



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:37 PM GMT

PDB ID : 3ZPV  
Title : Crystal structure of Drosophila Pygo PHD finger in complex with Legless HD1 domain  
Authors : Miller, T.C.R.; Mieszczanek, J.; Sanchez-Barrena, M.J.; Rutherford, T.J.; Fiedler, M.; Bienz, M.  
Deposited on : 2013-03-02  
Resolution : 2.68 Å(reported)

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

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

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

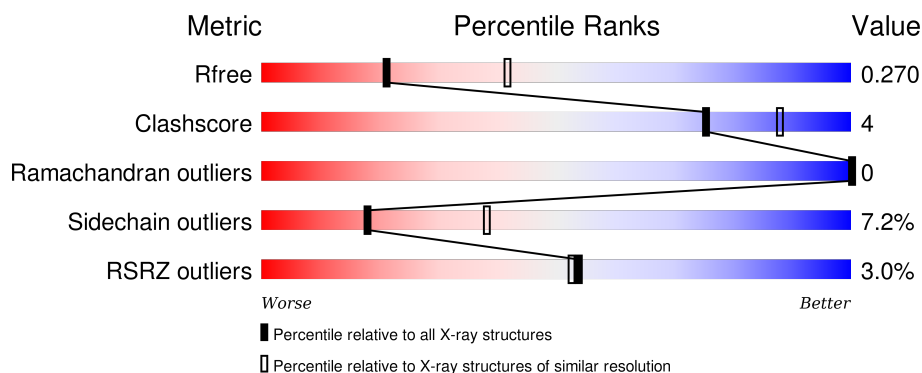
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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.






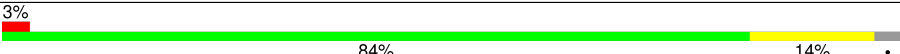

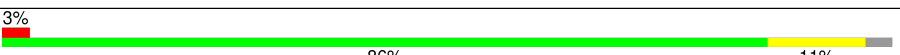

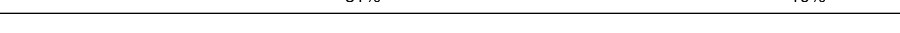



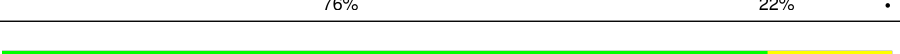
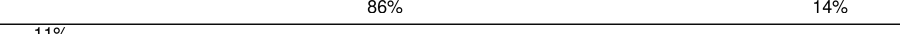

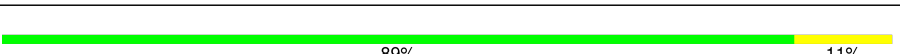



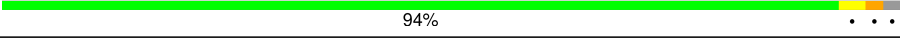


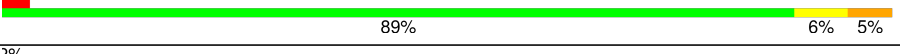

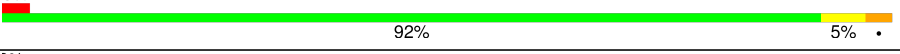
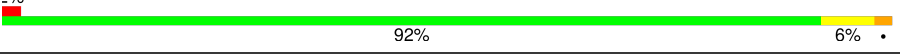
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	0	37	<div> <div>76%</div> <div>22%</div> <div>•</div> </div>
1	2	37	<div>16%</div> <div>86%</div> <div>14%</div>
1	4	37	<div>3%</div> <div>89%</div> <div>8%</div> <div>•</div>
1	6	37	<div>3%</div> <div>81%</div> <div>19%</div>
1	8	37	<div>24%</div> <div>81%</div> <div>16%</div> <div>•</div>

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Mol	Chain	Length	Quality of chain
1	B	37	
1	D	37	
1	F	37	
1	H	37	
1	J	37	
1	L	37	
1	N	37	
1	P	37	
1	R	37	
1	T	37	
1	V	37	
1	X	37	
1	Z	37	
2	1	62	
2	3	62	
2	5	62	
2	7	62	
2	9	62	
2	A	62	
2	C	62	
2	G	62	
2	I	62	
2	K	62	
2	M	62	
2	Q	62	

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Mol	Chain	Length	Quality of chain
2	S	62	<div><div></div><div>2%</div><div>89%</div><div>8%</div><div></div><div></div></div>
2	U	62	<div><div></div><div>3%</div><div>92%</div><div>5%</div><div></div><div></div></div>
2	W	62	<div><div></div><div>2%</div><div>87%</div><div>8%</div><div></div><div></div></div>
3	E	62	<div><div></div><div>3%</div><div>90%</div><div></div><div>5%</div><div></div></div>
3	O	62	<div><div></div><div>2%</div><div>87%</div><div>8%</div><div>5%</div><div></div></div>
3	Y	62	<div><div></div><div>5%</div><div>92%</div><div>5%</div><div></div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14064 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 PROTEIN BCL9 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	36	Total	C	N	O	S	0	0	0
			275	175	47	51	2			
1	2	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			
1	4	36	Total	C	N	O	S	0	0	0
			275	175	47	51	2			
1	6	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			
1	8	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			
1	B	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			
1	D	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			
1	F	36	Total	C	N	O	S	0	0	0
			275	175	47	51	2			
1	H	36	Total	C	N	O	S	0	0	0
			275	175	47	51	2			
1	J	36	Total	C	N	O	S	0	0	0
			275	175	47	51	2			
1	L	36	Total	C	N	O	S	0	0	0
			275	175	47	51	2			
1	N	37	Total	C	N	O	S	0	1	0
			288	182	49	55	2			
1	P	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			
1	R	36	Total	C	N	O	S	0	1	0
			281	179	47	53	2			
1	T	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			
1	V	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	37	Total	C	N	O	S	0	2	0
			291	184	50	55	2			
1	Z	37	Total	C	N	O	S	0	0	0
			279	177	48	52	2			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	317	GLY	-	EXPRESSION TAG	UNP Q961D9
0	318	ALA	-	EXPRESSION TAG	UNP Q961D9
0	319	MET	-	EXPRESSION TAG	UNP Q961D9
0	320	ALA	-	EXPRESSION TAG	UNP Q961D9
2	317	GLY	-	EXPRESSION TAG	UNP Q961D9
2	318	ALA	-	EXPRESSION TAG	UNP Q961D9
2	319	MET	-	EXPRESSION TAG	UNP Q961D9
2	320	ALA	-	EXPRESSION TAG	UNP Q961D9
4	317	GLY	-	EXPRESSION TAG	UNP Q961D9
4	318	ALA	-	EXPRESSION TAG	UNP Q961D9
4	319	MET	-	EXPRESSION TAG	UNP Q961D9
4	320	ALA	-	EXPRESSION TAG	UNP Q961D9
6	317	GLY	-	EXPRESSION TAG	UNP Q961D9
6	318	ALA	-	EXPRESSION TAG	UNP Q961D9
6	319	MET	-	EXPRESSION TAG	UNP Q961D9
6	320	ALA	-	EXPRESSION TAG	UNP Q961D9
8	317	GLY	-	EXPRESSION TAG	UNP Q961D9
8	318	ALA	-	EXPRESSION TAG	UNP Q961D9
8	319	MET	-	EXPRESSION TAG	UNP Q961D9
8	320	ALA	-	EXPRESSION TAG	UNP Q961D9
B	317	GLY	-	EXPRESSION TAG	UNP Q961D9
B	318	ALA	-	EXPRESSION TAG	UNP Q961D9
B	319	MET	-	EXPRESSION TAG	UNP Q961D9
B	320	ALA	-	EXPRESSION TAG	UNP Q961D9
D	317	GLY	-	EXPRESSION TAG	UNP Q961D9
D	318	ALA	-	EXPRESSION TAG	UNP Q961D9
D	319	MET	-	EXPRESSION TAG	UNP Q961D9
D	320	ALA	-	EXPRESSION TAG	UNP Q961D9
F	317	GLY	-	EXPRESSION TAG	UNP Q961D9
F	318	ALA	-	EXPRESSION TAG	UNP Q961D9
F	319	MET	-	EXPRESSION TAG	UNP Q961D9
F	320	ALA	-	EXPRESSION TAG	UNP Q961D9
H	317	GLY	-	EXPRESSION TAG	UNP Q961D9
H	318	ALA	-	EXPRESSION TAG	UNP Q961D9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	319	MET	-	EXPRESSION TAG	UNP Q961D9
H	320	ALA	-	EXPRESSION TAG	UNP Q961D9
J	317	GLY	-	EXPRESSION TAG	UNP Q961D9
J	318	ALA	-	EXPRESSION TAG	UNP Q961D9
J	319	MET	-	EXPRESSION TAG	UNP Q961D9
J	320	ALA	-	EXPRESSION TAG	UNP Q961D9
L	317	GLY	-	EXPRESSION TAG	UNP Q961D9
L	318	ALA	-	EXPRESSION TAG	UNP Q961D9
L	319	MET	-	EXPRESSION TAG	UNP Q961D9
L	320	ALA	-	EXPRESSION TAG	UNP Q961D9
N	317	GLY	-	EXPRESSION TAG	UNP Q961D9
N	318	ALA	-	EXPRESSION TAG	UNP Q961D9
N	319	MET	-	EXPRESSION TAG	UNP Q961D9
N	320	ALA	-	EXPRESSION TAG	UNP Q961D9
P	317	GLY	-	EXPRESSION TAG	UNP Q961D9
P	318	ALA	-	EXPRESSION TAG	UNP Q961D9
P	319	MET	-	EXPRESSION TAG	UNP Q961D9
P	320	ALA	-	EXPRESSION TAG	UNP Q961D9
R	317	GLY	-	EXPRESSION TAG	UNP Q961D9
R	318	ALA	-	EXPRESSION TAG	UNP Q961D9
R	319	MET	-	EXPRESSION TAG	UNP Q961D9
R	320	ALA	-	EXPRESSION TAG	UNP Q961D9
T	317	GLY	-	EXPRESSION TAG	UNP Q961D9
T	318	ALA	-	EXPRESSION TAG	UNP Q961D9
T	319	MET	-	EXPRESSION TAG	UNP Q961D9
T	320	ALA	-	EXPRESSION TAG	UNP Q961D9
V	317	GLY	-	EXPRESSION TAG	UNP Q961D9
V	318	ALA	-	EXPRESSION TAG	UNP Q961D9
V	319	MET	-	EXPRESSION TAG	UNP Q961D9
V	320	ALA	-	EXPRESSION TAG	UNP Q961D9
X	317	GLY	-	EXPRESSION TAG	UNP Q961D9
X	318	ALA	-	EXPRESSION TAG	UNP Q961D9
X	319	MET	-	EXPRESSION TAG	UNP Q961D9
X	320	ALA	-	EXPRESSION TAG	UNP Q961D9
Z	317	GLY	-	EXPRESSION TAG	UNP Q961D9
Z	318	ALA	-	EXPRESSION TAG	UNP Q961D9
Z	319	MET	-	EXPRESSION TAG	UNP Q961D9
Z	320	ALA	-	EXPRESSION TAG	UNP Q961D9

- Molecule 2 is a protein called PROTEIN PYGOPUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	3	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	5	61	Total 473	C 297	N 77	O 88	S 11	0	0	0
2	7	61	Total 473	C 297	N 77	O 88	S 11	0	0	0
2	9	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	A	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	C	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	G	62	Total 484	C 304	N 78	O 90	S 12	0	1	0
2	I	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	K	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	M	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	Q	62	Total 485	C 304	N 78	O 92	S 11	0	1	0
2	S	62	Total 485	C 304	N 78	O 92	S 11	0	1	0
2	U	62	Total 479	C 300	N 78	O 90	S 11	0	0	0
2	W	62	Total 479	C 300	N 78	O 90	S 11	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
1	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
1	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
1	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
3	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
3	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
3	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
3	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
5	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
5	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8

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Chain	Residue	Modelled	Actual	Comment	Reference
5	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
5	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
7	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
7	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
7	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
7	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
9	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
9	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
9	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
9	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
A	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
A	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
A	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
A	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
C	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
C	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
C	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
C	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
G	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
G	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
G	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
G	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
I	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
I	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
I	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
I	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
K	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
K	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
K	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
K	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
M	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
M	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
M	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
M	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
Q	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
Q	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
Q	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
Q	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
S	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
S	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
S	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
S	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8

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Chain	Residue	Modelled	Actual	Comment	Reference
U	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
U	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
U	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
U	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
W	743	GLY	-	EXPRESSION TAG	UNP Q9V9W8
W	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
W	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
W	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8

- Molecule 3 is a protein called PROTEIN PYGOPUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	62	Total	C	N	O	S	0	0	0
			480	301	78	90	11			
3	O	62	Total	C	N	O	S	0	1	0
			486	305	78	92	11			
3	Y	62	Total	C	N	O	S	0	0	0
			480	301	78	90	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	743	ALA	-	EXPRESSION TAG	UNP Q9V9W8
E	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
E	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
E	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
O	743	ALA	-	EXPRESSION TAG	UNP Q9V9W8
O	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
O	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
O	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8
Y	743	ALA	-	EXPRESSION TAG	UNP Q9V9W8
Y	744	ALA	-	EXPRESSION TAG	UNP Q9V9W8
Y	745	MET	-	EXPRESSION TAG	UNP Q9V9W8
Y	746	ALA	-	EXPRESSION TAG	UNP Q9V9W8

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Zn	0	0
			2	2		
4	Y	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	2	Total 2	Zn 2	0	0
4	K	2	Total 2	Zn 2	0	0
4	E	2	Total 2	Zn 2	0	0
4	Q	2	Total 2	Zn 2	0	0
4	I	2	Total 2	Zn 2	0	0
4	C	2	Total 2	Zn 2	0	0
4	S	2	Total 2	Zn 2	0	0
4	7	2	Total 2	Zn 2	0	0
4	A	2	Total 2	Zn 2	0	0
4	5	2	Total 2	Zn 2	0	0
4	O	2	Total 2	Zn 2	0	0
4	9	2	Total 2	Zn 2	0	0
4	W	2	Total 2	Zn 2	0	0
4	3	2	Total 2	Zn 2	0	0
4	U	2	Total 2	Zn 2	0	0
4	M	2	Total 2	Zn 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	0	5	Total 5	O 5	0	0
5	1	16	Total 16	O 16	0	0
5	2	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	3	12	Total O 12 12	0	0
5	4	5	Total O 5 5	0	0
5	5	19	Total O 19 19	0	0
5	6	11	Total O 11 11	0	0
5	7	17	Total O 17 17	0	0
5	8	5	Total O 5 5	0	0
5	9	12	Total O 12 12	0	0
5	A	23	Total O 23 23	0	0
5	B	6	Total O 6 6	0	0
5	C	23	Total O 23 23	0	0
5	D	6	Total O 6 6	0	0
5	E	31	Total O 31 31	0	0
5	F	4	Total O 4 4	0	0
5	G	20	Total O 20 20	0	0
5	H	2	Total O 2 2	0	0
5	I	18	Total O 18 18	0	0
5	J	1	Total O 1 1	0	0
5	K	12	Total O 12 12	0	0
5	L	2	Total O 2 2	0	0
5	M	19	Total O 19 19	0	0
5	N	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	17	Total 17	O 17	0	0
5	P	5	Total 5	O 5	0	0
5	Q	16	Total 16	O 16	0	0
5	R	2	Total 2	O 2	0	0
5	S	15	Total 15	O 15	0	0
5	T	2	Total 2	O 2	0	0
5	U	17	Total 17	O 17	0	0
5	V	3	Total 3	O 3	0	0
5	W	2	Total 2	O 2	0	0
5	X	3	Total 3	O 3	0	0
5	Y	10	Total 10	O 10	0	0
5	Z	2	Total 2	O 2	0	0

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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

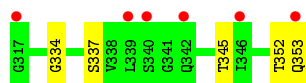
- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain 0: 




- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain 2: 




- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain 4: 




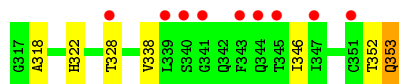
- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain 6: 




- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain 8: 

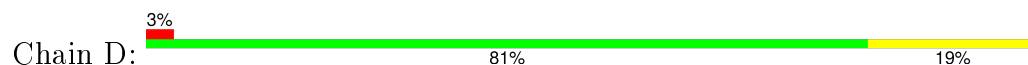


- Molecule 1: PROTEIN BCL9 HOMOLOG

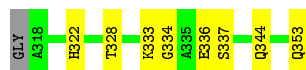
Chain B: 



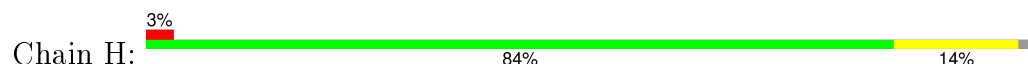
- Molecule 1: PROTEIN BCL9 HOMOLOG



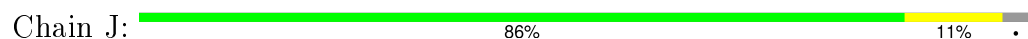
- Molecule 1: PROTEIN BCL9 HOMOLOG



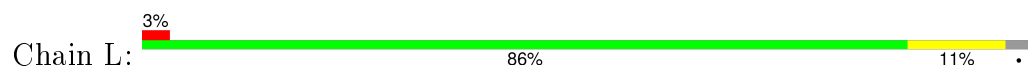
- Molecule 1: PROTEIN BCL9 HOMOLOG



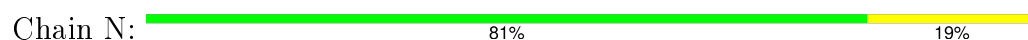
- Molecule 1: PROTEIN BCL9 HOMOLOG



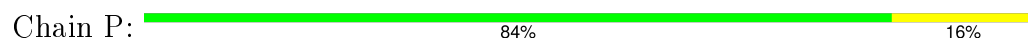
- Molecule 1: PROTEIN BCL9 HOMOLOG




- Molecule 1: PROTEIN BCL9 HOMOLOG

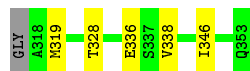


- Molecule 1: PROTEIN BCL9 HOMOLOG




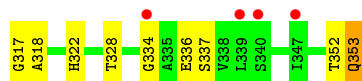
- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain R:  84% 14%




- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain T:  11% 76% 22%




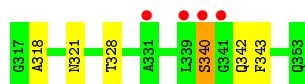
- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain V:  86% 14%




- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain X:  11% 84% 14%




- Molecule 1: PROTEIN BCL9 HOMOLOG

Chain Z:  89% 11%




- Molecule 2: PROTEIN PYGOPUS

Chain 1:  90% 8%



- Molecule 2: PROTEIN PYGOPUS

Chain 3:  3% 87% 10%




- Molecule 2: PROTEIN PYGOPUS



Chain 5:  94% . . .




• Molecule 2: PROTEIN PYGOPUS

Chain 7:  85% 11% . .




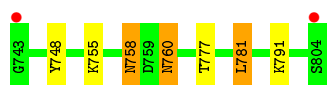
• Molecule 2: PROTEIN PYGOPUS

Chain 9:  3% 87% 11% .




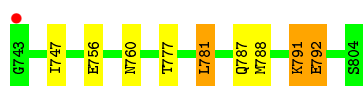
• Molecule 2: PROTEIN PYGOPUS

Chain A:  3% 89% 6% 5%

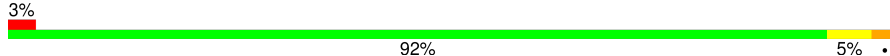


• Molecule 2: PROTEIN PYGOPUS

Chain C:  2% 85% 10% 5%



• Molecule 2: PROTEIN PYGOPUS

Chain G:  3% 92% 5% .



• Molecule 2: PROTEIN PYGOPUS

Chain I:  2% 92% 6% .



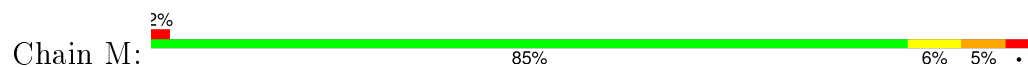
• Molecule 2: PROTEIN PYGOPUS

Chain K:  6% 89% 8% .

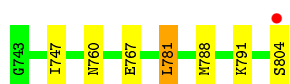
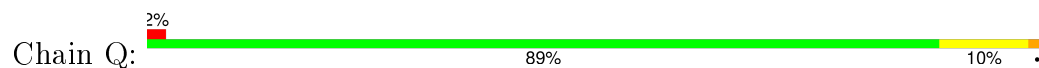




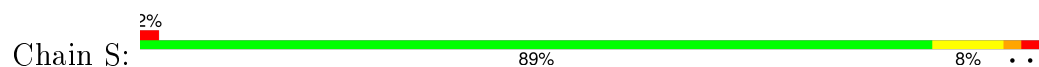
- Molecule 2: PROTEIN PYGOPUS



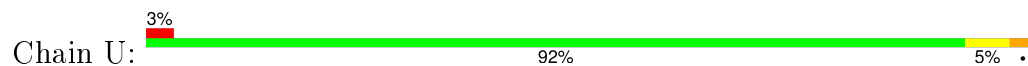
- Molecule 2: PROTEIN PYGOPUS



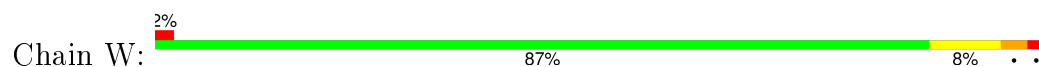
- Molecule 2: PROTEIN PYGOPUS



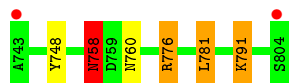
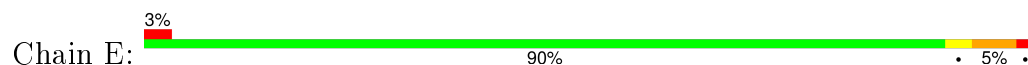
- Molecule 2: PROTEIN PYGOPUS



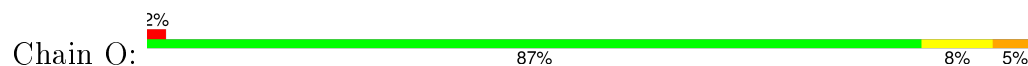
- Molecule 2: PROTEIN PYGOPUS



- Molecule 3: PROTEIN PYGOPUS



- Molecule 3: PROTEIN PYGOPUS





● Molecule 3: PROTEIN PYGOPUS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.21Å 111.96Å 190.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.24 – 2.68 46.19 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.24-2.68) 99.5 (46.19-2.68)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0024	Depositor
R, $R_{free}$	0.224 , 0.262 0.233 , 0.270	Depositor DCC
$R_{free}$ test set	3222 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	15 of 63676 reflections (0.024%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.07 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3563e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.61	0/280	0.69	0/378
1	2	0.60	0/284	0.70	0/383
1	4	0.60	0/280	0.70	0/378
1	6	0.56	0/284	0.66	0/383
1	8	0.55	0/284	0.66	0/383
1	B	0.75	1/284 (0.4%)	0.80	1/383 (0.3%)
1	D	0.68	0/284	0.71	1/383 (0.3%)
1	F	0.67	0/280	0.75	1/378 (0.3%)
1	H	0.59	0/280	0.65	0/378
1	J	0.59	0/280	0.62	0/378
1	L	0.67	0/280	0.76	0/378
1	N	0.58	0/293	0.62	0/395
1	P	0.59	0/284	0.66	0/383
1	R	0.56	0/289	0.68	0/390
1	T	0.50	0/284	0.61	0/383
1	V	0.77	1/284 (0.4%)	0.71	1/383 (0.3%)
1	X	0.95	2/299 (0.7%)	0.87	2/403 (0.5%)
1	Z	0.63	0/284	0.77	0/383
2	1	0.64	0/490	0.75	0/659
2	3	0.63	0/490	0.83	1/659 (0.2%)
2	5	0.72	0/484	0.74	0/651
2	7	0.68	1/484 (0.2%)	0.81	0/651
2	9	0.63	0/490	0.78	0/659
2	A	0.71	0/490	0.81	1/659 (0.2%)
2	C	0.73	1/490 (0.2%)	0.86	2/659 (0.3%)
2	G	0.61	0/498	0.74	0/669
2	I	0.64	0/490	0.76	0/659
2	K	0.66	0/490	0.81	1/659 (0.2%)
2	M	0.85	2/490 (0.4%)	0.89	2/659 (0.3%)
2	Q	0.61	0/499	0.82	0/671
2	S	0.67	0/499	0.79	1/671 (0.1%)
2	U	0.67	0/490	0.79	1/659 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	W	0.68	0/490	0.82	2/659 (0.3%)
3	E	0.75	0/491	0.92	3/661 (0.5%)
3	O	0.70	1/500 (0.2%)	0.86	0/673
3	Y	0.70	0/491	0.93	2/661 (0.3%)
All	All	0.67	9/13963 (0.1%)	0.78	22/18801 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	768	SER	CA-CB	9.32	1.67	1.52
1	X	340[A]	SER	CA-CB	7.60	1.64	1.52
1	X	340[B]	SER	CA-CB	7.60	1.64	1.52
1	V	340	SER	CA-CB	6.22	1.62	1.52
3	O	792	GLU	CD-OE2	5.80	1.32	1.25
2	7	792	GLU	CD-OE2	5.63	1.31	1.25
2	M	792	GLU	CD-OE2	5.54	1.31	1.25
1	B	336	GLU	CD-OE1	-5.34	1.19	1.25
2	C	756	GLU	CG-CD	5.02	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	752	MET	CA-CB-CG	8.97	128.55	113.30
2	K	791	LYS	CD-CE-NZ	8.40	131.02	111.70
3	E	776	ARG	CG-CD-NE	-7.52	96.01	111.80
3	Y	792	GLU	OE1-CD-OE2	-7.09	114.79	123.30
2	U	791	LYS	CD-CE-NZ	-6.85	95.95	111.70
2	W	791	LYS	CB-CG-CD	6.51	128.53	111.60
1	X	340[A]	SER	N-CA-CB	6.02	119.53	110.50
1	X	340[B]	SER	N-CA-CB	6.02	119.53	110.50
3	E	776	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	F	333	LYS	CG-CD-CE	5.86	129.48	111.90
1	B	336	GLU	OE1-CD-OE2	-5.84	116.29	123.30
2	C	760	ASN	CB-CA-C	-5.77	98.86	110.40
1	V	340	SER	N-CA-CB	5.76	119.14	110.50
2	M	768	SER	N-CA-CB	5.52	118.78	110.50
2	S	793	VAL	CB-CA-C	-5.44	101.07	111.40
2	3	792	GLU	CA-CB-CG	-5.27	101.80	113.40
1	D	336	GLU	OE1-CD-OE2	-5.20	117.06	123.30
2	W	793	VAL	CB-CA-C	-5.19	101.54	111.40
2	M	793	VAL	CB-CA-C	-5.19	101.55	111.40
2	C	756	GLU	OE1-CD-OE2	-5.14	117.13	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	758	ASN	CB-CG-OD1	-5.06	111.48	121.60
3	E	758	ASN	CB-CG-OD1	-5.03	111.54	121.60

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	0	275	0	266	9	0
1	2	279	0	269	3	0
1	4	275	0	266	1	0
1	6	279	0	269	4	0
1	8	279	0	269	10	0
1	B	279	0	269	3	0
1	D	279	0	269	5	0
1	F	275	0	266	4	0
1	H	275	0	266	4	0
1	J	275	0	266	3	0
1	L	275	0	266	4	0
1	N	288	0	274	4	0
1	P	279	0	269	3	0
1	R	281	0	272	7	0
1	T	279	0	269	7	0
1	V	279	0	269	2	0
1	X	291	0	281	6	0
1	Z	279	0	269	5	0
2	1	479	0	429	7	0
2	3	479	0	429	2	0
2	5	473	0	424	1	0
2	7	473	0	424	5	0
2	9	479	0	429	9	0
2	A	479	0	429	7	0
2	C	479	0	429	7	0
2	G	484	0	438	2	0
2	I	479	0	429	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	479	0	429	4	0
2	M	479	0	429	6	0
2	Q	485	0	435	9	0
2	S	485	0	435	4	0
2	U	479	0	429	2	0
2	W	479	0	430	7	0
3	E	480	0	431	4	0
3	O	486	0	437	4	0
3	Y	480	0	431	1	0
4	1	2	0	0	0	0
4	3	2	0	0	0	0
4	5	2	0	0	0	0
4	7	2	0	0	0	0
4	9	2	0	0	0	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
4	I	2	0	0	0	0
4	K	2	0	0	0	0
4	M	2	0	0	0	0
4	O	2	0	0	0	0
4	Q	2	0	0	0	0
4	S	2	0	0	0	0
4	U	2	0	0	0	0
4	W	2	0	0	0	0
4	Y	2	0	0	0	0
5	0	5	0	0	1	0
5	1	16	0	0	0	0
5	2	3	0	0	0	0
5	3	12	0	0	1	0
5	4	5	0	0	0	0
5	5	19	0	0	1	0
5	6	11	0	0	2	0
5	7	17	0	0	2	0
5	8	5	0	0	0	0
5	9	12	0	0	0	0
5	A	23	0	0	0	0
5	B	6	0	0	0	1
5	C	23	0	0	1	0
5	D	6	0	0	0	0
5	E	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	4	0	0	0	0
5	G	20	0	0	2	0
5	H	2	0	0	0	0
5	I	18	0	0	0	0
5	J	1	0	0	0	0
5	K	12	0	0	0	0
5	L	2	0	0	0	0
5	M	19	0	0	1	1
5	N	5	0	0	1	0
5	O	17	0	0	1	0
5	P	5	0	0	0	0
5	Q	16	0	0	1	0
5	R	2	0	0	0	0
5	S	15	0	0	0	0
5	T	2	0	0	0	0
5	U	17	0	0	0	0
5	V	3	0	0	0	0
5	W	2	0	0	0	0
5	X	3	0	0	1	0
5	Y	10	0	0	0	0
5	Z	2	0	0	0	0
All	All	14064	0	12590	103	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (103) 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:A:755:LYS:HE3	1:Z:340:SER:O	1.42	1.19
1:X:321:ASN:OD1	5:X:2001:HOH:O	1.64	1.14
1:8:346:ILE:HG23	2:9:788:MET:HE2	1.31	1.12
1:0:346:ILE:HG23	2:1:788:MET:HE2	1.32	1.09
2:A:755:LYS:CE	1:Z:340:SER:O	2.04	1.05
2:Q:788:MET:HE2	1:R:346:ILE:HG23	1.34	1.05
1:0:346:ILE:HG23	2:1:788:MET:CE	1.87	1.03
2:Q:788:MET:CE	1:R:346:ILE:HG23	1.91	1.00
1:8:346:ILE:HG23	2:9:788:MET:CE	1.90	1.00
2:M:768:SER:OG	2:M:798:CYS:SG	2.22	0.95
1:8:346:ILE:CG2	2:9:788:MET:HE2	2.02	0.90
1:0:346:ILE:CG2	2:1:788:MET:HE2	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:352:THR:HG22	5:N:2005:HOH:O	1.73	0.88
2:Q:788:MET:HE2	1:R:346:ILE:CG2	2.09	0.81
1:L:352:THR:O	1:L:353:GLN:HB2	1.83	0.77
2:M:792:GLU:OE1	1:N:347:ILE:HG12	1.88	0.74
2:A:755:LYS:HE3	1:Z:340:SER:C	2.10	0.71
1:6:347:ILE:HG12	2:7:792:GLU:OE1	1.90	0.71
2:S:793:VAL:HG21	2:W:763:ALA:HB3	1.73	0.71
1:2:345:THR:HB	2:3:792:GLU:OE1	1.94	0.67
2:A:755:LYS:HE2	1:Z:340:SER:O	1.95	0.66
3:O:792:GLU:OE1	1:P:347:ILE:HG12	1.95	0.66
2:S:763:ALA:HB3	2:W:793:VAL:HG21	1.78	0.64
2:Q:804:SER:HA	5:Q:2016:HOH:O	2.00	0.62
2:M:793:VAL:HG21	2:U:763:ALA:HB3	1.81	0.62
2:C:791:LYS:HG3	2:C:792:GLU:OE1	2.00	0.61
1:B:352:THR:O	1:B:353:GLN:HB3	2.01	0.61
1:T:318:ALA:HA	2:W:747:ILE:HD13	1.82	0.60
2:3:777:THR:HB	5:3:2007:HOH:O	2.02	0.59
2:C:792:GLU:HG3	5:G:2004:HOH:O	2.02	0.59
2:W:781:LEU:HD13	1:X:328:THR:HG23	1.85	0.59
2:C:747:ILE:HD13	1:H:318:ALA:HA	1.86	0.58
1:D:352:THR:O	1:D:353:GLN:HG3	2.04	0.58
1:2:352:THR:O	1:2:353:GLN:HB3	2.04	0.58
1:8:346:ILE:CG2	2:9:788:MET:CE	2.71	0.57
2:1:763:ALA:HB3	3:O:793:VAL:HG21	1.87	0.56
1:0:346:ILE:CG2	2:1:788:MET:CE	2.70	0.56
2:7:783:GLU:HG2	5:7:2007:HOH:O	2.04	0.56
2:Q:788:MET:HE3	1:R:338:VAL:HG21	1.89	0.55
1:D:352:THR:O	1:D:353:GLN:CG	2.55	0.55
3:E:791:LYS:HG2	5:E:2027:HOH:O	2.07	0.54
2:Q:788:MET:CE	1:R:346:ILE:CG2	2.74	0.52
1:X:342[B]:GLN:HG3	1:X:343:PHE:CD2	2.44	0.52
2:C:787:GLN:HB3	5:C:2010:HOH:O	2.09	0.52
1:T:318:ALA:HA	2:W:747:ILE:CD1	2.39	0.52
2:C:781:LEU:HD13	1:D:328:THR:HG23	1.92	0.51
1:D:339:LEU:HB3	1:P:339:LEU:HB3	1.94	0.49
2:G:791:LYS:HG2	5:G:2015:HOH:O	2.12	0.49
1:T:322:HIS:HB3	2:W:748:TYR:CZ	2.47	0.49
2:K:781:LEU:HD13	1:L:328:THR:HG23	1.94	0.49
1:J:318:ALA:HA	2:K:747:ILE:HD13	1.95	0.49
2:7:783:GLU:CG	5:7:2007:HOH:O	2.61	0.48
2:M:791:LYS:HG2	5:M:2013:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:318:ALA:HA	2:9:747:ILE:HD13	1.96	0.48
3:Y:781:LEU:HD13	1:Z:328:THR:HG23	1.95	0.48
1:8:338:VAL:HG21	2:9:788:MET:HE3	1.96	0.48
1:X:340[A]:SER:OG	1:X:342[A]:GLN:HG3	2.14	0.48
2:Q:788:MET:CE	1:R:338:VAL:HG21	2.44	0.47
2:7:748:TYR:CZ	1:8:322:HIS:HB3	2.50	0.47
2:U:781:LEU:HD13	1:V:328:THR:HG23	1.95	0.47
3:O:777:THR:HB	5:O:2007:HOH:O	2.14	0.46
2:5:791:LYS:HG2	5:5:2014:HOH:O	2.16	0.46
2:I:748:TYR:CZ	1:L:322:HIS:HB3	2.50	0.46
1:8:338:VAL:HG21	2:9:788:MET:CE	2.46	0.45
2:A:760:ASN:ND2	1:F:344:GLN:NE2	2.64	0.45
2:M:781:LEU:HD13	1:N:328:THR:HG23	1.98	0.45
1:0:328:THR:HG23	2:1:781:LEU:HD13	1.99	0.45
2:S:747:ILE:HD13	1:X:318:ALA:HA	1.99	0.45
1:8:352:THR:O	1:8:353:GLN:C	2.55	0.44
1:0:346:ILE:HG12	5:0:2005:HOH:O	2.18	0.44
2:A:781:LEU:HD13	1:B:328:THR:HG23	1.98	0.44
1:X:342[B]:GLN:HG3	1:X:343:PHE:CE2	2.53	0.44
1:T:352:THR:O	1:T:353:GLN:C	2.55	0.44
1:4:318:ALA:HA	2:Q:747:ILE:HD13	2.00	0.43
3:E:781:LEU:HD13	1:F:328:THR:HG23	1.98	0.43
2:C:747:ILE:CD1	1:H:318:ALA:HA	2.48	0.43
1:8:328:THR:HG23	2:9:781:LEU:HD13	2.00	0.43
1:6:339:LEU:HD23	5:6:2011:HOH:O	2.18	0.43
2:7:747:ILE:HD13	1:8:318:ALA:HA	2.01	0.43
2:Q:781:LEU:HD13	1:R:328:THR:HG23	2.01	0.42
2:G:781:LEU:HD13	1:H:328:THR:HG23	2.00	0.42
1:0:318:ALA:HA	3:O:747:ILE:HD13	2.01	0.42
1:B:322:HIS:HB3	3:E:748:TYR:CZ	2.55	0.41
2:A:748:TYR:CZ	1:F:322:HIS:HB3	2.55	0.41
2:K:779:VAL:O	1:L:328:THR:HG21	2.20	0.41
5:6:2002:HOH:O	2:9:743:GLY:HA2	2.21	0.41
1:J:322:HIS:HB3	2:K:748:TYR:CZ	2.55	0.41
2:M:748:TYR:CZ	1:V:322:HIS:HB3	2.55	0.41
2:S:781:LEU:HD13	1:T:328:THR:HG23	2.02	0.41
2:C:788:MET:HA	2:C:791:LYS:HG2	2.02	0.41
1:N:334:GLY:O	1:N:337:SER:HB2	2.21	0.41
2:I:781:LEU:HD13	1:J:328:THR:HG23	2.03	0.41
1:H:334:GLY:O	1:H:337:SER:HB2	2.21	0.41
1:0:334:GLY:O	1:0:337:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:334:GLY:O	1:P:337:SER:HB2	2.21	0.41
1:D:334:GLY:O	1:D:337:SER:HB2	2.22	0.40
3:E:758:ASN:HD22	3:E:760:ASN:H	1.70	0.40
1:6:334:GLY:O	1:6:337:SER:HB2	2.22	0.40
1:2:334:GLY:O	1:2:337:SER:HB2	2.22	0.40
1:0:338:VAL:HG21	2:1:788:MET:CE	2.52	0.40
1:T:334:GLY:O	1:T:337:SER:HB2	2.22	0.40
1:F:334:GLY:O	1:F:337:SER:HB2	2.22	0.40
1:T:317:GLY:O	2:W:756:GLU:OE2	2.40	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2004:HOH:O	5:M:2008:HOH:O[4_545]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
1	2	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
1	4	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
1	6	35/37 (95%)	35 (100%)	0	0	100	100
1	8	35/37 (95%)	35 (100%)	0	0	100	100
1	B	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
1	D	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
1	F	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
1	H	34/37 (92%)	33 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	34/37 (92%)	34 (100%)	0	0	100	100
1	L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
1	N	36/37 (97%)	36 (100%)	0	0	100	100
1	P	35/37 (95%)	35 (100%)	0	0	100	100
1	R	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
1	T	35/37 (95%)	35 (100%)	0	0	100	100
1	V	35/37 (95%)	35 (100%)	0	0	100	100
1	X	37/37 (100%)	37 (100%)	0	0	100	100
1	Z	35/37 (95%)	35 (100%)	0	0	100	100
2	1	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	3	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	5	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
2	7	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
2	9	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	A	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	C	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	G	61/62 (98%)	58 (95%)	3 (5%)	0	100	100
2	I	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	K	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	M	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	Q	61/62 (98%)	59 (97%)	2 (3%)	0	100	100
2	S	61/62 (98%)	59 (97%)	2 (3%)	0	100	100
2	U	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
2	W	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
3	E	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
3	O	61/62 (98%)	59 (97%)	2 (3%)	0	100	100
3	Y	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	1709/1782 (96%)	1663 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	0	29/29 (100%)	27 (93%)	2 (7%)	19	40
1	2	29/29 (100%)	29 (100%)	0	100	100
1	4	29/29 (100%)	27 (93%)	2 (7%)	19	40
1	6	29/29 (100%)	27 (93%)	2 (7%)	19	40
1	8	29/29 (100%)	28 (97%)	1 (3%)	44	73
1	B	29/29 (100%)	29 (100%)	0	100	100
1	D	29/29 (100%)	29 (100%)	0	100	100
1	F	29/29 (100%)	27 (93%)	2 (7%)	19	40
1	H	29/29 (100%)	28 (97%)	1 (3%)	44	73
1	J	29/29 (100%)	28 (97%)	1 (3%)	44	73
1	L	29/29 (100%)	29 (100%)	0	100	100
1	N	30/29 (103%)	27 (90%)	3 (10%)	9	20
1	P	29/29 (100%)	27 (93%)	2 (7%)	19	40
1	R	30/29 (103%)	27 (90%)	3 (10%)	9	20
1	T	29/29 (100%)	27 (93%)	2 (7%)	19	40
1	V	29/29 (100%)	27 (93%)	2 (7%)	19	40
1	X	31/29 (107%)	31 (100%)	0	100	100
1	Z	29/29 (100%)	27 (93%)	2 (7%)	19	40
2	1	52/52 (100%)	48 (92%)	4 (8%)	16	34
2	3	52/52 (100%)	45 (86%)	7 (14%)	5	10
2	5	51/52 (98%)	48 (94%)	3 (6%)	24	49
2	7	51/52 (98%)	47 (92%)	4 (8%)	16	33
2	9	52/52 (100%)	47 (90%)	5 (10%)	10	22
2	A	52/52 (100%)	47 (90%)	5 (10%)	10	22
2	C	52/52 (100%)	48 (92%)	4 (8%)	16	34
2	G	53/52 (102%)	48 (91%)	5 (9%)	11	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	52/52 (100%)	48 (92%)	4 (8%)	16	34
2	K	52/52 (100%)	48 (92%)	4 (8%)	16	34
2	M	52/52 (100%)	46 (88%)	6 (12%)	7	15
2	Q	53/52 (102%)	49 (92%)	4 (8%)	17	36
2	S	53/52 (102%)	47 (89%)	6 (11%)	7	15
2	U	52/52 (100%)	48 (92%)	4 (8%)	16	34
2	W	52/52 (100%)	48 (92%)	4 (8%)	16	34
3	E	52/52 (100%)	48 (92%)	4 (8%)	16	34
3	O	53/52 (102%)	47 (89%)	6 (11%)	7	15
3	Y	52/52 (100%)	48 (92%)	4 (8%)	16	34
All	All	1464/1458 (100%)	1356 (93%)	108 (7%)	18	36

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	336	GLU
1	0	353	GLN
2	1	760	ASN
2	1	777	THR
2	1	781	LEU
2	1	791	LYS
2	3	752	MET
2	3	758	ASN
2	3	760	ASN
2	3	767	GLU
2	3	777	THR
2	3	781	LEU
2	3	791	LYS
1	4	336	GLU
1	4	353	GLN
2	5	760	ASN
2	5	781	LEU
2	5	791	LYS
1	6	336	GLU
1	6	353	GLN
2	7	760	ASN
2	7	767	GLU
2	7	777	THR

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Mol	Chain	Res	Type
2	7	781	LEU
1	8	353	GLN
2	9	760	ASN
2	9	767	GLU
2	9	777	THR
2	9	781	LEU
2	9	791	LYS
2	A	758	ASN
2	A	760	ASN
2	A	777	THR
2	A	781	LEU
2	A	791	LYS
2	C	777	THR
2	C	781	LEU
2	C	791	LYS
2	C	792	GLU
3	E	758	ASN
3	E	776	ARG
3	E	781	LEU
3	E	791	LYS
1	F	336	GLU
1	F	353	GLN
2	G	760	ASN
2	G	767	GLU
2	G	777	THR
2	G	781	LEU
2	G	791	LYS
1	H	336	GLU
2	I	760	ASN
2	I	767	GLU
2	I	781	LEU
2	I	791	LYS
1	J	336	GLU
2	K	760	ASN
2	K	767	GLU
2	K	781	LEU
2	K	791	LYS
2	M	760	ASN
2	M	767	GLU
2	M	768	SER
2	M	781	LEU
2	M	791	LYS

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Mol	Chain	Res	Type
2	M	793	VAL
1	N	336[A]	GLU
1	N	336[B]	GLU
1	N	353	GLN
3	O	760	ASN
3	O	767	GLU
3	O	777	THR
3	O	781	LEU
3	O	791	LYS
3	O	793	VAL
1	P	336	GLU
1	P	353	GLN
2	Q	760	ASN
2	Q	767	GLU
2	Q	781	LEU
2	Q	791	LYS
1	R	319	MET
1	R	336[A]	GLU
1	R	336[B]	GLU
2	S	760	ASN
2	S	767[A]	GLU
2	S	767[B]	GLU
2	S	781	LEU
2	S	791	LYS
2	S	793	VAL
1	T	336	GLU
1	T	353	GLN
2	U	760	ASN
2	U	777	THR
2	U	781	LEU
2	U	791	LYS
1	V	336	GLU
1	V	353	GLN
2	W	767	GLU
2	W	781	LEU
2	W	791	LYS
2	W	793	VAL
3	Y	777	THR
3	Y	781	LEU
3	Y	791	LYS
3	Y	792	GLU
1	Z	319	MET

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Mol	Chain	Res	Type
1	Z	353	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	353	GLN
1	4	353	GLN
2	A	758	ASN
2	A	760	ASN
3	E	758	ASN
1	F	342	GLN
1	F	344	GLN
2	G	754	HIS
1	H	353	GLN
1	L	322	HIS
1	R	342	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 36 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	36/37 (97%)	0.17	0 100 100	30, 43, 66, 78	0
1	2	37/37 (100%)	1.22	6 (16%) 3 2	41, 60, 84, 107	0
1	4	36/37 (97%)	0.31	1 (2%) 56 55	30, 45, 67, 82	0
1	6	37/37 (100%)	0.41	1 (2%) 58 57	28, 42, 66, 73	0
1	8	37/37 (100%)	1.28	9 (24%) 1 1	40, 54, 73, 90	0
1	B	37/37 (100%)	0.16	0 100 100	25, 40, 62, 84	0
1	D	37/37 (100%)	0.35	1 (2%) 58 57	27, 42, 64, 86	0
1	F	36/37 (97%)	0.17	0 100 100	18, 27, 51, 71	0
1	H	36/37 (97%)	0.34	1 (2%) 56 55	20, 33, 55, 63	0
1	J	36/37 (97%)	0.14	0 100 100	21, 37, 57, 72	0
1	L	36/37 (97%)	0.64	1 (2%) 56 55	31, 47, 73, 95	0
1	N	37/37 (100%)	0.13	0 100 100	21, 34, 55, 76	0
1	P	37/37 (100%)	0.24	0 100 100	24, 38, 68, 78	0
1	R	36/37 (97%)	0.30	0 100 100	31, 42, 66, 82	0
1	T	37/37 (100%)	0.95	4 (10%) 8 5	37, 64, 91, 95	0
1	V	37/37 (100%)	0.05	0 100 100	22, 36, 64, 74	0
1	X	37/37 (100%)	0.82	4 (10%) 8 5	31, 52, 79, 83	0
1	Z	37/37 (100%)	0.64	0 100 100	33, 42, 62, 82	0
2	1	62/62 (100%)	0.07	0 100 100	17, 30, 51, 101	0
2	3	62/62 (100%)	0.25	2 (3%) 51 50	25, 39, 59, 104	0
2	5	61/62 (98%)	-0.15	0 100 100	21, 33, 52, 61	0
2	7	61/62 (98%)	0.20	0 100 100	28, 41, 59, 77	0
2	9	62/62 (100%)	0.25	2 (3%) 51 50	24, 41, 60, 101	0
2	A	62/62 (100%)	0.00	2 (3%) 51 50	19, 32, 52, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	C	62/62 (100%)	0.19	1 (1%) 74 74	24, 37, 54, 98	0
2	G	62/62 (100%)	0.07	2 (3%) 51 50	19, 32, 49, 93	0
2	I	62/62 (100%)	0.12	1 (1%) 74 74	20, 33, 51, 97	0
2	K	62/62 (100%)	0.38	4 (6%) 22 20	26, 41, 58, 107	0
2	M	62/62 (100%)	0.01	1 (1%) 74 74	18, 30, 45, 90	0
2	Q	62/62 (100%)	0.03	1 (1%) 74 74	25, 39, 55, 93	0
2	S	62/62 (100%)	0.15	1 (1%) 74 74	21, 37, 60, 94	0
2	U	62/62 (100%)	0.01	2 (3%) 51 50	15, 28, 47, 103	0
2	W	62/62 (100%)	0.42	1 (1%) 74 74	27, 48, 72, 110	0
3	E	62/62 (100%)	0.09	2 (3%) 51 50	16, 27, 45, 86	0
3	O	62/62 (100%)	0.09	1 (1%) 74 74	25, 38, 56, 83	0
3	Y	62/62 (100%)	0.30	3 (4%) 34 32	26, 40, 61, 96	0
All	All	1773/1782 (99%)	0.26	54 (3%) 54 52	15, 39, 70, 110	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	804	SER	8.6
2	3	804	SER	7.5
2	G	804	SER	7.2
2	I	804	SER	5.7
1	2	353	GLN	4.9
2	K	804	SER	4.8
1	8	347	ILE	4.2
1	2	340	SER	4.1
2	Q	804	SER	3.9
2	9	804	SER	3.8
1	8	341	GLY	3.7
2	S	804	SER	3.7
3	E	804	SER	3.7
2	9	803	VAL	3.5
2	U	804	SER	3.5
3	O	804	SER	3.4
3	E	743	ALA	3.3
3	Y	759	ASP	3.3
1	8	340	SER	3.0
2	A	804	SER	3.0
1	T	347	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	Y	804	SER	2.9
1	X	331	ALA	2.9
1	8	345	THR	2.8
2	3	803	VAL	2.7
2	K	803	VAL	2.7
2	M	804	SER	2.7
1	T	340	SER	2.7
1	2	346	ILE	2.6
3	Y	743	ALA	2.5
2	U	743	GLY	2.5
1	2	339	LEU	2.4
1	X	339	LEU	2.4
2	K	752	MET	2.4
1	8	351	CYS	2.4
1	2	342	GLN	2.3
1	T	339	LEU	2.3
1	D	353	GLN	2.3
1	8	339	LEU	2.2
1	H	320	ALA	2.2
1	T	334	GLY	2.2
1	X	341	GLY	2.2
2	K	744	ALA	2.1
1	6	342	GLN	2.1
1	L	353	GLN	2.1
1	8	343	PHE	2.1
1	4	353	GLN	2.1
1	8	344	GLN	2.1
2	C	743	GLY	2.1
2	G	743	GLY	2.1
1	X	340[A]	SER	2.1
1	2	317	GLY	2.0
1	8	328	THR	2.0
2	A	743	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ZN	Y	805	1/1	0.98	0.18	0.04	39,39,39,39	0
4	ZN	K	806	1/1	0.97	0.16	-0.58	33,33,33,33	0
4	ZN	C	805	1/1	0.98	0.12	-1.14	33,33,33,33	0
4	ZN	O	805	1/1	0.98	0.06	-1.89	32,32,32,32	0
4	ZN	C	806	1/1	0.98	0.08	-2.06	38,38,38,38	0
4	ZN	Q	805	1/1	0.95	0.05	-2.12	40,40,40,40	0
4	ZN	7	806	1/1	0.95	0.12	-2.29	48,48,48,48	0
4	ZN	O	806	1/1	0.99	0.07	-2.30	31,31,31,31	0
4	ZN	A	806	1/1	0.97	0.06	-2.41	26,26,26,26	0
4	ZN	7	805	1/1	0.98	0.08	-2.53	31,31,31,31	0
4	ZN	Q	806	1/1	0.98	0.08	-2.69	35,35,35,35	0
4	ZN	I	805	1/1	0.98	0.07	-2.70	30,30,30,30	0
4	ZN	5	805	1/1	0.97	0.06	-2.72	32,32,32,32	0
4	ZN	E	806	1/1	0.98	0.05	-2.80	19,19,19,19	0
4	ZN	Y	806	1/1	0.98	0.10	-2.92	32,32,32,32	0
4	ZN	K	805	1/1	0.96	0.10	-2.96	44,44,44,44	0
4	ZN	5	806	1/1	0.97	0.05	-3.00	23,23,23,23	0
4	ZN	3	806	1/1	0.97	0.06	-3.07	31,31,31,31	0
4	ZN	9	805	1/1	0.98	0.07	-3.15	33,33,33,33	0
4	ZN	E	805	1/1	0.98	0.07	-3.40	28,28,28,28	0
4	ZN	G	806	1/1	0.97	0.05	-3.48	25,25,25,25	0
4	ZN	G	805	1/1	0.95	0.07	-3.53	35,35,35,35	0
4	ZN	1	805	1/1	0.97	0.04	-3.78	26,26,26,26	0
4	ZN	S	805	1/1	0.96	0.06	-3.83	30,30,30,30	0
4	ZN	M	805	1/1	0.96	0.05	-3.83	33,33,33,33	0
4	ZN	M	806	1/1	0.97	0.05	-3.85	27,27,27,27	0
4	ZN	U	806	1/1	0.99	0.05	-3.89	20,20,20,20	0
4	ZN	9	806	1/1	0.97	0.06	-4.44	34,34,34,34	0
4	ZN	1	806	1/1	0.99	0.04	-4.57	19,19,19,19	0
4	ZN	W	805	1/1	0.98	0.06	-5.38	39,39,39,39	0
4	ZN	A	805	1/1	0.98	0.07	-5.38	27,27,27,27	0
4	ZN	U	805	1/1	0.97	0.04	-5.95	26,26,26,26	0
4	ZN	W	806	1/1	0.93	0.10	-	50,50,50,50	0
4	ZN	I	806	1/1	0.97	0.07	-	31,31,31,31	0
4	ZN	S	806	1/1	0.98	0.05	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	3	805	1/1	0.94	0.07	-	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.