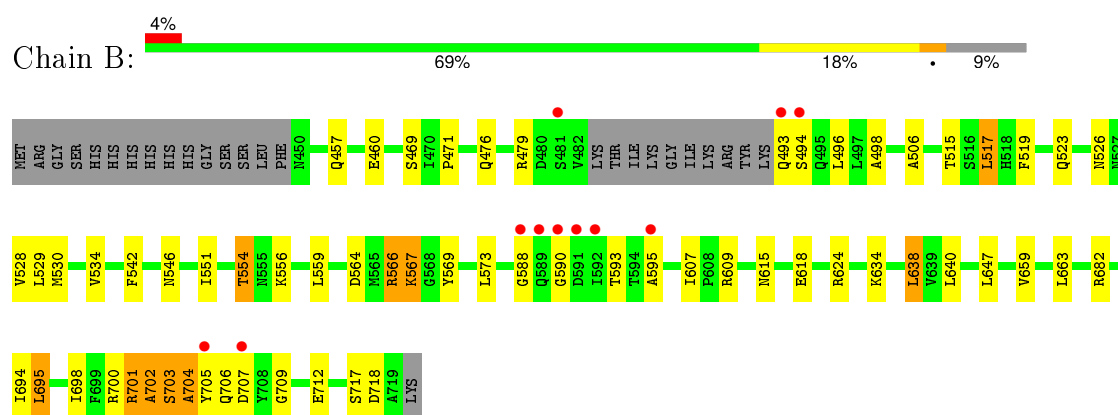
3 Residue-property plots

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.

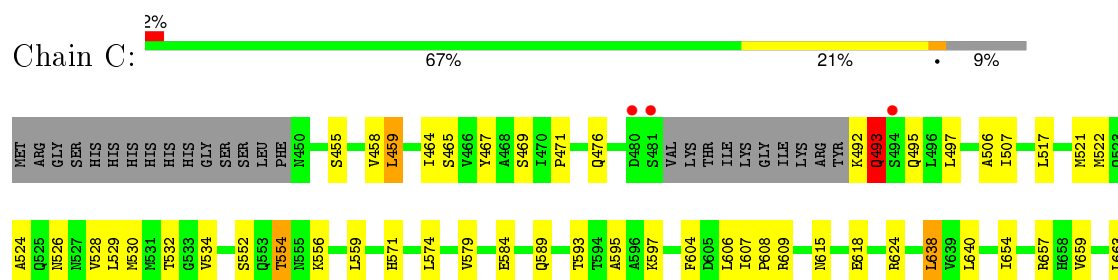
• Molecule 1: Tyrosine-protein kinase wzc



• Molecule 1: Tyrosine-protein kinase wzc

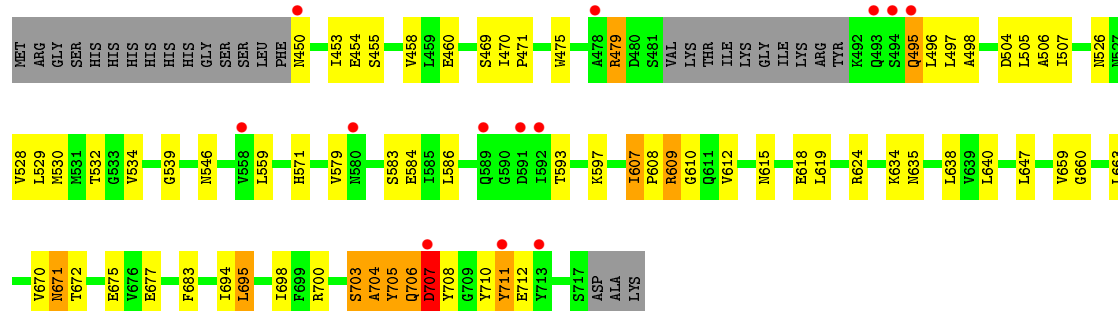


• Molecule 1: Tyrosine-protein kinase wzc

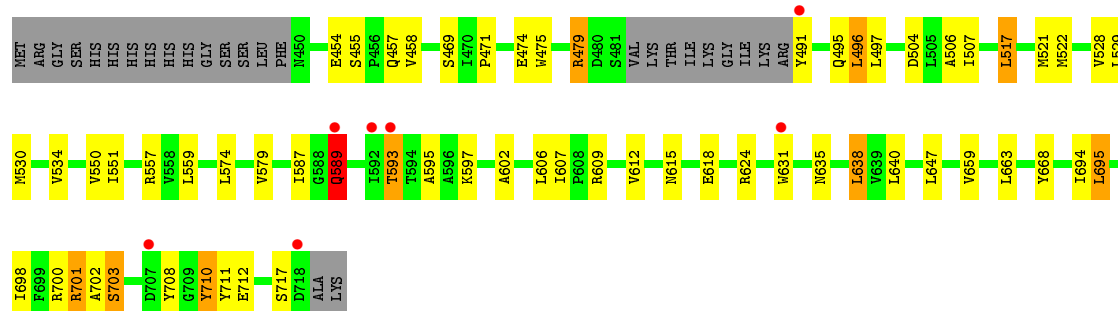




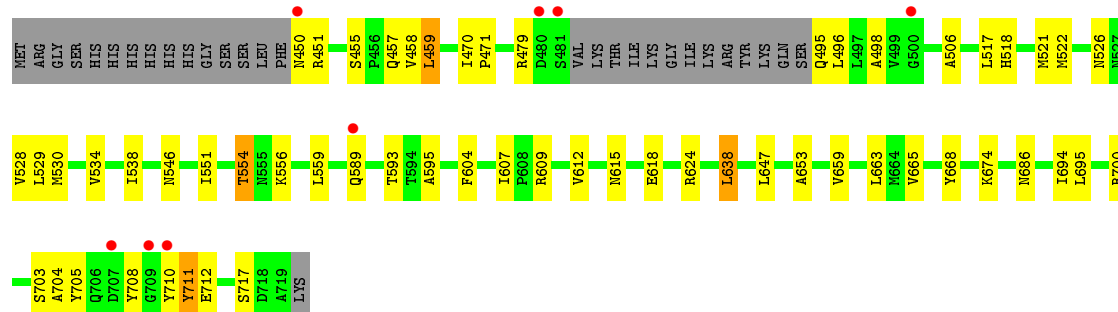
- Molecule 1: Tyrosine-protein kinase wzc



- Molecule 1: Tyrosine-protein kinase wzc

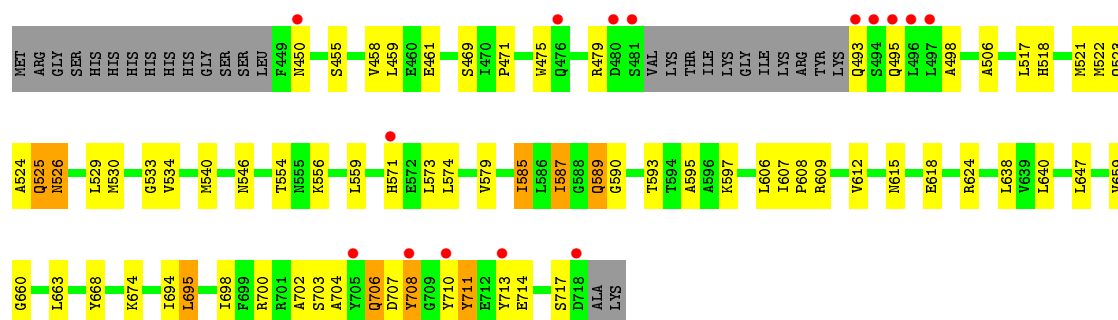


- Molecule 1: Tyrosine-protein kinase wzc

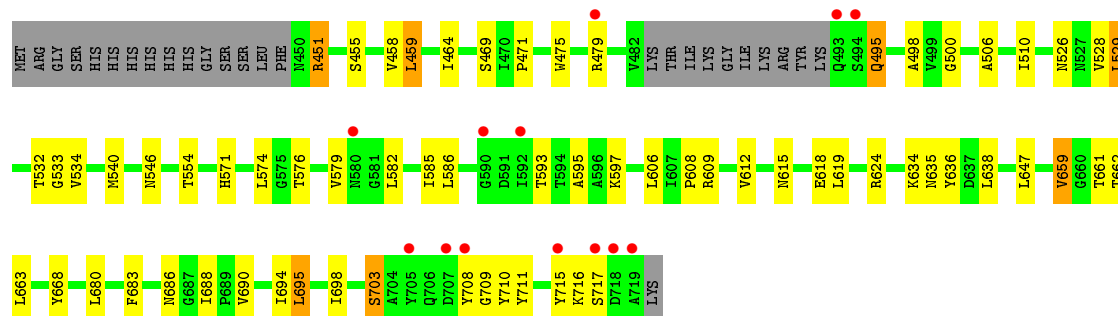


- Molecule 1: Tyrosine-protein kinase wzc

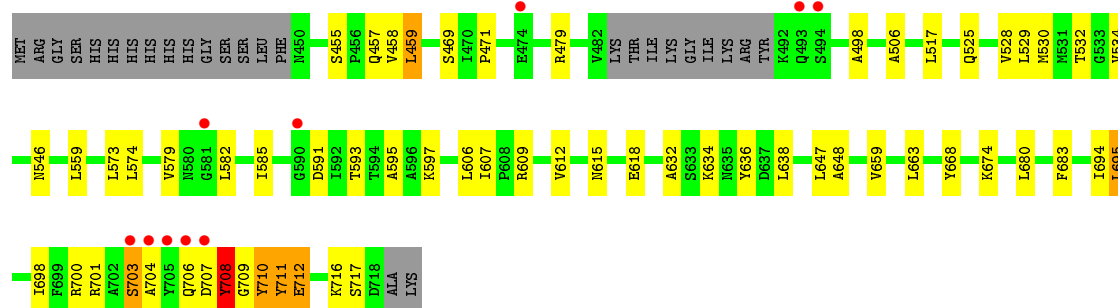




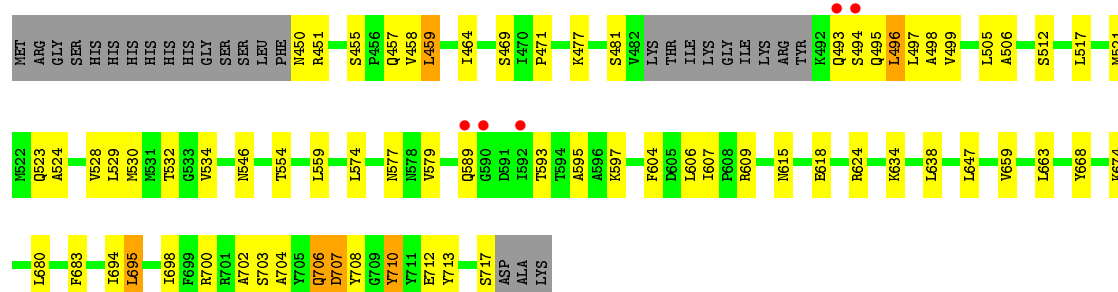
• Molecule 1: Tyrosine-protein kinase wzc




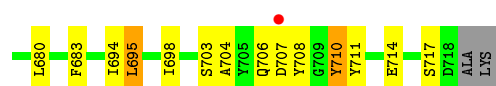
• Molecule 1: Tyrosine-protein kinase wzc



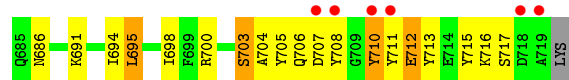
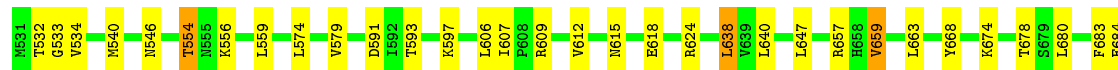
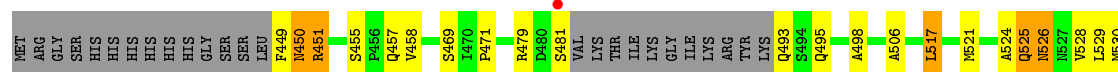
• Molecule 1: Tyrosine-protein kinase wzc



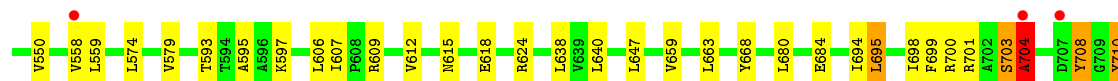
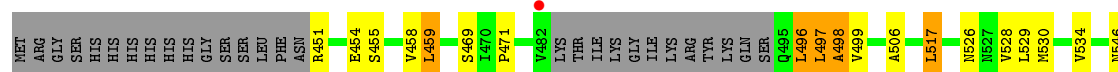
- Chain N: 
- Horizontal bar chart showing the distribution of Chain N across various categories. The chart is divided into four segments: 67% (green), 21% (yellow), 3% (red), and 9% (grey). The categories are listed on the left and right sides of the chart.
- | Category | Percentage |
|----------|------------|
| NET | 67% |
| ARG | 67% |
| GLY | 67% |
| SER | 67% |
| HIS | 67% |
| HIS | 67% |
| HIS | 67% |
| HIS | 67% |
| GLY | 67% |
| SER | 67% |
| SER | 67% |
| LEU | 67% |
| PHE | 67% |
| M450 | 67% |
| S485 | 67% |
| P456 | 67% |
| Q457 | 67% |
| V488 | 67% |
| L459 | 67% |
| P460 | 67% |
| P461 | 67% |
| S469 | 67% |
| I470 | 67% |
| P471 | 67% |
| S481 | 67% |
| V482 | 67% |
| LYS | 67% |
| THR | 67% |
| ILE | 67% |
| LYS | 67% |
| GLY | 67% |
| ILE | 67% |
| LYS | 67% |
| ARG | 67% |
| TYR | 67% |
| K492 | 67% |
| Q493 | 67% |
| S494 | 67% |
| Q495 | 67% |
| L496 | 67% |
| L497 | 67% |
| A498 | 67% |
| A506 | 67% |
| I510 | 67% |
| T515 | 67% |
| S516 | 67% |
| L517 | 67% |
| M521 | 67% |
| M526 | 67% |
| L529 | 67% |
| M30 | 67% |
| M31 | 67% |
| T32 | 67% |
| G33 | 67% |
| V34 | 67% |
| N346 | 67% |
| I551 | 67% |
| T554 | 67% |
| N555 | 67% |
| K556 | 67% |
| L559 | 67% |
| H571 | 67% |
| L574 | 67% |
| V579 | 67% |
| L586 | 67% |
| I587 | 67% |
| G588 | 67% |
| Q589 | 67% |
| G590 | 67% |
| D591 | 67% |
| I592 | 67% |
| T593 | 67% |
| K597 | 67% |
| L606 | 67% |
| I607 | 67% |
| P608 | 67% |
| R609 | 67% |
| V612 | 67% |
| N615 | 67% |
| E618 | 67% |
| L619 | 67% |
| R624 | 67% |
| I638 | 67% |
| V639 | 67% |
| L640 | 67% |
| L647 | 67% |
| V659 | 67% |
| G660 | 67% |
| L663 | 67% |
| L668 | 67% |



- Molecule 1: Tyrosine-protein kinase wzc



- Molecule 1: Tyrosine-protein kinase wzc



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.16Å 137.78Å 158.96Å 90.00° 92.99° 90.00°	Depositor
Resolution (Å)	49.74 – 3.20 49.74 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.74-3.20) 96.3 (49.74-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.186 , 0.223 0.202 , 0.243	Depositor DCC
R_{free} test set	833 reflections (1.00%)	DCC
Wilson B-factor (Å ²)	85.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.9	EDS
Estimated twinning fraction	0.003 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.004 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.006 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.006 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.012 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 83937 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32420	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

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

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	0.52	0/2032	0.77	1/2759 (0.0%)
1	B	0.51	0/2038	0.76	1/2769 (0.0%)
1	C	0.52	0/2040	0.76	0/2770
1	D	0.50	0/2027	0.77	1/2752 (0.0%)
1	E	0.52	0/2048	0.75	0/2781
1	F	0.50	0/2016	0.75	0/2739
1	G	0.47	0/2038	0.71	0/2768
1	H	0.51	0/2038	0.76	0/2769
1	I	0.49	0/2042	0.74	0/2773
1	J	0.51	0/2034	0.76	0/2762
1	K	0.53	0/2027	0.78	1/2752 (0.0%)
1	L	0.51	0/2033	0.76	0/2760
1	M	0.50	0/2011	0.75	1/2732 (0.0%)
1	N	0.52	0/2042	0.76	0/2773
1	O	0.52	0/2043	0.77	1/2775 (0.0%)
1	P	0.51	0/2010	0.78	2/2731 (0.1%)
All	All	0.51	0/32519	0.76	8/44165 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	712	GLU	C-N-CA	5.81	136.22	121.70
1	M	705	TYR	C-N-CA	5.76	136.11	121.70
1	B	705	TYR	C-N-CA	5.58	135.65	121.70
1	A	705	TYR	C-N-CA	5.51	135.48	121.70
1	K	702	ALA	C-N-CA	5.37	135.12	121.70
1	P	704	ALA	C-N-CA	5.27	134.88	121.70
1	D	703	SER	C-N-CA	5.26	134.85	121.70
1	P	496	LEU	CA-CB-CG	5.15	127.15	115.30

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	1998	0	2015	63	0
1	B	2004	0	2017	35	0
1	C	2006	0	2021	30	0
1	D	1993	0	2012	48	0
1	E	2013	0	2025	30	0
1	F	1982	0	1995	26	0
1	G	2003	0	2012	42	0
1	H	2004	0	2017	32	0
1	I	2008	0	2025	29	0
1	J	2000	0	2021	37	0
1	K	1993	0	2012	33	0
1	L	1999	0	2024	22	0
1	M	1977	0	1990	41	0
1	N	2008	0	2025	50	0
1	O	2008	0	2017	50	0
1	P	1976	0	1993	34	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	2	0
2	D	27	0	12	1	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	1	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	1	0
2	K	27	0	12	0	0
2	L	27	0	12	0	0
2	M	27	0	12	0	0
2	N	27	0	12	1	0
2	O	27	0	12	1	0
2	P	27	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
All	All	32420	0	32413	541	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 8.

All (541) 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:A:454:GLU:CG	1:A:701:ARG:HH22	1.00	1.58
1:A:454:GLU:HG2	1:A:701:ARG:NH2	0.91	1.23
1:N:587:ILE:CG2	1:N:619:LEU:HD22	1.71	1.20
1:N:587:ILE:CG2	1:N:619:LEU:CD2	2.22	1.17
1:A:497:LEU:HG	1:A:507:ILE:HD11	1.26	1.15
1:N:587:ILE:HG21	1:N:619:LEU:HD21	1.32	1.10
1:J:577:ASN:ND2	1:J:579:VAL:HG22	1.69	1.08
1:N:588:GLY:O	1:N:589:GLN:HG2	1.49	1.07
1:E:497:LEU:HG	1:E:507:ILE:HD11	1.37	1.06
1:O:525:GLN:HG3	1:O:526:ASN:H	1.17	1.04
1:A:454:GLU:CB	1:A:701:ARG:HH22	1.70	1.04
1:A:454:GLU:HG2	1:A:701:ARG:CZ	1.92	1.00
1:D:706:GLN:HE22	1:D:711:TYR:CB	1.73	1.00
1:A:706:GLN:HB3	1:A:711:TYR:HD1	1.27	0.99
1:D:497:LEU:HG	1:D:507:ILE:HD11	1.44	0.99
1:N:587:ILE:HG21	1:N:619:LEU:CD2	1.89	0.98
1:K:700:ARG:HG2	1:K:710:TYR:HE1	1.29	0.98
1:N:587:ILE:O	1:N:587:ILE:HD12	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:587:ILE:HG22	1:N:619:LEU:HD22	1.48	0.95
1:D:706:GLN:HE22	1:D:711:TYR:HB3	1.31	0.95
1:A:701:ARG:NH1	1:O:451:ARG:NH2	2.15	0.94
1:A:454:GLU:CG	1:A:701:ARG:NH2	1.78	0.91
1:A:497:LEU:HG	1:A:507:ILE:CD1	2.02	0.89
1:N:588:GLY:C	1:N:589:GLN:HG2	1.89	0.88
1:A:493:GLN:HB2	1:A:494:SER:HA	1.55	0.88
1:O:525:GLN:HG3	1:O:526:ASN:N	1.93	0.84
1:C:702:ALA:HA	1:N:704:ALA:HA	1.60	0.83
1:H:528:VAL:HG12	1:H:659:VAL:HG23	1.61	0.82
1:K:700:ARG:HG2	1:K:710:TYR:CE1	2.14	0.82
1:A:706:GLN:HB3	1:A:711:TYR:CD1	2.15	0.81
1:N:587:ILE:HG22	1:N:619:LEU:CD2	2.04	0.80
1:N:587:ILE:CG2	1:N:619:LEU:HD21	1.98	0.80
1:L:705:TYR:H	1:L:706:GLN:HA	1.46	0.80
1:N:587:ILE:CG1	1:N:587:ILE:O	2.30	0.80
1:N:587:ILE:CD1	1:N:587:ILE:O	2.29	0.80
1:J:577:ASN:HD22	1:J:579:VAL:HG22	1.45	0.79
1:E:504:ASP:HB3	1:E:507:ILE:HD12	1.64	0.79
1:L:612:VAL:HG11	1:M:717:SER:HB3	1.63	0.79
1:M:612:VAL:HG11	1:N:717:SER:HB3	1.65	0.78
1:D:706:GLN:HE22	1:D:711:TYR:HB2	1.48	0.77
1:A:612:VAL:HG11	1:B:717:SER:HB3	1.67	0.77
1:D:706:GLN:NE2	1:D:711:TYR:CB	2.47	0.76
1:N:588:GLY:O	1:N:589:GLN:CG	2.30	0.76
1:D:704:ALA:HB1	1:M:702:ALA:HB1	1.68	0.76
1:J:707:ASP:HB3	1:J:708:TYR:HA	1.67	0.76
1:A:703:SER:H	1:P:704:ALA:HB3	1.51	0.76
1:A:527:ASN:HD21	1:A:633:SER:HA	1.51	0.76
1:O:707:ASP:HB2	1:O:708:TYR:HA	1.68	0.76
1:N:587:ILE:HG23	1:N:619:LEU:HD22	1.68	0.75
1:K:700:ARG:HH21	1:K:712:GLU:HB3	1.51	0.74
1:C:455:SER:OG	1:C:458:VAL:HG23	1.87	0.74
1:G:707:ASP:H	1:G:711:TYR:HD2	1.35	0.73
1:N:530:MET:HB2	1:N:659:VAL:HG11	1.70	0.73
1:D:703:SER:H	1:M:704:ALA:HA	1.54	0.72
1:O:525:GLN:CG	1:O:526:ASN:H	2.00	0.72
1:I:717:SER:HB3	1:P:612:VAL:HG11	1.70	0.72
1:F:612:VAL:HG11	1:G:717:SER:HB3	1.71	0.71
1:A:701:ARG:HH11	1:O:451:ARG:HH21	1.38	0.71
1:D:706:GLN:NE2	1:D:711:TYR:HB3	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:GLN:HG3	1:C:711:TYR:HB3	1.71	0.71
1:D:504:ASP:HB3	1:D:507:ILE:HD12	1.73	0.70
1:P:700:ARG:HG3	1:P:710:TYR:HE1	1.57	0.70
1:M:469:SER:HB3	1:M:698:ILE:HD12	1.73	0.69
1:I:469:SER:HB3	1:I:698:ILE:HD12	1.76	0.68
1:L:469:SER:HB3	1:L:698:ILE:HD12	1.75	0.68
1:N:469:SER:HB3	1:N:698:ILE:HD12	1.75	0.68
1:A:701:ARG:NH1	1:O:451:ARG:HH22	1.89	0.68
1:M:592:ILE:C	1:M:594:THR:H	1.97	0.68
1:C:469:SER:HB3	1:C:698:ILE:HD12	1.76	0.68
1:A:469:SER:HB3	1:A:698:ILE:HD12	1.74	0.67
1:D:670:VAL:HG12	1:D:671:ASN:H	1.58	0.67
1:P:528:VAL:HG12	1:P:659:VAL:HG23	1.77	0.67
1:A:497:LEU:CG	1:A:507:ILE:HD11	2.16	0.67
1:D:706:GLN:NE2	1:D:711:TYR:HB2	2.08	0.66
1:B:704:ALA:HA	1:O:703:SER:H	1.60	0.66
1:C:704:ALA:HB3	1:N:703:SER:N	2.10	0.66
1:E:528:VAL:HG12	1:E:659:VAL:HG23	1.78	0.66
1:G:469:SER:HB3	1:G:698:ILE:HD12	1.77	0.66
1:E:475:TRP:O	1:E:479:ARG:HG2	1.96	0.66
1:K:469:SER:HB3	1:K:698:ILE:HD12	1.79	0.65
1:A:518:HIS:O	1:A:519:PHE:HB3	1.96	0.65
1:K:455:SER:HB3	1:K:458:VAL:HG23	1.79	0.65
1:B:469:SER:HB3	1:B:698:ILE:HD12	1.78	0.64
1:O:469:SER:HB3	1:O:698:ILE:HD12	1.78	0.64
1:D:671:ASN:O	1:D:675:GLU:HB2	1.98	0.64
1:K:663:LEU:HD23	1:K:694:ILE:HD11	1.80	0.64
1:G:498:ALA:H	1:G:546:ASN:ND2	1.96	0.64
1:A:706:GLN:CB	1:A:711:TYR:HD1	2.08	0.64
1:J:469:SER:HB3	1:J:698:ILE:HD12	1.78	0.63
1:G:663:LEU:HD23	1:G:694:ILE:HD11	1.80	0.63
1:G:554:THR:HG22	1:G:556:LYS:HG3	1.81	0.63
1:H:469:SER:HB3	1:H:698:ILE:HD12	1.80	0.63
1:D:469:SER:HB3	1:D:698:ILE:HD12	1.79	0.63
1:O:663:LEU:HD23	1:O:694:ILE:HD11	1.81	0.63
1:M:663:LEU:HD23	1:M:694:ILE:HD11	1.81	0.62
1:A:516:SER:HA	1:H:686:ASN:ND2	2.15	0.62
1:L:663:LEU:HD23	1:L:694:ILE:HD11	1.79	0.62
1:E:469:SER:HB3	1:E:698:ILE:HD12	1.80	0.62
1:J:528:VAL:HG12	1:J:659:VAL:HG23	1.81	0.62
1:D:528:VAL:HG12	1:D:659:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:459:LEU:HD23	1:P:459:LEU:H	1.64	0.62
1:P:469:SER:HB3	1:P:698:ILE:HD12	1.80	0.62
1:F:459:LEU:HD23	1:F:459:LEU:H	1.65	0.62
1:C:530:MET:HB2	1:C:659:VAL:HG11	1.82	0.62
1:M:457:GLN:NE2	1:M:709:GLY:HA2	2.15	0.61
1:H:663:LEU:HD23	1:H:694:ILE:HD11	1.82	0.61
1:D:612:VAL:HG11	1:E:717:SER:HB3	1.82	0.61
1:I:528:VAL:HG12	1:I:659:VAL:HG23	1.81	0.61
1:D:539:GLY:HA2	2:D:1000:ADP:H5'1	1.83	0.61
1:F:615:ASN:HB2	1:F:618:GLU:HB2	1.83	0.61
1:G:615:ASN:HB2	1:G:618:GLU:HB2	1.82	0.61
1:B:566:ARG:O	1:B:567:LYS:HB2	2.01	0.61
1:F:518:HIS:O	1:F:522:MET:HG2	2.00	0.61
1:F:528:VAL:HG12	1:F:659:VAL:HG23	1.81	0.61
1:B:528:VAL:HG12	1:B:659:VAL:HG23	1.82	0.60
1:D:663:LEU:HD23	1:D:694:ILE:HD11	1.83	0.60
1:F:538:ILE:HD12	1:F:665:VAL:HG12	1.82	0.60
1:P:497:LEU:HG	1:P:498:ALA:H	1.65	0.60
1:P:574:LEU:HD12	1:P:606:LEU:HD22	1.84	0.60
1:A:663:LEU:HD23	1:A:694:ILE:HD11	1.82	0.60
1:N:615:ASN:HB2	1:N:618:GLU:HB2	1.84	0.60
1:H:459:LEU:H	1:H:459:LEU:HD23	1.67	0.60
1:J:577:ASN:HD21	1:J:579:VAL:HG22	1.64	0.60
1:D:705:TYR:HD1	1:M:701:ARG:O	1.85	0.60
1:K:612:VAL:HG11	1:L:717:SER:HB3	1.84	0.60
1:G:571:HIS:HB3	1:G:608:PRO:HB3	1.84	0.59
1:L:528:VAL:HG12	1:L:659:VAL:HG23	1.83	0.59
1:E:454:GLU:HG2	1:E:701:ARG:HH21	1.67	0.59
1:J:521:MET:HA	1:J:524:ALA:HB2	1.84	0.59
1:I:574:LEU:HD12	1:I:606:LEU:HD22	1.85	0.59
1:A:454:GLU:CB	1:A:701:ARG:NH2	2.47	0.59
1:P:663:LEU:HD23	1:P:694:ILE:HD11	1.84	0.59
1:H:615:ASN:HB2	1:H:618:GLU:HB2	1.84	0.59
1:C:663:LEU:HD23	1:C:694:ILE:HD11	1.85	0.59
1:E:663:LEU:HD23	1:E:694:ILE:HD11	1.84	0.59
1:K:700:ARG:NH2	1:K:712:GLU:HB3	2.18	0.58
1:O:657:ARG:HH21	1:O:686:ASN:HB3	1.69	0.58
1:O:498:ALA:H	1:O:546:ASN:ND2	2.01	0.58
1:N:517:LEU:O	1:N:521:MET:HG2	2.03	0.58
1:P:615:ASN:HB2	1:P:618:GLU:HB2	1.85	0.58
1:N:459:LEU:HD23	1:N:459:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:615:ASN:HB2	1:O:618:GLU:HB2	1.85	0.58
1:E:615:ASN:HB2	1:E:618:GLU:HB2	1.85	0.58
1:I:663:LEU:HD23	1:I:694:ILE:HD11	1.86	0.58
1:O:524:ALA:O	1:O:525:GLN:HG2	2.04	0.58
1:A:615:ASN:HB2	1:A:618:GLU:HB2	1.86	0.58
1:C:654:ILE:O	1:C:657:ARG:HG2	2.03	0.58
1:N:695:LEU:HB3	1:N:698:ILE:HD11	1.86	0.57
1:J:496:LEU:HB3	1:J:499:VAL:HG22	1.86	0.57
1:I:615:ASN:HB2	1:I:618:GLU:HB2	1.86	0.57
1:N:498:ALA:HB2	1:N:546:ASN:HD22	1.68	0.57
1:F:526:ASN:HD21	1:F:528:VAL:HB	1.68	0.57
1:A:717:SER:HB3	1:H:612:VAL:HG11	1.86	0.57
1:K:615:ASN:HB2	1:K:618:GLU:HB2	1.85	0.57
1:D:559:LEU:HD11	1:D:607:ILE:HG23	1.87	0.57
1:O:707:ASP:HB2	1:O:708:TYR:CA	2.35	0.57
1:B:534:VAL:O	1:B:647:LEU:HB2	2.04	0.57
1:C:615:ASN:HB2	1:C:618:GLU:HB2	1.86	0.57
1:C:521:MET:HE1	1:C:638:LEU:HD21	1.87	0.57
1:P:695:LEU:HB3	1:P:698:ILE:HD11	1.87	0.57
1:F:663:LEU:HD23	1:F:694:ILE:HD11	1.87	0.57
1:M:534:VAL:O	1:M:647:LEU:HB2	2.05	0.57
1:B:663:LEU:HD23	1:B:694:ILE:HD11	1.85	0.57
1:J:615:ASN:HB2	1:J:618:GLU:HB2	1.85	0.57
1:H:695:LEU:HB3	1:H:698:ILE:HD11	1.87	0.57
1:M:700:ARG:HG3	1:M:710:TYR:HE2	1.70	0.57
1:M:498:ALA:HB2	1:M:546:ASN:HD22	1.68	0.57
1:I:695:LEU:HB3	1:I:698:ILE:HD11	1.87	0.56
1:D:615:ASN:HB2	1:D:618:GLU:HB2	1.85	0.56
1:M:615:ASN:HB2	1:M:618:GLU:HB2	1.86	0.56
1:B:615:ASN:HB2	1:B:618:GLU:HB2	1.86	0.56
1:P:526:ASN:HD21	1:P:528:VAL:HB	1.70	0.56
1:L:559:LEU:HD11	1:L:607:ILE:HG13	1.87	0.56
1:K:705:TYR:H	1:K:706:GLN:HA	1.69	0.56
1:J:663:LEU:HD23	1:J:694:ILE:HD11	1.87	0.56
1:J:498:ALA:HB2	1:J:546:ASN:HD22	1.71	0.56
1:A:530:MET:HB2	1:A:659:VAL:HG11	1.86	0.56
1:D:707:ASP:CB	1:D:708:TYR:HA	2.35	0.56
1:G:518:HIS:O	1:G:522:MET:HG2	2.05	0.56
1:A:703:SER:H	1:P:704:ALA:CB	2.18	0.56
1:K:534:VAL:O	1:K:647:LEU:HB2	2.06	0.55
1:N:663:LEU:HD23	1:N:694:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:534:VAL:O	1:J:647:LEU:HB2	2.06	0.55
1:J:695:LEU:HB3	1:J:698:ILE:HD11	1.88	0.55
1:A:517:LEU:HD21	1:A:529:LEU:HD22	1.88	0.55
1:D:498:ALA:H	1:D:546:ASN:ND2	2.04	0.55
1:E:534:VAL:O	1:E:647:LEU:HB2	2.06	0.55
1:H:534:VAL:O	1:H:647:LEU:HB2	2.07	0.55
1:I:534:VAL:O	1:I:647:LEU:HB2	2.07	0.55
1:A:534:VAL:O	1:A:647:LEU:HB2	2.07	0.55
1:L:615:ASN:HB2	1:L:618:GLU:HB2	1.88	0.55
1:O:612:VAL:HG11	1:P:717:SER:HB3	1.88	0.55
1:E:454:GLU:HG2	1:E:701:ARG:NH2	2.22	0.55
1:L:534:VAL:O	1:L:647:LEU:HB2	2.06	0.55
1:D:704:ALA:HB2	1:M:704:ALA:HB2	1.88	0.55
1:A:703:SER:OG	1:P:703:SER:HB2	2.07	0.55
1:B:695:LEU:HB3	1:B:698:ILE:HD11	1.89	0.55
1:H:586:LEU:HD23	1:H:619:LEU:HB3	1.88	0.55
1:D:534:VAL:O	1:D:647:LEU:HB2	2.07	0.55
1:P:497:LEU:C	1:P:499:VAL:H	2.11	0.54
1:G:704:ALA:HB3	1:J:703:SER:H	1.72	0.54
1:D:695:LEU:HB3	1:D:698:ILE:HD11	1.89	0.54
1:A:701:ARG:HH11	1:O:451:ARG:NH2	1.90	0.54
1:C:526:ASN:HD21	1:C:528:VAL:HB	1.73	0.54
1:G:695:LEU:HB3	1:G:698:ILE:HD11	1.90	0.54
1:P:534:VAL:O	1:P:647:LEU:HB2	2.07	0.54
1:D:526:ASN:HB3	1:D:660:GLY:HA3	1.88	0.54
1:L:695:LEU:HB3	1:L:698:ILE:HD11	1.90	0.54
1:O:695:LEU:HB3	1:O:698:ILE:HD11	1.88	0.54
1:A:453:ILE:HG13	1:A:671:ASN:O	2.08	0.53
1:F:534:VAL:O	1:F:647:LEU:HB2	2.07	0.53
1:G:612:VAL:HG11	1:H:717:SER:HB3	1.90	0.53
1:H:634:LYS:O	1:H:636:TYR:N	2.38	0.53
1:O:534:VAL:O	1:O:647:LEU:HB2	2.08	0.53
1:C:695:LEU:HB3	1:C:698:ILE:HD11	1.89	0.53
1:G:706:GLN:O	1:G:711:TYR:HB3	2.09	0.53
1:J:577:ASN:HD22	1:J:579:VAL:CG2	2.19	0.53
1:M:530:MET:HB2	1:M:659:VAL:HG11	1.91	0.53
1:D:479:ARG:CZ	1:D:495:GLN:HB2	2.39	0.53
1:N:534:VAL:O	1:N:647:LEU:HB2	2.09	0.52
1:F:498:ALA:H	1:F:546:ASN:ND2	2.07	0.52
1:M:695:LEU:HB3	1:M:698:ILE:HD11	1.90	0.52
1:M:612:VAL:CG1	1:N:717:SER:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:559:LEU:HD11	1:N:607:ILE:HG13	1.92	0.52
1:M:706:GLN:HB2	1:M:711:TYR:HD1	1.74	0.52
1:O:450:ASN:HD21	1:O:674:LYS:HB2	1.74	0.52
1:H:529:LEU:HD12	1:H:661:THR:HB	1.92	0.52
1:N:587:ILE:HG13	1:N:587:ILE:O	2.07	0.52
1:G:533:GLY:HA3	1:G:540:MET:SD	2.50	0.52
1:D:707:ASP:HB3	1:D:708:TYR:HA	1.92	0.52
1:G:534:VAL:O	1:G:647:LEU:HB2	2.10	0.52
1:A:516:SER:HA	1:H:686:ASN:HD22	1.75	0.52
1:K:661:THR:HG23	1:K:691:LYS:HG3	1.90	0.52
1:B:701:ARG:HD3	1:O:705:TYR:HE2	1.74	0.52
1:F:471:PRO:HD2	1:F:506:ALA:HA	1.92	0.52
1:J:471:PRO:HD2	1:J:506:ALA:HA	1.92	0.52
1:E:551:ILE:HG21	1:E:638:LEU:HD11	1.92	0.51
1:N:612:VAL:HG11	1:O:717:SER:HB3	1.93	0.51
1:L:705:TYR:H	1:L:706:GLN:CA	2.19	0.51
1:P:498:ALA:HB2	1:P:546:ASN:HD22	1.75	0.51
1:G:455:SER:HB3	1:G:458:VAL:HG23	1.93	0.51
1:M:471:PRO:HD2	1:M:506:ALA:HA	1.92	0.51
1:G:530:MET:HB2	1:G:659:VAL:HG11	1.91	0.51
1:M:455:SER:OG	1:M:457:GLN:HG2	2.11	0.51
1:M:559:LEU:HD11	1:M:607:ILE:HG13	1.92	0.51
1:D:455:SER:OG	1:D:458:VAL:HG23	2.11	0.51
1:E:455:SER:OG	1:E:457:GLN:HG2	2.10	0.51
1:C:459:LEU:HB2	1:C:464:ILE:HB	1.92	0.51
1:G:700:ARG:HD3	1:G:707:ASP:OD1	2.11	0.51
1:K:695:LEU:HB3	1:K:698:ILE:HD11	1.91	0.50
1:H:498:ALA:H	1:H:546:ASN:ND2	2.08	0.50
1:G:498:ALA:H	1:G:546:ASN:HD21	1.57	0.50
1:J:577:ASN:ND2	1:J:579:VAL:CG2	2.58	0.50
1:M:457:GLN:HE21	1:M:709:GLY:HA2	1.76	0.50
1:M:700:ARG:HG3	1:M:710:TYR:CE2	2.46	0.50
1:I:559:LEU:HD11	1:I:607:ILE:HG13	1.94	0.50
1:L:459:LEU:H	1:L:459:LEU:HD23	1.76	0.50
1:N:471:PRO:HD2	1:N:506:ALA:HA	1.92	0.50
1:I:471:PRO:HD2	1:I:506:ALA:HA	1.93	0.50
1:E:559:LEU:HD11	1:E:607:ILE:HG13	1.94	0.50
1:K:559:LEU:HD11	1:K:607:ILE:HG13	1.94	0.50
1:A:498:ALA:HB2	1:A:546:ASN:HD22	1.77	0.50
1:A:563:CYS:SG	1:A:641:ILE:CG2	3.00	0.50
1:A:635:ASN:HD22	1:A:635:ASN:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:559:LEU:HD11	1:J:607:ILE:HG13	1.93	0.50
1:N:506:ALA:O	1:N:510:ILE:HG13	2.12	0.50
1:E:695:LEU:HB3	1:E:698:ILE:HD11	1.93	0.50
1:A:703:SER:N	1:P:704:ALA:HB3	2.22	0.50
1:G:704:ALA:HB3	1:J:702:ALA:HA	1.94	0.50
1:I:498:ALA:H	1:I:546:ASN:ND2	2.09	0.50
1:J:700:ARG:HG3	1:J:710:TYR:HE1	1.77	0.49
1:I:612:VAL:HG11	1:J:717:SER:HB3	1.94	0.49
1:G:521:MET:HA	1:G:524:ALA:HB3	1.94	0.49
1:G:526:ASN:HB3	1:G:660:GLY:HA3	1.93	0.49
1:A:695:LEU:HB3	1:A:698:ILE:HD11	1.94	0.49
1:B:498:ALA:H	1:B:546:ASN:ND2	2.10	0.49
1:D:707:ASP:HA	1:D:711:TYR:HD1	1.78	0.49
1:O:559:LEU:HD11	1:O:607:ILE:HG13	1.94	0.49
1:B:519:PHE:O	1:B:523:GLN:HB2	2.12	0.49
1:B:471:PRO:HD2	1:B:506:ALA:HA	1.94	0.49
1:B:559:LEU:HD11	1:B:607:ILE:HG13	1.94	0.49
1:H:703:SER:HB2	1:I:703:SER:OG	2.11	0.49
1:G:471:PRO:HD2	1:G:506:ALA:HA	1.94	0.49
1:H:455:SER:HB3	1:H:458:VAL:HG23	1.94	0.49
2:N:1000:ADP:H5'1	2:N:1000:ADP:H8	1.77	0.49
1:L:471:PRO:HD2	1:L:506:ALA:HA	1.94	0.49
1:F:559:LEU:HD11	1:F:607:ILE:HG13	1.94	0.49
1:G:585:ILE:HG22	1:G:590:GLY:HA3	1.94	0.49
1:B:702:ALA:CB	1:O:704:ALA:HA	2.43	0.49
1:E:471:PRO:HD2	1:E:506:ALA:HA	1.94	0.49
1:K:579:VAL:O	1:K:597:LYS:NZ	2.45	0.49
1:H:532:THR:HG21	1:H:683:PHE:CZ	2.47	0.49
1:G:525:GLN:O	1:G:526:ASN:HB2	2.11	0.48
1:O:532:THR:HG21	1:O:683:PHE:CZ	2.48	0.48
1:M:700:ARG:NH2	1:M:712:GLU:HB3	2.28	0.48
1:F:498:ALA:HB2	1:F:546:ASN:HD22	1.78	0.48
1:E:574:LEU:HD12	1:E:606:LEU:HD22	1.95	0.48
1:M:459:LEU:HD12	1:M:673:LEU:HD13	1.95	0.48
1:D:471:PRO:HD2	1:D:506:ALA:HA	1.95	0.48
1:O:528:VAL:HG12	1:O:659:VAL:HG23	1.95	0.48
1:I:457:GLN:NE2	1:I:709:GLY:HA2	2.28	0.48
1:C:471:PRO:HD2	1:C:506:ALA:HA	1.93	0.48
1:K:667:ARG:HB3	1:K:670:VAL:HB	1.95	0.48
1:N:517:LEU:HD21	1:N:529:LEU:HD22	1.95	0.48
1:F:521:MET:HE1	1:F:638:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PRO:HD2	1:A:506:ALA:HA	1.96	0.48
1:O:521:MET:HE1	1:O:638:LEU:HD21	1.95	0.48
1:J:459:LEU:HB2	1:J:464:ILE:HB	1.93	0.48
1:A:559:LEU:HD11	1:A:607:ILE:HG13	1.95	0.48
1:M:521:MET:HE1	1:M:638:LEU:HD21	1.95	0.48
1:A:584:GLU:O	1:A:587:ILE:HG22	2.13	0.48
1:K:530:MET:HB2	1:K:659:VAL:HG11	1.94	0.48
1:K:526:ASN:ND2	1:K:660:GLY:HA3	2.28	0.48
1:L:498:ALA:H	1:L:546:ASN:ND2	2.12	0.48
1:J:455:SER:OG	1:J:457:GLN:HG2	2.14	0.48
1:G:493:GLN:HG3	2:G:1000:ADP:C2'	2.43	0.48
1:A:493:GLN:CB	1:A:494:SER:HA	2.37	0.47
1:B:517:LEU:HD21	1:B:529:LEU:HD22	1.95	0.47
1:K:455:SER:OG	1:K:457:GLN:HG2	2.14	0.47
1:O:498:ALA:H	1:O:546:ASN:HD21	1.61	0.47
1:G:498:ALA:HB2	1:G:546:ASN:HD22	1.78	0.47
1:B:530:MET:N	1:B:659:VAL:HG21	2.29	0.47
1:C:554:THR:HG22	1:C:556:LYS:HG3	1.96	0.47
1:I:701:ARG:NH1	1:I:708:TYR:OH	2.47	0.47
1:K:471:PRO:HD2	1:K:506:ALA:HA	1.96	0.47
1:N:703:SER:HB2	1:N:706:GLN:HA	1.97	0.47
1:M:592:ILE:C	1:M:594:THR:N	2.65	0.47
1:E:455:SER:HB3	1:E:458:VAL:HG23	1.97	0.47
1:B:476:GLN:HG3	1:B:542:PHE:HE1	1.79	0.47
1:N:571:HIS:HB3	1:N:608:PRO:HB3	1.97	0.47
1:O:471:PRO:HD2	1:O:506:ALA:HA	1.97	0.47
1:E:700:ARG:HG3	1:E:710:TYR:HE1	1.79	0.47
1:A:579:VAL:O	1:A:597:LYS:NZ	2.48	0.47
1:J:505:LEU:HD22	1:J:712:GLU:HG2	1.96	0.47
1:B:564:ASP:OD1	1:B:566:ARG:O	2.32	0.47
1:O:554:THR:HG22	1:O:556:LYS:HG3	1.97	0.47
1:O:528:VAL:HG12	1:O:659:VAL:CG2	2.45	0.47
1:A:554:THR:HG22	1:A:556:LYS:HG3	1.97	0.47
1:C:493:GLN:HG3	2:C:1000:ADP:O2'	2.15	0.47
1:K:667:ARG:HH11	1:K:667:ARG:HG2	1.80	0.46
1:P:579:VAL:O	1:P:597:LYS:NZ	2.48	0.46
1:F:455:SER:HB3	1:F:458:VAL:HG23	1.96	0.46
1:G:704:ALA:CB	1:J:703:SER:H	2.28	0.46
1:C:559:LEU:HD11	1:C:607:ILE:HG13	1.97	0.46
1:P:471:PRO:HD2	1:P:506:ALA:HA	1.96	0.46
1:I:459:LEU:HD23	1:I:459:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:ARG:HD2	1:C:715:TYR:HD2	1.81	0.46
1:O:449:PHE:HE2	1:O:674:LYS:HG3	1.80	0.46
1:F:455:SER:OG	1:F:457:GLN:HG2	2.16	0.46
1:E:587:ILE:HD11	1:E:589:GLN:HE21	1.81	0.46
1:E:612:VAL:HG11	1:F:717:SER:HB3	1.97	0.46
1:G:579:VAL:O	1:G:597:LYS:NZ	2.48	0.46
1:N:579:VAL:O	1:N:597:LYS:NZ	2.49	0.46
1:F:700:ARG:HG3	1:F:710:TYR:CE1	2.50	0.46
1:H:574:LEU:HD12	1:H:606:LEU:HD22	1.96	0.46
1:B:704:ALA:HA	1:O:703:SER:N	2.28	0.46
1:O:455:SER:OG	1:O:457:GLN:HG2	2.16	0.46
1:D:498:ALA:HB2	1:D:546:ASN:HD22	1.81	0.46
1:E:579:VAL:O	1:E:597:LYS:NZ	2.48	0.46
1:D:700:ARG:NH2	1:D:703:SER:HA	2.31	0.46
1:A:563:CYS:SG	1:A:641:ILE:HG23	2.56	0.46
1:A:493:GLN:HB2	1:A:494:SER:CA	2.34	0.46
1:O:529:LEU:HD23	1:O:640:LEU:HG	1.97	0.46
1:M:674:LYS:HE3	1:N:707:ASP:HB3	1.98	0.46
1:J:455:SER:HB3	1:J:458:VAL:HG23	1.98	0.45
1:N:455:SER:OG	1:N:457:GLN:HG2	2.16	0.45
1:C:529:LEU:HD23	1:C:640:LEU:HG	1.98	0.45
1:P:455:SER:HB3	1:P:458:VAL:HG23	1.99	0.45
1:P:529:LEU:HD23	1:P:640:LEU:HG	1.98	0.45
1:D:607:ILE:O	1:D:607:ILE:HG13	2.16	0.45
1:L:498:ALA:HB2	1:L:546:ASN:HD22	1.81	0.45
1:M:686:ASN:ND2	1:N:515:THR:HG22	2.31	0.45
1:M:706:GLN:NE2	1:M:712:GLU:O	2.50	0.45
1:I:498:ALA:HB2	1:I:546:ASN:HD22	1.81	0.45
1:G:459:LEU:HD23	1:G:459:LEU:H	1.82	0.45
1:D:586:LEU:HD13	1:D:619:LEU:HB3	1.97	0.45
1:B:702:ALA:HB1	1:O:704:ALA:HA	1.98	0.45
1:A:702:ALA:HA	1:P:704:ALA:HB3	1.99	0.45
1:M:455:SER:HB3	1:M:458:VAL:HG23	1.99	0.45
1:N:551:ILE:HD13	1:N:638:LEU:HD22	1.99	0.45
1:H:471:PRO:HD2	1:H:506:ALA:HA	1.98	0.45
1:B:479:ARG:HE	1:B:494:SER:HB2	1.82	0.45
1:L:530:MET:N	1:L:659:VAL:HG21	2.31	0.45
1:E:517:LEU:HD21	1:E:529:LEU:HD22	1.99	0.45
1:J:493:GLN:HB3	2:J:1000:ADP:O2'	2.16	0.45
1:J:579:VAL:O	1:J:597:LYS:NZ	2.49	0.44
1:J:530:MET:N	1:J:659:VAL:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:455:SER:HB3	1:I:458:VAL:HG23	1.99	0.44
1:H:579:VAL:O	1:H:597:LYS:NZ	2.50	0.44
1:M:579:VAL:O	1:M:597:LYS:NZ	2.50	0.44
1:O:493:GLN:HB2	2:O:1000:ADP:H3'	1.99	0.44
1:P:517:LEU:HD21	1:P:529:LEU:HD22	2.00	0.44
1:L:579:VAL:O	1:L:597:LYS:NZ	2.50	0.44
1:O:710:TYR:CE1	1:O:712:GLU:HG2	2.52	0.44
1:H:686:ASN:HB2	1:H:688:ILE:HD12	2.00	0.44
1:N:455:SER:HB3	1:N:458:VAL:HG23	1.98	0.44
1:I:532:THR:HG21	1:I:683:PHE:CZ	2.53	0.44
1:H:533:GLY:N	1:H:540:MET:SD	2.90	0.44
1:H:662:THR:HB	1:H:690:VAL:HA	1.99	0.44
1:D:498:ALA:H	1:D:546:ASN:HD21	1.65	0.44
1:H:475:TRP:CH2	1:H:500:GLY:HA3	2.52	0.44
1:G:587:ILE:HD11	1:G:589:GLN:HB2	2.00	0.44
1:F:703:SER:OG	1:K:703:SER:O	2.21	0.44
1:A:519:PHE:O	1:A:523:GLN:HB3	2.18	0.44
1:A:703:SER:CB	1:P:703:SER:HB2	2.47	0.44
1:I:530:MET:N	1:I:659:VAL:HG21	2.32	0.44
1:I:700:ARG:NH2	1:I:712:GLU:HB3	2.33	0.44
1:E:496:LEU:HD23	1:E:496:LEU:HA	1.89	0.44
1:F:498:ALA:H	1:F:546:ASN:HD21	1.65	0.44
1:C:574:LEU:HD12	1:C:606:LEU:HD22	2.00	0.44
1:A:662:THR:H	1:A:691:LYS:HZ3	1.66	0.44
1:J:706:GLN:NE2	1:J:712:GLU:O	2.51	0.44
1:H:571:HIS:HB3	1:H:608:PRO:HB3	2.00	0.44
1:D:584:GLU:OE1	1:D:610:GLY:HA3	2.18	0.44
1:K:496:LEU:HD13	1:K:546:ASN:ND2	2.32	0.44
1:B:498:ALA:HB2	1:B:546:ASN:HD22	1.83	0.44
1:O:517:LEU:HD21	1:O:529:LEU:HD22	2.00	0.44
1:H:498:ALA:HB2	1:H:546:ASN:HD22	1.82	0.43
1:A:498:ALA:H	1:A:546:ASN:ND2	2.16	0.43
1:E:551:ILE:HD13	1:E:638:LEU:HD11	1.99	0.43
1:N:532:THR:HG21	1:N:683:PHE:CZ	2.54	0.43
1:B:554:THR:HG22	1:B:556:LYS:HG3	2.01	0.43
1:G:574:LEU:HD12	1:G:606:LEU:HD22	2.00	0.43
1:D:530:MET:N	1:D:659:VAL:HG21	2.33	0.43
1:K:705:TYR:N	1:K:706:GLN:HA	2.33	0.43
1:O:455:SER:HB3	1:O:458:VAL:HG23	1.99	0.43
1:H:533:GLY:HA3	1:H:540:MET:SD	2.59	0.43
1:I:706:GLN:HB3	1:I:711:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:MET:N	1:E:659:VAL:HG21	2.33	0.43
1:F:530:MET:N	1:F:659:VAL:HG21	2.33	0.43
1:F:554:THR:HG22	1:F:556:LYS:HG3	2.00	0.43
1:G:702:ALA:HA	1:J:704:ALA:HA	2.01	0.43
1:H:582:LEU:HA	1:H:585:ILE:HD12	2.00	0.43
1:K:674:LYS:HD2	1:L:707:ASP:OD2	2.18	0.43
1:M:551:ILE:HD13	1:M:638:LEU:HD22	2.01	0.43
1:M:574:LEU:HD12	1:M:606:LEU:HD22	2.00	0.43
1:A:496:LEU:HD21	1:A:549:ALA:HB2	2.00	0.43
1:C:534:VAL:HG11	1:C:675:GLU:HB3	2.01	0.43
1:G:706:GLN:HB2	1:G:713:TYR:CE1	2.53	0.43
1:O:450:ASN:ND2	1:O:674:LYS:HB2	2.34	0.43
1:D:579:VAL:O	1:D:597:LYS:NZ	2.51	0.43
1:F:551:ILE:HD13	1:F:638:LEU:HD22	2.01	0.43
1:C:492:LYS:O	2:C:1000:ADP:H3'	2.19	0.43
1:N:574:LEU:HD12	1:N:606:LEU:HD22	2.01	0.43
1:I:648:ALA:HB2	1:J:713:TYR:HB2	2.01	0.43
1:M:532:THR:HG21	1:M:683:PHE:CZ	2.54	0.43
1:C:579:VAL:O	1:C:597:LYS:NZ	2.51	0.43
1:E:593:THR:HG23	1:E:631:TRP:HE1	1.83	0.43
1:I:455:SER:OG	1:I:457:GLN:HG2	2.19	0.43
1:J:574:LEU:HD12	1:J:606:LEU:HD22	2.00	0.43
1:A:521:MET:HG2	1:A:661:THR:HG21	1.99	0.43
1:G:529:LEU:HD23	1:G:640:LEU:HG	2.00	0.43
1:D:529:LEU:HD23	1:D:640:LEU:HG	2.00	0.43
1:B:702:ALA:CB	1:O:705:TYR:H	2.31	0.42
1:I:700:ARG:HG3	1:I:710:TYR:HE2	1.84	0.42
1:A:686:ASN:HD22	1:B:515:THR:HG22	1.84	0.42
1:F:653:ALA:HB1	1:F:686:ASN:HD22	1.84	0.42
1:B:493:GLN:HG2	2:B:1000:ADP:O2'	2.18	0.42
1:M:498:ALA:H	1:M:546:ASN:ND2	2.17	0.42
1:O:530:MET:HB2	1:O:659:VAL:HG21	2.00	0.42
1:G:559:LEU:HD11	1:G:607:ILE:HG13	2.01	0.42
1:C:675:GLU:OE2	1:D:706:GLN:HB3	2.19	0.42
1:B:457:GLN:HE22	1:B:709:GLY:HA2	1.84	0.42
1:H:459:LEU:HB2	1:H:464:ILE:HB	2.02	0.42
1:N:529:LEU:HD23	1:N:640:LEU:HG	2.01	0.42
1:D:470:ILE:HA	1:D:471:PRO:HD3	1.97	0.42
1:C:532:THR:HG21	1:C:683:PHE:CZ	2.55	0.42
1:A:532:THR:HG21	1:A:683:PHE:CZ	2.54	0.42
1:I:674:LYS:HA	1:I:674:LYS:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:579:VAL:O	1:O:597:LYS:NZ	2.53	0.42
1:P:530:MET:N	1:P:659:VAL:HG21	2.34	0.42
1:E:702:ALA:HA	1:L:704:ALA:HA	2.02	0.42
1:F:450:ASN:HD22	1:F:674:LYS:HB2	1.84	0.42
1:P:497:LEU:O	1:P:499:VAL:N	2.40	0.42
1:G:703:SER:C	1:J:703:SER:HB2	2.40	0.42
1:G:533:GLY:N	1:G:540:MET:SD	2.93	0.42
1:E:529:LEU:HD23	1:E:640:LEU:HG	2.02	0.42
1:G:475:TRP:CE2	1:G:479:ARG:HD2	2.55	0.42
1:N:554:THR:HG22	1:N:556:LYS:HG3	2.01	0.42
1:B:551:ILE:HD13	1:B:638:LEU:HD22	2.00	0.42
1:A:475:TRP:CE3	1:A:497:LEU:HD13	2.55	0.42
1:B:526:ASN:ND2	1:B:528:VAL:H	2.17	0.42
1:K:706:GLN:O	1:K:711:TYR:HD1	2.02	0.42
1:L:532:THR:HG21	1:L:683:PHE:CZ	2.54	0.42
1:K:459:LEU:HB2	1:K:464:ILE:HB	2.02	0.42
1:C:476:GLN:HE21	1:C:497:LEU:HB2	1.84	0.42
1:N:586:LEU:O	1:N:588:GLY:HA2	2.20	0.41
1:D:475:TRP:CE3	1:D:497:LEU:HD13	2.55	0.41
1:D:609:ARG:NH2	1:D:612:VAL:HG23	2.36	0.41
1:H:479:ARG:NH1	1:H:495:GLN:HB3	2.35	0.41
1:A:703:SER:HB2	1:P:703:SER:CB	2.50	0.41
1:O:700:ARG:HH22	1:O:703:SER:HB3	1.85	0.41
1:C:700:ARG:CG	1:C:710:TYR:HE2	2.34	0.41
1:D:532:THR:HG21	1:D:683:PHE:CZ	2.55	0.41
1:E:557:ARG:NH1	1:E:635:ASN:O	2.54	0.41
1:K:532:THR:HG21	1:K:683:PHE:CZ	2.56	0.41
1:I:579:VAL:O	1:I:597:LYS:NZ	2.51	0.41
1:P:700:ARG:HG3	1:P:710:TYR:CE1	2.46	0.41
1:A:529:LEU:HD23	1:A:640:LEU:HG	2.02	0.41
1:A:707:ASP:CG	1:A:708:TYR:H	2.24	0.41
1:I:582:LEU:HA	1:I:585:ILE:HD12	2.03	0.41
1:N:498:ALA:H	1:N:546:ASN:ND2	2.18	0.41
1:M:686:ASN:HD22	1:N:515:THR:HG22	1.85	0.41
1:B:566:ARG:O	1:B:567:LYS:CB	2.68	0.41
1:M:470:ILE:HD13	1:M:543:VAL:HG22	2.03	0.41
1:P:699:PHE:HE2	1:P:701:ARG:HE	1.68	0.41
1:N:710:TYR:C	1:N:710:TYR:CD1	2.94	0.41
1:B:701:ARG:HD3	1:O:705:TYR:CE2	2.55	0.41
1:F:470:ILE:HA	1:F:471:PRO:HD3	1.96	0.41
1:K:644:PRO:HB3	1:L:715:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:526:ASN:ND2	1:N:660:GLY:HA3	2.35	0.41
1:M:592:ILE:HG22	1:M:593:THR:H	1.85	0.41
1:K:526:ASN:HD22	1:K:660:GLY:HA3	1.86	0.41
1:C:700:ARG:HG2	1:C:710:TYR:CE2	2.56	0.41
1:C:710:TYR:CE1	1:C:712:GLU:HG2	2.56	0.41
1:L:554:THR:HG22	1:L:556:LYS:HG3	2.01	0.41
1:O:574:LEU:HD12	1:O:606:LEU:HD22	2.02	0.41
1:O:525:GLN:HE21	1:O:526:ASN:HB3	1.86	0.41
1:M:498:ALA:H	1:M:546:ASN:HD21	1.69	0.41
1:G:703:SER:O	1:J:703:SER:HB2	2.20	0.41
1:J:532:THR:HG21	1:J:683:PHE:CZ	2.56	0.41
1:D:505:LEU:HD23	1:D:712:GLU:HB3	2.02	0.41
1:M:496:LEU:HA	1:M:496:LEU:HD23	1.89	0.41
1:D:571:HIS:HB3	1:D:608:PRO:HB3	2.03	0.40
1:P:559:LEU:HD11	1:P:607:ILE:HG13	2.03	0.40
1:O:533:GLY:HA3	1:O:540:MET:SD	2.61	0.40
1:A:612:VAL:CG1	1:B:717:SER:HB3	2.45	0.40
1:A:703:SER:HB2	1:P:703:SER:HB2	2.02	0.40
1:A:703:SER:HB2	1:P:703:SER:OG	2.21	0.40
1:O:498:ALA:HB2	1:O:546:ASN:HD22	1.85	0.40
1:K:498:ALA:H	1:K:546:ASN:ND2	2.19	0.40
1:C:571:HIS:HB3	1:C:608:PRO:HB3	2.03	0.40
1:A:470:ILE:HD12	1:A:694:ILE:CG2	2.51	0.40
1:I:632:ALA:O	1:I:636:TYR:HB2	2.22	0.40
1:D:634:LYS:HD3	1:D:635:ASN:ND2	2.36	0.40
1:G:458:VAL:O	1:G:461:GLU:HG2	2.22	0.40
1:K:667:ARG:HD3	1:K:670:VAL:HG21	2.03	0.40
1:B:529:LEU:HD23	1:B:640:LEU:HG	2.03	0.40
1:G:674:LYS:HZ1	1:H:709:GLY:H	1.68	0.40
1:K:668:TYR:HB2	1:K:698:ILE:HG12	2.04	0.40
1:J:477:LYS:O	1:J:481:SER:HB2	2.22	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	255/286 (89%)	235 (92%)	14 (6%)	6 (2%)	7	43
1	B	256/286 (90%)	233 (91%)	14 (6%)	9 (4%)	4	31
1	C	256/286 (90%)	231 (90%)	20 (8%)	5 (2%)	9	48
1	D	254/286 (89%)	237 (93%)	11 (4%)	6 (2%)	7	43
1	E	256/286 (90%)	234 (91%)	16 (6%)	6 (2%)	8	44
1	F	253/286 (88%)	234 (92%)	13 (5%)	6 (2%)	7	43
1	G	255/286 (89%)	233 (91%)	15 (6%)	7 (3%)	6	39
1	H	256/286 (90%)	231 (90%)	19 (7%)	6 (2%)	8	44
1	I	256/286 (90%)	237 (93%)	14 (6%)	5 (2%)	9	48
1	J	255/286 (89%)	232 (91%)	19 (8%)	4 (2%)	12	54
1	K	254/286 (89%)	232 (91%)	13 (5%)	9 (4%)	4	31
1	L	255/286 (89%)	238 (93%)	15 (6%)	2 (1%)	24	69
1	M	252/286 (88%)	228 (90%)	18 (7%)	6 (2%)	7	43
1	N	256/286 (90%)	236 (92%)	16 (6%)	4 (2%)	12	54
1	O	256/286 (90%)	234 (91%)	16 (6%)	6 (2%)	8	44
1	P	252/286 (88%)	231 (92%)	14 (6%)	7 (3%)	6	37
All	All	4077/4576 (89%)	3736 (92%)	247 (6%)	94 (2%)	8	44

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	TYR
1	A	708	TYR
1	B	496	LEU
1	B	703	SER
1	B	704	ALA
1	C	493	GLN
1	D	704	ALA
1	D	706	GLN
1	D	707	ASP
1	E	589	GLN
1	E	602	ALA
1	E	668	TYR
1	E	703	SER
1	E	708	TYR

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Mol	Chain	Res	Type
1	F	668	TYR
1	F	704	ALA
1	F	711	TYR
1	G	526	ASN
1	G	668	TYR
1	H	495	GLN
1	H	668	TYR
1	I	668	TYR
1	I	704	ALA
1	I	708	TYR
1	J	668	TYR
1	K	495	GLN
1	K	595	ALA
1	K	703	SER
1	K	709	GLY
1	K	711	TYR
1	K	715	TYR
1	L	668	TYR
1	L	708	TYR
1	M	592	ILE
1	M	668	TYR
1	M	703	SER
1	M	706	GLN
1	N	591	ASP
1	N	668	TYR
1	N	708	TYR
1	O	525	GLN
1	O	593	THR
1	O	668	TYR
1	P	668	TYR
1	P	708	TYR
1	A	706	GLN
1	A	707	ASP
1	B	567	LYS
1	B	706	GLN
1	C	524	ALA
1	F	589	GLN
1	I	703	SER
1	J	706	GLN
1	K	497	LEU
1	K	714	GLU
1	M	496	LEU

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Mol	Chain	Res	Type
1	M	589	GLN
1	P	497	LEU
1	P	715	TYR
1	B	590	GLY
1	C	707	ASP
1	D	453	ILE
1	D	671	ASN
1	D	672	THR
1	F	595	ALA
1	G	706	GLN
1	H	451	ARG
1	H	595	ALA
1	H	715	TYR
1	I	595	ALA
1	K	710	TYR
1	P	704	ALA
1	B	595	ALA
1	C	595	ALA
1	C	704	ALA
1	E	595	ALA
1	G	525	GLN
1	J	595	ALA
1	O	591	ASP
1	O	706	GLN
1	P	498	ALA
1	P	595	ALA
1	F	708	TYR
1	G	708	TYR
1	H	526	ASN
1	A	453	ILE
1	A	595	ALA
1	B	702	ALA
1	G	495	GLN
1	G	595	ALA
1	J	497	LEU
1	N	590	GLY
1	O	713	TYR
1	B	588	GLY

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	220/244 (90%)	203 (92%)	17 (8%)	16	54
1	B	221/244 (91%)	202 (91%)	19 (9%)	13	46
1	C	221/244 (91%)	199 (90%)	22 (10%)	9	37
1	D	220/244 (90%)	202 (92%)	18 (8%)	14	50
1	E	222/244 (91%)	202 (91%)	20 (9%)	12	43
1	F	218/244 (89%)	201 (92%)	17 (8%)	16	53
1	G	221/244 (91%)	205 (93%)	16 (7%)	18	57
1	H	221/244 (91%)	202 (91%)	19 (9%)	13	46
1	I	222/244 (91%)	203 (91%)	19 (9%)	13	46
1	J	221/244 (91%)	198 (90%)	23 (10%)	9	35
1	K	220/244 (90%)	202 (92%)	18 (8%)	14	50
1	L	220/244 (90%)	199 (90%)	21 (10%)	11	40
1	M	218/244 (89%)	201 (92%)	17 (8%)	16	53
1	N	222/244 (91%)	205 (92%)	17 (8%)	16	54
1	O	221/244 (91%)	199 (90%)	22 (10%)	9	37
1	P	218/244 (89%)	200 (92%)	18 (8%)	14	49
All	All	3526/3904 (90%)	3223 (91%)	303 (9%)	13	46

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	SER
1	A	474	GLU
1	A	477	LYS
1	A	480	ASP
1	A	492	LYS
1	A	493	GLN
1	A	517	LEU
1	A	523	GLN

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Mol	Chain	Res	Type
1	A	554	THR
1	A	609	ARG
1	A	635	ASN
1	A	638	LEU
1	A	700	ARG
1	A	703	SER
1	A	710	TYR
1	A	712	GLU
1	A	716	LYS
1	B	460	GLU
1	B	517	LEU
1	B	554	THR
1	B	566	ARG
1	B	569	TYR
1	B	573	LEU
1	B	593	THR
1	B	609	ARG
1	B	624	ARG
1	B	634	LYS
1	B	638	LEU
1	B	682	ARG
1	B	695	LEU
1	B	700	ARG
1	B	701	ARG
1	B	703	SER
1	B	707	ASP
1	B	712	GLU
1	B	718	ASP
1	C	459	LEU
1	C	465	SER
1	C	467	TYR
1	C	493	GLN
1	C	495	GLN
1	C	507	ILE
1	C	517	LEU
1	C	522	MET
1	C	552	SER
1	C	554	THR
1	C	584	GLU
1	C	589	GLN
1	C	593	THR
1	C	604	PHE

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Mol	Chain	Res	Type
1	C	609	ARG
1	C	624	ARG
1	C	638	LEU
1	C	679	SER
1	C	695	LEU
1	C	705	TYR
1	C	710	TYR
1	C	711	TYR
1	D	450	ASN
1	D	454	GLU
1	D	460	GLU
1	D	479	ARG
1	D	495	GLN
1	D	496	LEU
1	D	583	SER
1	D	593	THR
1	D	607	ILE
1	D	609	ARG
1	D	624	ARG
1	D	638	LEU
1	D	677	GLU
1	D	695	LEU
1	D	705	TYR
1	D	707	ASP
1	D	710	TYR
1	D	711	TYR
1	E	474	GLU
1	E	479	ARG
1	E	491	TYR
1	E	495	GLN
1	E	496	LEU
1	E	517	LEU
1	E	521	MET
1	E	522	MET
1	E	550	VAL
1	E	589	GLN
1	E	593	THR
1	E	609	ARG
1	E	624	ARG
1	E	638	LEU
1	E	695	LEU
1	E	701	ARG

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Mol	Chain	Res	Type
1	E	703	SER
1	E	710	TYR
1	E	711	TYR
1	E	712	GLU
1	F	451	ARG
1	F	459	LEU
1	F	479	ARG
1	F	495	GLN
1	F	496	LEU
1	F	517	LEU
1	F	529	LEU
1	F	554	THR
1	F	593	THR
1	F	604	PHE
1	F	609	ARG
1	F	624	ARG
1	F	638	LEU
1	F	695	LEU
1	F	705	TYR
1	F	711	TYR
1	F	712	GLU
1	G	450	ASN
1	G	517	LEU
1	G	523	GLN
1	G	573	LEU
1	G	585	ILE
1	G	587	ILE
1	G	589	GLN
1	G	593	THR
1	G	609	ARG
1	G	624	ARG
1	G	638	LEU
1	G	695	LEU
1	G	708	TYR
1	G	710	TYR
1	G	711	TYR
1	G	714	GLU
1	H	451	ARG
1	H	459	LEU
1	H	510	ILE
1	H	529	LEU
1	H	554	THR

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Mol	Chain	Res	Type
1	H	576	THR
1	H	593	THR
1	H	609	ARG
1	H	624	ARG
1	H	635	ASN
1	H	638	LEU
1	H	659	VAL
1	H	680	LEU
1	H	695	LEU
1	H	703	SER
1	H	708	TYR
1	H	710	TYR
1	H	711	TYR
1	H	716	LYS
1	I	459	LEU
1	I	479	ARG
1	I	517	LEU
1	I	525	GLN
1	I	529	LEU
1	I	573	LEU
1	I	591	ASP
1	I	593	THR
1	I	609	ARG
1	I	634	LYS
1	I	638	LEU
1	I	680	LEU
1	I	695	LEU
1	I	707	ASP
1	I	708	TYR
1	I	710	TYR
1	I	711	TYR
1	I	712	GLU
1	I	716	LYS
1	J	450	ASN
1	J	451	ARG
1	J	459	LEU
1	J	494	SER
1	J	495	GLN
1	J	496	LEU
1	J	512	SER
1	J	517	LEU
1	J	523	GLN

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Mol	Chain	Res	Type
1	J	529	LEU
1	J	554	THR
1	J	589	GLN
1	J	593	THR
1	J	604	PHE
1	J	609	ARG
1	J	624	ARG
1	J	634	LYS
1	J	638	LEU
1	J	674	LYS
1	J	680	LEU
1	J	695	LEU
1	J	707	ASP
1	J	710	TYR
1	K	459	LEU
1	K	496	LEU
1	K	517	LEU
1	K	525	GLN
1	K	526	ASN
1	K	529	LEU
1	K	576	THR
1	K	593	THR
1	K	609	ARG
1	K	624	ARG
1	K	638	LEU
1	K	680	LEU
1	K	695	LEU
1	K	706	GLN
1	K	707	ASP
1	K	708	TYR
1	K	711	TYR
1	K	716	LYS
1	L	479	ARG
1	L	495	GLN
1	L	517	LEU
1	L	522	MET
1	L	525	GLN
1	L	529	LEU
1	L	572	GLU
1	L	573	LEU
1	L	593	THR
1	L	594	THR

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Mol	Chain	Res	Type
1	L	609	ARG
1	L	624	ARG
1	L	638	LEU
1	L	680	LEU
1	L	695	LEU
1	L	701	ARG
1	L	705	TYR
1	L	706	GLN
1	L	707	ASP
1	L	708	TYR
1	L	711	TYR
1	M	459	LEU
1	M	517	LEU
1	M	522	MET
1	M	529	LEU
1	M	550	VAL
1	M	554	THR
1	M	573	LEU
1	M	593	THR
1	M	609	ARG
1	M	624	ARG
1	M	638	LEU
1	M	680	LEU
1	M	695	LEU
1	M	701	ARG
1	M	707	ASP
1	M	708	TYR
1	M	716	LYS
1	N	450	ASN
1	N	459	LEU
1	N	482	VAL
1	N	492	LYS
1	N	496	LEU
1	N	517	LEU
1	N	526	ASN
1	N	593	THR
1	N	609	ARG
1	N	624	ARG
1	N	638	LEU
1	N	659	VAL
1	N	680	LEU
1	N	695	LEU

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Mol	Chain	Res	Type
1	N	710	TYR
1	N	711	TYR
1	N	714	GLU
1	O	450	ASN
1	O	451	ARG
1	O	479	ARG
1	O	481	SER
1	O	495	GLN
1	O	517	LEU
1	O	526	ASN
1	O	554	THR
1	O	609	ARG
1	O	624	ARG
1	O	638	LEU
1	O	659	VAL
1	O	678	THR
1	O	680	LEU
1	O	684	GLU
1	O	691	LYS
1	O	695	LEU
1	O	703	SER
1	O	710	TYR
1	O	711	TYR
1	O	715	TYR
1	O	716	LYS
1	P	451	ARG
1	P	454	GLU
1	P	459	LEU
1	P	496	LEU
1	P	517	LEU
1	P	550	VAL
1	P	558	VAL
1	P	593	THR
1	P	609	ARG
1	P	624	ARG
1	P	638	LEU
1	P	680	LEU
1	P	684	GLU
1	P	695	LEU
1	P	703	SER
1	P	708	TYR
1	P	710	TYR

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Mol	Chain	Res	Type
1	P	711	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	GLN
1	A	476	GLN
1	A	526	ASN
1	A	527	ASN
1	A	546	ASN
1	B	493	GLN
1	B	526	ASN
1	B	546	ASN
1	B	589	GLN
1	C	476	GLN
1	C	526	ASN
1	C	589	GLN
1	D	457	GLN
1	D	476	GLN
1	D	495	GLN
1	D	546	ASN
1	D	706	GLN
1	E	457	GLN
1	E	476	GLN
1	E	495	GLN
1	E	580	ASN
1	E	589	GLN
1	F	450	ASN
1	F	457	GLN
1	F	476	GLN
1	F	526	ASN
1	F	546	ASN
1	F	589	GLN
1	G	546	ASN
1	H	476	GLN
1	H	546	ASN
1	H	555	ASN
1	H	686	ASN
1	I	457	GLN
1	I	525	GLN
1	I	546	ASN
1	I	635	ASN

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Mol	Chain	Res	Type
1	J	546	ASN
1	J	577	ASN
1	K	457	GLN
1	K	476	GLN
1	K	493	GLN
1	K	526	ASN
1	K	546	ASN
1	K	706	GLN
1	L	476	GLN
1	L	546	ASN
1	L	580	ASN
1	L	589	GLN
1	L	685	GLN
1	L	686	ASN
1	M	450	ASN
1	M	457	GLN
1	M	476	GLN
1	M	546	ASN
1	N	457	GLN
1	N	476	GLN
1	N	495	GLN
1	N	526	ASN
1	N	546	ASN
1	N	577	ASN
1	O	450	ASN
1	O	457	GLN
1	O	493	GLN
1	O	525	GLN
1	O	546	ASN
1	O	577	ASN
1	O	580	ASN
1	P	526	ASN
1	P	546	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	A	1000	3	22,29,29	1.35	3 (13%)	27,45,45	0.93	1 (3%)
2	ADP	B	1000	3	22,29,29	1.46	3 (13%)	27,45,45	1.04	3 (11%)
2	ADP	C	1000	3	22,29,29	1.48	4 (18%)	27,45,45	1.03	3 (11%)
2	ADP	D	1000	3	22,29,29	1.65	5 (22%)	27,45,45	1.42	3 (11%)
2	ADP	E	1000	3	22,29,29	1.28	3 (13%)	27,45,45	1.08	4 (14%)
2	ADP	F	1000	3	22,29,29	1.52	4 (18%)	27,45,45	1.07	2 (7%)
2	ADP	G	1000	3	22,29,29	1.73	5 (22%)	27,45,45	1.87	6 (22%)
2	ADP	H	1000	3	22,29,29	1.31	4 (18%)	27,45,45	1.18	4 (14%)
2	ADP	I	1000	3	22,29,29	1.34	3 (13%)	27,45,45	0.87	0
2	ADP	J	1000	3	22,29,29	1.43	4 (18%)	27,45,45	1.16	2 (7%)
2	ADP	K	1000	3	22,29,29	1.46	3 (13%)	27,45,45	0.95	1 (3%)
2	ADP	L	1000	3	22,29,29	1.65	4 (18%)	27,45,45	0.96	0
2	ADP	M	1000	3	22,29,29	1.34	4 (18%)	27,45,45	1.05	2 (7%)
2	ADP	N	1000	3	22,29,29	1.57	4 (18%)	27,45,45	1.32	4 (14%)
2	ADP	O	1000	3	22,29,29	1.71	3 (13%)	27,45,45	0.97	2 (7%)
2	ADP	P	1000	3	22,29,29	1.49	4 (18%)	27,45,45	0.91	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	B	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	C	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	D	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	E	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	F	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	G	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	H	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	I	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	J	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	K	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	L	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	M	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	N	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	O	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	P	1000	3	-	0/12/32/32	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1000	ADP	C8-N7	-2.75	1.29	1.34
2	D	1000	ADP	C8-N7	-2.28	1.30	1.34
2	N	1000	ADP	C8-N7	-2.27	1.30	1.34
2	J	1000	ADP	C2-N3	2.06	1.35	1.32
2	H	1000	ADP	O4'-C1'	2.10	1.43	1.41
2	M	1000	ADP	C2-N1	2.11	1.37	1.33
2	J	1000	ADP	C4-N3	2.13	1.38	1.35
2	E	1000	ADP	C2-N1	2.32	1.38	1.33
2	E	1000	ADP	O4'-C1'	2.34	1.44	1.41
2	H	1000	ADP	C2-N1	2.40	1.38	1.33
2	P	1000	ADP	C4-N3	2.45	1.39	1.35
2	M	1000	ADP	C4-N3	2.51	1.39	1.35
2	A	1000	ADP	O4'-C1'	2.51	1.44	1.41
2	H	1000	ADP	C4-N3	2.54	1.39	1.35
2	D	1000	ADP	C4-N3	2.59	1.39	1.35
2	F	1000	ADP	C4-N3	2.59	1.39	1.35
2	C	1000	ADP	C4-N3	2.65	1.39	1.35
2	P	1000	ADP	C2-N1	2.67	1.39	1.33
2	C	1000	ADP	C2-N3	2.68	1.36	1.32
2	N	1000	ADP	C2-N1	2.69	1.39	1.33
2	D	1000	ADP	C2-N3	2.69	1.37	1.32
2	M	1000	ADP	C2-N3	2.71	1.37	1.32
2	I	1000	ADP	O4'-C1'	2.73	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1000	ADP	C2-N1	2.78	1.39	1.33
2	J	1000	ADP	C2-N1	2.80	1.39	1.33
2	I	1000	ADP	C2-N1	2.84	1.39	1.33
2	G	1000	ADP	C2-N3	2.85	1.37	1.32
2	K	1000	ADP	C2-N1	2.87	1.39	1.33
2	L	1000	ADP	C4-N3	2.95	1.40	1.35
2	G	1000	ADP	C2-N1	2.95	1.39	1.33
2	N	1000	ADP	C2-N3	2.98	1.37	1.32
2	O	1000	ADP	C4-N3	3.04	1.40	1.35
2	B	1000	ADP	C2-N1	3.06	1.39	1.33
2	F	1000	ADP	C2-N1	3.09	1.39	1.33
2	C	1000	ADP	C2-N1	3.10	1.39	1.33
2	B	1000	ADP	C4-N3	3.15	1.40	1.35
2	M	1000	ADP	O4'-C1'	3.31	1.45	1.41
2	I	1000	ADP	C2-N3	3.37	1.38	1.32
2	L	1000	ADP	O4'-C1'	3.40	1.45	1.41
2	P	1000	ADP	O4'-C1'	3.45	1.45	1.41
2	L	1000	ADP	C2-N3	3.47	1.38	1.32
2	G	1000	ADP	C4-N3	3.49	1.40	1.35
2	F	1000	ADP	O4'-C1'	3.50	1.45	1.41
2	A	1000	ADP	C2-N3	3.50	1.38	1.32
2	P	1000	ADP	C2-N3	3.59	1.38	1.32
2	F	1000	ADP	C2-N3	3.60	1.38	1.32
2	A	1000	ADP	C2-N1	3.62	1.40	1.33
2	L	1000	ADP	C2-N1	3.63	1.40	1.33
2	E	1000	ADP	C2-N3	3.65	1.38	1.32
2	K	1000	ADP	O4'-C1'	3.68	1.45	1.41
2	H	1000	ADP	C2-N3	3.75	1.38	1.32
2	B	1000	ADP	C2-N3	3.77	1.38	1.32
2	O	1000	ADP	C2-N3	3.89	1.39	1.32
2	K	1000	ADP	C2-N3	3.93	1.39	1.32
2	C	1000	ADP	O4'-C1'	3.99	1.46	1.41
2	G	1000	ADP	O4'-C1'	4.27	1.46	1.41
2	J	1000	ADP	O4'-C1'	4.41	1.46	1.41
2	N	1000	ADP	O4'-C1'	4.57	1.47	1.41
2	O	1000	ADP	C2-N1	4.62	1.42	1.33
2	D	1000	ADP	O4'-C1'	4.64	1.47	1.41

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1000	ADP	N3-C2-N1	-5.28	124.85	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1000	ADP	C4'-O4'-C1'	-4.01	105.31	109.72
2	D	1000	ADP	C2'-C1'-N9	-3.69	108.66	114.29
2	J	1000	ADP	C4'-O4'-C1'	-3.29	106.11	109.72
2	D	1000	ADP	N3-C2-N1	-3.25	126.41	128.89
2	G	1000	ADP	O3B-PB-O1B	-3.22	100.21	110.58
2	B	1000	ADP	N3-C2-N1	-2.68	126.84	128.89
2	N	1000	ADP	N3-C2-N1	-2.54	126.95	128.89
2	G	1000	ADP	C2'-C3'-C4'	-2.47	97.54	102.61
2	H	1000	ADP	O3B-PB-O1B	-2.39	102.87	110.58
2	E	1000	ADP	N3-C2-N1	-2.38	127.07	128.89
2	E	1000	ADP	O3B-PB-O1B	-2.33	103.07	110.58
2	C	1000	ADP	C4'-O4'-C1'	-2.33	107.16	109.72
2	N	1000	ADP	C1'-N9-C4	-2.32	123.44	126.94
2	N	1000	ADP	O3B-PB-O1B	-2.18	103.55	110.58
2	H	1000	ADP	C4'-O4'-C1'	-2.13	107.38	109.72
2	O	1000	ADP	O3B-PB-O1B	-2.04	104.00	110.58
2	N	1000	ADP	O4'-C4'-C3'	-2.03	101.05	105.15
2	M	1000	ADP	O3B-PB-O1B	-2.01	104.10	110.58
2	G	1000	ADP	C4-C5-N7	2.05	111.36	109.48
2	B	1000	ADP	O2A-PA-O3A	2.06	114.43	105.09
2	E	1000	ADP	O2A-PA-O3A	2.07	114.47	105.09
2	A	1000	ADP	O2A-PA-O3A	2.09	114.58	105.09
2	C	1000	ADP	O3B-PB-O3A	2.12	114.70	105.09
2	B	1000	ADP	O4'-C4'-C3'	2.14	109.45	105.15
2	C	1000	ADP	O2A-PA-O3A	2.16	114.89	105.09
2	P	1000	ADP	O3B-PB-O3A	2.19	115.04	105.09
2	F	1000	ADP	O3B-PB-O3A	2.26	115.36	105.09
2	H	1000	ADP	O2A-PA-O3A	2.29	115.48	105.09
2	K	1000	ADP	O2A-PA-O3A	2.31	115.56	105.09
2	P	1000	ADP	O2A-PA-O3A	2.33	115.65	105.09
2	J	1000	ADP	O2A-PA-O3A	2.44	116.18	105.09
2	M	1000	ADP	O3B-PB-O3A	2.55	116.68	105.09
2	F	1000	ADP	O2A-PA-O3A	2.60	116.88	105.09
2	E	1000	ADP	O3B-PB-O3A	2.61	116.94	105.09
2	O	1000	ADP	O3B-PB-O3A	2.69	117.28	105.09
2	H	1000	ADP	O3B-PB-O3A	2.78	117.69	105.09
2	G	1000	ADP	O3B-PB-O3A	2.95	118.49	105.09
2	D	1000	ADP	O3A-PA-O5'	3.39	111.93	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	ADP	1	0
2	C	1000	ADP	2	0
2	D	1000	ADP	1	0
2	G	1000	ADP	1	0
2	J	1000	ADP	1	0
2	N	1000	ADP	1	0
2	O	1000	ADP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	259/286 (90%)	0.02	9 (3%) 48 32	48, 72, 112, 127	0
1	B	260/286 (90%)	0.21	11 (4%) 40 26	57, 83, 119, 129	0
1	C	260/286 (90%)	0.04	7 (2%) 58 44	51, 79, 112, 141	0
1	D	258/286 (90%)	0.36	13 (5%) 32 19	62, 90, 120, 148	0
1	E	260/286 (90%)	0.11	7 (2%) 58 44	60, 85, 117, 139	0
1	F	257/286 (89%)	0.08	8 (3%) 52 38	58, 80, 110, 139	0
1	G	259/286 (90%)	0.20	15 (5%) 26 15	67, 91, 120, 143	0
1	H	260/286 (90%)	0.21	13 (5%) 32 19	64, 88, 124, 144	0
1	I	260/286 (90%)	0.16	10 (3%) 44 29	57, 83, 117, 136	0
1	J	259/286 (90%)	0.10	5 (1%) 70 55	57, 80, 115, 133	0
1	K	258/286 (90%)	0.01	4 (1%) 74 62	54, 73, 112, 147	0
1	L	259/286 (90%)	-0.06	6 (2%) 64 49	51, 72, 112, 140	0
1	M	256/286 (89%)	0.05	9 (3%) 48 32	48, 74, 106, 128	0
1	N	260/286 (90%)	-0.01	9 (3%) 48 32	50, 70, 111, 131	0
1	O	260/286 (90%)	-0.00	7 (2%) 58 44	51, 74, 113, 133	0
1	P	256/286 (89%)	0.00	4 (1%) 74 62	53, 76, 108, 136	0
All	All	4141/4576 (90%)	0.09	137 (3%) 50 35	48, 80, 116, 148	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	494	SER	5.7
1	J	494	SER	5.6
1	D	707	ASP	5.5
1	B	494	SER	5.2
1	K	707	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	493	GLN	4.2
1	H	708	TYR	4.2
1	G	493	GLN	4.0
1	G	710	TYR	4.0
1	F	709	GLY	4.0
1	B	493	GLN	4.0
1	D	493	GLN	4.0
1	A	589	GLN	4.0
1	H	707	ASP	3.9
1	H	493	GLN	3.9
1	C	480	ASP	3.8
1	H	719	ALA	3.8
1	B	705	TYR	3.7
1	F	481	SER	3.7
1	G	495	GLN	3.6
1	O	708	TYR	3.6
1	M	717	SER	3.6
1	N	482	VAL	3.6
1	E	707	ASP	3.6
1	B	591	ASP	3.5
1	J	592	ILE	3.5
1	G	718	ASP	3.5
1	H	718	ASP	3.5
1	C	718	ASP	3.4
1	N	592	ILE	3.4
1	P	482	VAL	3.4
1	G	708	TYR	3.3
1	N	495	GLN	3.3
1	H	494	SER	3.3
1	E	592	ILE	3.3
1	J	493	GLN	3.3
1	K	711	TYR	3.2
1	H	592	ILE	3.2
1	I	705	TYR	3.2
1	D	580	ASN	3.1
1	B	592	ILE	3.1
1	O	718	ASP	3.1
1	K	708	TYR	3.1
1	O	711	TYR	3.1
1	A	718	ASP	3.1
1	O	707	ASP	3.1
1	I	707	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	706	GLN	3.0
1	N	481	SER	3.0
1	G	480	ASP	3.0
1	L	720	LYS	3.0
1	F	589	GLN	3.0
1	J	589	GLN	3.0
1	C	494	SER	2.9
1	M	589	GLN	2.9
1	F	707	ASP	2.9
1	N	494	SER	2.9
1	D	450	ASN	2.9
1	C	481	SER	2.9
1	F	450	ASN	2.9
1	F	500	GLY	2.9
1	M	478	ALA	2.9
1	N	590	GLY	2.9
1	E	593	THR	2.9
1	M	703	SER	2.9
1	I	494	SER	2.8
1	B	590	GLY	2.8
1	D	494	SER	2.8
1	A	592	ILE	2.8
1	G	481	SER	2.8
1	B	481	SER	2.8
1	D	478	ALA	2.8
1	L	706	GLN	2.7
1	B	588	GLY	2.7
1	E	589	GLN	2.7
1	N	461	GLU	2.7
1	H	590	GLY	2.7
1	J	590	GLY	2.6
1	A	494	SER	2.6
1	K	705	TYR	2.6
1	O	719	ALA	2.6
1	D	495	GLN	2.6
1	L	461	GLU	2.6
1	B	707	ASP	2.5
1	F	710	TYR	2.5
1	I	704	ALA	2.5
1	D	589	GLN	2.5
1	N	493	GLN	2.5
1	L	707	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	496	LEU	2.5
1	G	705	TYR	2.4
1	A	711	TYR	2.4
1	G	571	HIS	2.4
1	C	719	ALA	2.4
1	D	711	TYR	2.4
1	A	708	TYR	2.4
1	P	558	VAL	2.4
1	M	475	TRP	2.4
1	E	718	ASP	2.4
1	P	704	ALA	2.3
1	D	558	VAL	2.3
1	H	717	SER	2.3
1	N	707	ASP	2.3
1	B	595	ALA	2.3
1	C	710	TYR	2.3
1	P	707	ASP	2.3
1	A	461	GLU	2.2
1	L	482	VAL	2.2
1	I	590	GLY	2.2
1	G	476	GLN	2.2
1	L	718	ASP	2.2
1	M	502	PRO	2.2
1	H	705	TYR	2.2
1	H	479	ARG	2.2
1	F	480	ASP	2.2
1	E	631	TRP	2.1
1	H	715	TYR	2.1
1	A	590	GLY	2.1
1	B	589	GLN	2.1
1	C	709	GLY	2.1
1	D	591	ASP	2.1
1	D	592	ILE	2.1
1	I	703	SER	2.1
1	G	497	LEU	2.1
1	I	581	GLY	2.1
1	G	450	ASN	2.1
1	I	474	GLU	2.1
1	M	718	ASP	2.1
1	A	701	ARG	2.1
1	O	481	SER	2.1
1	M	503	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	580	ASN	2.0
1	D	713	TYR	2.0
1	O	710	TYR	2.0
1	G	713	TYR	2.0
1	E	491	TYR	2.0
1	M	500	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CA	A	1001	1/1	0.96	0.33	6.47	79,79,79,79	0
3	CA	N	1001	1/1	0.97	0.26	1.65	70,70,70,70	0
3	CA	J	1001	1/1	0.96	0.26	1.24	81,81,81,81	0
3	CA	E	1001	1/1	0.94	0.22	0.91	86,86,86,86	0
3	CA	O	1001	1/1	0.94	0.26	0.77	64,64,64,64	0
3	CA	F	1001	1/1	0.98	0.24	0.63	83,83,83,83	0
3	CA	M	1001	1/1	0.97	0.23	0.39	74,74,74,74	0
3	CA	K	1001	1/1	0.98	0.21	0.27	69,69,69,69	0
3	CA	C	1001	1/1	0.93	0.19	-0.42	80,80,80,80	0
2	ADP	M	1000	27/27	0.94	0.22	-0.54	72,74,76,78	0
2	ADP	G	1000	27/27	0.95	0.24	-0.55	83,86,88,90	0
2	ADP	A	1000	27/27	0.96	0.18	-0.62	53,57,63,64	0
2	ADP	I	1000	27/27	0.92	0.21	-0.63	84,85,87,89	0
2	ADP	H	1000	27/27	0.95	0.20	-0.65	81,83,85,88	0
2	ADP	D	1000	27/27	0.94	0.19	-0.66	79,83,85,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ADP	N	1000	27/27	0.97	0.18	-0.73	58,60,62,64	0
2	ADP	E	1000	27/27	0.95	0.18	-0.75	74,76,78,79	0
2	ADP	B	1000	27/27	0.96	0.16	-0.75	82,83,85,86	0
2	ADP	C	1000	27/27	0.95	0.20	-0.77	72,75,77,79	0
2	ADP	J	1000	27/27	0.95	0.18	-0.79	74,77,80,82	0
3	CA	B	1001	1/1	0.93	0.18	-0.92	73,73,73,73	0
2	ADP	K	1000	27/27	0.97	0.18	-0.96	67,69,72,72	0
3	CA	L	1001	1/1	0.97	0.16	-0.96	71,71,71,71	0
3	CA	P	1001	1/1	0.92	0.15	-1.01	76,76,76,76	0
2	ADP	P	1000	27/27	0.96	0.17	-1.03	66,69,71,72	0
2	ADP	L	1000	27/27	0.96	0.17	-1.04	75,76,78,80	0
3	CA	G	1001	1/1	0.94	0.14	-1.10	89,89,89,89	0
2	ADP	F	1000	27/27	0.96	0.18	-1.10	72,74,76,77	0
2	ADP	O	1000	27/27	0.97	0.16	-1.14	55,58,61,62	0
3	CA	I	1001	1/1	0.94	0.13	-1.25	82,82,82,82	0
3	CA	H	1001	1/1	0.91	0.16	-1.33	79,79,79,79	0
3	CA	D	1001	1/1	0.94	0.14	-1.66	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.