



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 06:12 AM EDT

PDB ID : 5JR9  
Title : Crystal structure of apo-NeC3PO  
Authors : Zhang, J.; Gan, J.  
Deposited on : 2016-05-06  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

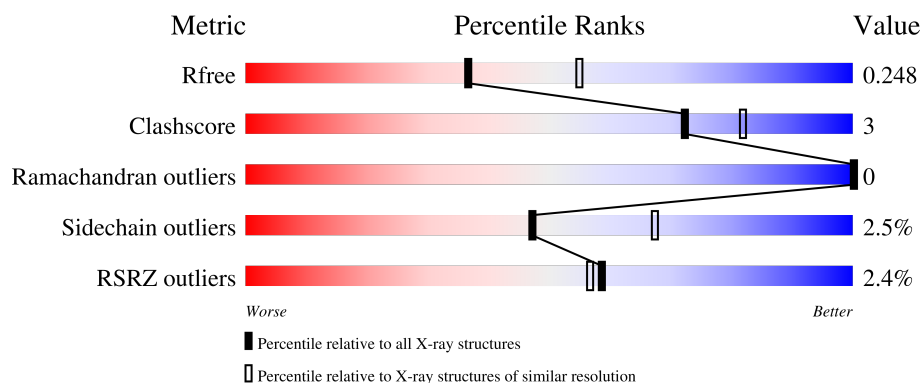
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	219	<div> <div>75%</div> <div>10%</div> <div>14%</div> </div>
2	B	218	<div> <div>74%</div> <div>11%</div> <div>15%</div> </div>
2	D	218	<div> <div>7%</div> <div>74%</div> <div>11%</div> <div>15%</div> </div>
2	E	218	<div> <div>73%</div> <div>12%</div> <div>15%</div> </div>
2	F	218	<div> <div>73%</div> <div>11%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	218	<div><div>%</div><div><div></div><div>79%</div><div>6%</div><div>15%</div></div></div>
2	H	218	<div><div>3%</div><div><div></div><div>75%</div><div>9%</div><div>15%</div></div></div>
3	C	219	<div><div>2%</div><div><div></div><div>77%</div><div>7%</div><div>16%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12286 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 NEQ131.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1548	1005	241	298	4			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP Q74ML9
A	-32	GLY	-	expression tag	UNP Q74ML9
A	-31	SER	-	expression tag	UNP Q74ML9
A	-30	SER	-	expression tag	UNP Q74ML9
A	-29	HIS	-	expression tag	UNP Q74ML9
A	-28	HIS	-	expression tag	UNP Q74ML9
A	-27	HIS	-	expression tag	UNP Q74ML9
A	-26	HIS	-	expression tag	UNP Q74ML9
A	-25	HIS	-	expression tag	UNP Q74ML9
A	-24	HIS	-	expression tag	UNP Q74ML9
A	-23	SER	-	expression tag	UNP Q74ML9
A	-22	SER	-	expression tag	UNP Q74ML9
A	-21	GLY	-	expression tag	UNP Q74ML9
A	-20	LEU	-	expression tag	UNP Q74ML9
A	-19	VAL	-	expression tag	UNP Q74ML9
A	-18	PRO	-	expression tag	UNP Q74ML9
A	-17	ARG	-	expression tag	UNP Q74ML9
A	-16	GLY	-	expression tag	UNP Q74ML9
A	-15	SER	-	expression tag	UNP Q74ML9
A	-14	HIS	-	expression tag	UNP Q74ML9
A	-13	MET	-	expression tag	UNP Q74ML9
A	-12	ALA	-	expression tag	UNP Q74ML9
A	-11	SER	-	expression tag	UNP Q74ML9
A	-10	MET	-	expression tag	UNP Q74ML9
A	-9	THR	-	expression tag	UNP Q74ML9
A	-8	GLY	-	expression tag	UNP Q74ML9
A	-7	GLY	-	expression tag	UNP Q74ML9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLN	-	expression tag	UNP Q74ML9
A	-5	GLN	-	expression tag	UNP Q74ML9
A	-4	MET	-	expression tag	UNP Q74ML9
A	-3	GLY	-	expression tag	UNP Q74ML9
A	-2	ARG	-	expression tag	UNP Q74ML9
A	-1	GLY	-	expression tag	UNP Q74ML9
A	0	SER	-	expression tag	UNP Q74ML9
A	185	ALA	-	expression tag	UNP Q74ML9

- Molecule 2 is a protein called NEQ131.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	0	0
			1534	997	239	294	4			
2	D	185	Total	C	N	O	S	0	0	0
			1488	967	226	291	4			
2	E	186	Total	C	N	O	S	0	0	0
			1543	1002	241	296	4			
2	F	185	Total	C	N	O	S	0	0	0
			1536	998	239	295	4			
2	G	186	Total	C	N	O	S	0	0	0
			1544	1003	241	296	4			
2	H	185	Total	C	N	O	S	0	0	0
			1515	986	234	291	4			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	MET	-	initiating methionine	UNP Q74ML9
B	-32	GLY	-	expression tag	UNP Q74ML9
B	-31	SER	-	expression tag	UNP Q74ML9
B	-30	SER	-	expression tag	UNP Q74ML9
B	-29	HIS	-	expression tag	UNP Q74ML9
B	-28	HIS	-	expression tag	UNP Q74ML9
B	-27	HIS	-	expression tag	UNP Q74ML9
B	-26	HIS	-	expression tag	UNP Q74ML9
B	-25	HIS	-	expression tag	UNP Q74ML9
B	-24	HIS	-	expression tag	UNP Q74ML9
B	-23	SER	-	expression tag	UNP Q74ML9
B	-22	SER	-	expression tag	UNP Q74ML9
B	-21	GLY	-	expression tag	UNP Q74ML9
B	-20	LEU	-	expression tag	UNP Q74ML9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	VAL	-	expression tag	UNP Q74ML9
B	-18	PRO	-	expression tag	UNP Q74ML9
B	-17	ARG	-	expression tag	UNP Q74ML9
B	-16	GLY	-	expression tag	UNP Q74ML9
B	-15	SER	-	expression tag	UNP Q74ML9
B	-14	HIS	-	expression tag	UNP Q74ML9
B	-13	MET	-	expression tag	UNP Q74ML9
B	-12	ALA	-	expression tag	UNP Q74ML9
B	-11	SER	-	expression tag	UNP Q74ML9
B	-10	MET	-	expression tag	UNP Q74ML9
B	-9	THR	-	expression tag	UNP Q74ML9
B	-8	GLY	-	expression tag	UNP Q74ML9
B	-7	GLY	-	expression tag	UNP Q74ML9
B	-6	GLN	-	expression tag	UNP Q74ML9
B	-5	GLN	-	expression tag	UNP Q74ML9
B	-4	MET	-	expression tag	UNP Q74ML9
B	-3	GLY	-	expression tag	UNP Q74ML9
B	-2	ARG	-	expression tag	UNP Q74ML9
B	-1	GLY	-	expression tag	UNP Q74ML9
B	0	SER	-	expression tag	UNP Q74ML9
D	-33	MET	-	initiating methionine	UNP Q74ML9
D	-32	GLY	-	expression tag	UNP Q74ML9
D	-31	SER	-	expression tag	UNP Q74ML9
D	-30	SER	-	expression tag	UNP Q74ML9
D	-29	HIS	-	expression tag	UNP Q74ML9
D	-28	HIS	-	expression tag	UNP Q74ML9
D	-27	HIS	-	expression tag	UNP Q74ML9
D	-26	HIS	-	expression tag	UNP Q74ML9
D	-25	HIS	-	expression tag	UNP Q74ML9
D	-24	HIS	-	expression tag	UNP Q74ML9
D	-23	SER	-	expression tag	UNP Q74ML9
D	-22	SER	-	expression tag	UNP Q74ML9
D	-21	GLY	-	expression tag	UNP Q74ML9
D	-20	LEU	-	expression tag	UNP Q74ML9
D	-19	VAL	-	expression tag	UNP Q74ML9
D	-18	PRO	-	expression tag	UNP Q74ML9
D	-17	ARG	-	expression tag	UNP Q74ML9
D	-16	GLY	-	expression tag	UNP Q74ML9
D	-15	SER	-	expression tag	UNP Q74ML9
D	-14	HIS	-	expression tag	UNP Q74ML9
D	-13	MET	-	expression tag	UNP Q74ML9
D	-12	ALA	-	expression tag	UNP Q74ML9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	SER	-	expression tag	UNP Q74ML9
D	-10	MET	-	expression tag	UNP Q74ML9
D	-9	THR	-	expression tag	UNP Q74ML9
D	-8	GLY	-	expression tag	UNP Q74ML9
D	-7	GLY	-	expression tag	UNP Q74ML9
D	-6	GLN	-	expression tag	UNP Q74ML9
D	-5	GLN	-	expression tag	UNP Q74ML9
D	-4	MET	-	expression tag	UNP Q74ML9
D	-3	GLY	-	expression tag	UNP Q74ML9
D	-2	ARG	-	expression tag	UNP Q74ML9
D	-1	GLY	-	expression tag	UNP Q74ML9
D	0	SER	-	expression tag	UNP Q74ML9
E	-33	MET	-	initiating methionine	UNP Q74ML9
E	-32	GLY	-	expression tag	UNP Q74ML9
E	-31	SER	-	expression tag	UNP Q74ML9
E	-30	SER	-	expression tag	UNP Q74ML9
E	-29	HIS	-	expression tag	UNP Q74ML9
E	-28	HIS	-	expression tag	UNP Q74ML9
E	-27	HIS	-	expression tag	UNP Q74ML9
E	-26	HIS	-	expression tag	UNP Q74ML9
E	-25	HIS	-	expression tag	UNP Q74ML9
E	-24	HIS	-	expression tag	UNP Q74ML9
E	-23	SER	-	expression tag	UNP Q74ML9
E	-22	SER	-	expression tag	UNP Q74ML9
E	-21	GLY	-	expression tag	UNP Q74ML9
E	-20	LEU	-	expression tag	UNP Q74ML9
E	-19	VAL	-	expression tag	UNP Q74ML9
E	-18	PRO	-	expression tag	UNP Q74ML9
E	-17	ARG	-	expression tag	UNP Q74ML9
E	-16	GLY	-	expression tag	UNP Q74ML9
E	-15	SER	-	expression tag	UNP Q74ML9
E	-14	HIS	-	expression tag	UNP Q74ML9
E	-13	MET	-	expression tag	UNP Q74ML9
E	-12	ALA	-	expression tag	UNP Q74ML9
E	-11	SER	-	expression tag	UNP Q74ML9
E	-10	MET	-	expression tag	UNP Q74ML9
E	-9	THR	-	expression tag	UNP Q74ML9
E	-8	GLY	-	expression tag	UNP Q74ML9
E	-7	GLY	-	expression tag	UNP Q74ML9
E	-6	GLN	-	expression tag	UNP Q74ML9
E	-5	GLN	-	expression tag	UNP Q74ML9
E	-4	MET	-	expression tag	UNP Q74ML9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q74ML9
E	-2	ARG	-	expression tag	UNP Q74ML9
E	-1	GLY	-	expression tag	UNP Q74ML9
E	0	SER	-	expression tag	UNP Q74ML9
F	-33	MET	-	initiating methionine	UNP Q74ML9
F	-32	GLY	-	expression tag	UNP Q74ML9
F	-31	SER	-	expression tag	UNP Q74ML9
F	-30	SER	-	expression tag	UNP Q74ML9
F	-29	HIS	-	expression tag	UNP Q74ML9
F	-28	HIS	-	expression tag	UNP Q74ML9
F	-27	HIS	-	expression tag	UNP Q74ML9
F	-26	HIS	-	expression tag	UNP Q74ML9
F	-25	HIS	-	expression tag	UNP Q74ML9
F	-24	HIS	-	expression tag	UNP Q74ML9
F	-23	SER	-	expression tag	UNP Q74ML9
F	-22	SER	-	expression tag	UNP Q74ML9
F	-21	GLY	-	expression tag	UNP Q74ML9
F	-20	LEU	-	expression tag	UNP Q74ML9
F	-19	VAL	-	expression tag	UNP Q74ML9
F	-18	PRO	-	expression tag	UNP Q74ML9
F	-17	ARG	-	expression tag	UNP Q74ML9
F	-16	GLY	-	expression tag	UNP Q74ML9
F	-15	SER	-	expression tag	UNP Q74ML9
F	-14	HIS	-	expression tag	UNP Q74ML9
F	-13	MET	-	expression tag	UNP Q74ML9
F	-12	ALA	-	expression tag	UNP Q74ML9
F	-11	SER	-	expression tag	UNP Q74ML9
F	-10	MET	-	expression tag	UNP Q74ML9
F	-9	THR	-	expression tag	UNP Q74ML9
F	-8	GLY	-	expression tag	UNP Q74ML9
F	-7	GLY	-	expression tag	UNP Q74ML9
F	-6	GLN	-	expression tag	UNP Q74ML9
F	-5	GLN	-	expression tag	UNP Q74ML9
F	-4	MET	-	expression tag	UNP Q74ML9
F	-3	GLY	-	expression tag	UNP Q74ML9
F	-2	ARG	-	expression tag	UNP Q74ML9
F	-1	GLY	-	expression tag	UNP Q74ML9
F	0	SER	-	expression tag	UNP Q74ML9
G	-33	MET	-	initiating methionine	UNP Q74ML9
G	-32	GLY	-	expression tag	UNP Q74ML9
G	-31	SER	-	expression tag	UNP Q74ML9
G	-30	SER	-	expression tag	UNP Q74ML9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-29	HIS	-	expression tag	UNP Q74ML9
G	-28	HIS	-	expression tag	UNP Q74ML9
G	-27	HIS	-	expression tag	UNP Q74ML9
G	-26	HIS	-	expression tag	UNP Q74ML9
G	-25	HIS	-	expression tag	UNP Q74ML9
G	-24	HIS	-	expression tag	UNP Q74ML9
G	-23	SER	-	expression tag	UNP Q74ML9
G	-22	SER	-	expression tag	UNP Q74ML9
G	-21	GLY	-	expression tag	UNP Q74ML9
G	-20	LEU	-	expression tag	UNP Q74ML9
G	-19	VAL	-	expression tag	UNP Q74ML9
G	-18	PRO	-	expression tag	UNP Q74ML9
G	-17	ARG	-	expression tag	UNP Q74ML9
G	-16	GLY	-	expression tag	UNP Q74ML9
G	-15	SER	-	expression tag	UNP Q74ML9
G	-14	HIS	-	expression tag	UNP Q74ML9
G	-13	MET	-	expression tag	UNP Q74ML9
G	-12	ALA	-	expression tag	UNP Q74ML9
G	-11	SER	-	expression tag	UNP Q74ML9
G	-10	MET	-	expression tag	UNP Q74ML9
G	-9	THR	-	expression tag	UNP Q74ML9
G	-8	GLY	-	expression tag	UNP Q74ML9
G	-7	GLY	-	expression tag	UNP Q74ML9
G	-6	GLN	-	expression tag	UNP Q74ML9
G	-5	GLN	-	expression tag	UNP Q74ML9
G	-4	MET	-	expression tag	UNP Q74ML9
G	-3	GLY	-	expression tag	UNP Q74ML9
G	-2	ARG	-	expression tag	UNP Q74ML9
G	-1	GLY	-	expression tag	UNP Q74ML9
G	0	SER	-	expression tag	UNP Q74ML9
H	-33	MET	-	initiating methionine	UNP Q74ML9
H	-32	GLY	-	expression tag	UNP Q74ML9
H	-31	SER	-	expression tag	UNP Q74ML9
H	-30	SER	-	expression tag	UNP Q74ML9
H	-29	HIS	-	expression tag	UNP Q74ML9
H	-28	HIS	-	expression tag	UNP Q74ML9
H	-27	HIS	-	expression tag	UNP Q74ML9
H	-26	HIS	-	expression tag	UNP Q74ML9
H	-25	HIS	-	expression tag	UNP Q74ML9
H	-24	HIS	-	expression tag	UNP Q74ML9
H	-23	SER	-	expression tag	UNP Q74ML9
H	-22	SER	-	expression tag	UNP Q74ML9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-21	GLY	-	expression tag	UNP Q74ML9
H	-20	LEU	-	expression tag	UNP Q74ML9
H	-19	VAL	-	expression tag	UNP Q74ML9
H	-18	PRO	-	expression tag	UNP Q74ML9
H	-17	ARG	-	expression tag	UNP Q74ML9
H	-16	GLY	-	expression tag	UNP Q74ML9
H	-15	SER	-	expression tag	UNP Q74ML9
H	-14	HIS	-	expression tag	UNP Q74ML9
H	-13	MET	-	expression tag	UNP Q74ML9
H	-12	ALA	-	expression tag	UNP Q74ML9
H	-11	SER	-	expression tag	UNP Q74ML9
H	-10	MET	-	expression tag	UNP Q74ML9
H	-9	THR	-	expression tag	UNP Q74ML9
H	-8	GLY	-	expression tag	UNP Q74ML9
H	-7	GLY	-	expression tag	UNP Q74ML9
H	-6	GLN	-	expression tag	UNP Q74ML9
H	-5	GLN	-	expression tag	UNP Q74ML9
H	-4	MET	-	expression tag	UNP Q74ML9
H	-3	GLY	-	expression tag	UNP Q74ML9
H	-2	ARG	-	expression tag	UNP Q74ML9
H	-1	GLY	-	expression tag	UNP Q74ML9
H	0	SER	-	expression tag	UNP Q74ML9

- Molecule 3 is a protein called NEQ131.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	185	Total	C	N	O	S	0	0	0
			1526	992	235	295	4			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-33	MET	-	initiating methionine	UNP Q74ML9
C	-32	GLY	-	expression tag	UNP Q74ML9
C	-31	SER	-	expression tag	UNP Q74ML9
C	-30	SER	-	expression tag	UNP Q74ML9
C	-29	HIS	-	expression tag	UNP Q74ML9
C	-28	HIS	-	expression tag	UNP Q74ML9
C	-27	HIS	-	expression tag	UNP Q74ML9
C	-26	HIS	-	expression tag	UNP Q74ML9
C	-25	HIS	-	expression tag	UNP Q74ML9
C	-24	HIS	-	expression tag	UNP Q74ML9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	SER	-	expression tag	UNP Q74ML9
C	-22	SER	-	expression tag	UNP Q74ML9
C	-21	GLY	-	expression tag	UNP Q74ML9
C	-20	LEU	-	expression tag	UNP Q74ML9
C	-19	VAL	-	expression tag	UNP Q74ML9
C	-18	PRO	-	expression tag	UNP Q74ML9
C	-17	ARG	-	expression tag	UNP Q74ML9
C	-16	GLY	-	expression tag	UNP Q74ML9
C	-15	SER	-	expression tag	UNP Q74ML9
C	-14	HIS	-	expression tag	UNP Q74ML9
C	-13	MET	-	expression tag	UNP Q74ML9
C	-12	ALA	-	expression tag	UNP Q74ML9
C	-11	SER	-	expression tag	UNP Q74ML9
C	-10	MET	-	expression tag	UNP Q74ML9
C	-9	THR	-	expression tag	UNP Q74ML9
C	-8	GLY	-	expression tag	UNP Q74ML9
C	-7	GLY	-	expression tag	UNP Q74ML9
C	-6	GLN	-	expression tag	UNP Q74ML9
C	-5	GLN	-	expression tag	UNP Q74ML9
C	-4	MET	-	expression tag	UNP Q74ML9
C	-3	GLY	-	expression tag	UNP Q74ML9
C	-2	ARG	-	expression tag	UNP Q74ML9
C	-1	GLY	-	expression tag	UNP Q74ML9
C	0	SER	-	expression tag	UNP Q74ML9

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	6	Total O 6 6	0	0
4	C	4	Total O 4 4	0	0
4	D	1	Total O 1 1	0	0
4	E	12	Total O 12 12	0	0
4	F	7	Total O 7 7	0	0
4	G	7	Total O 7 7	0	0

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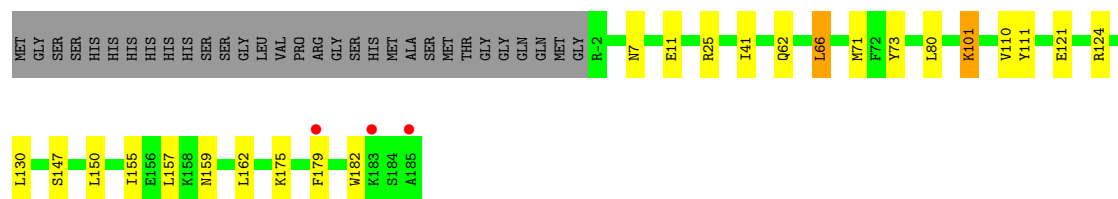
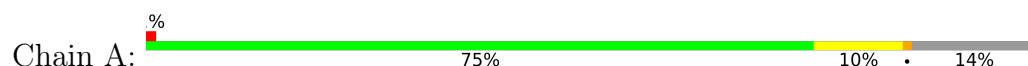
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total	O	0	0
			2	2		

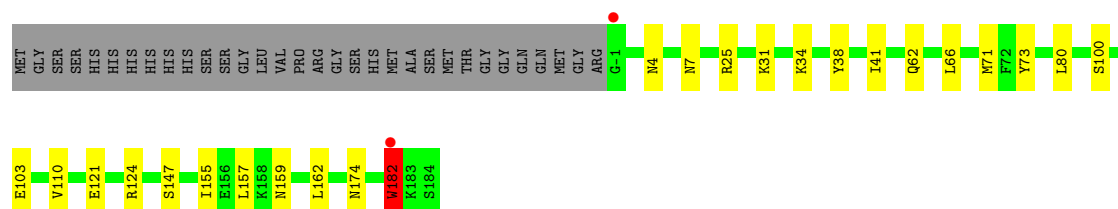
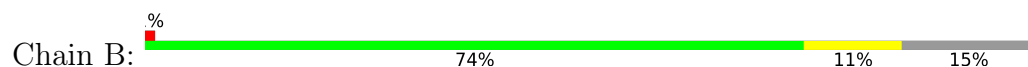
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

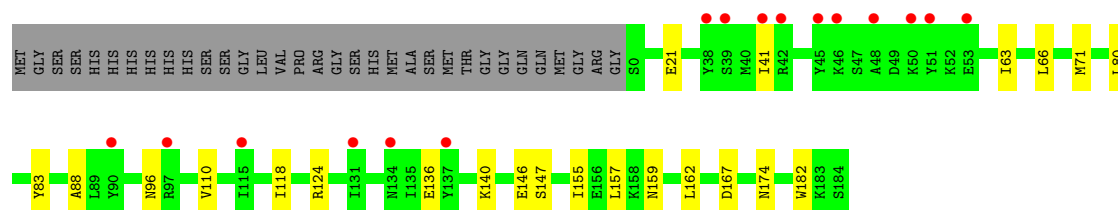
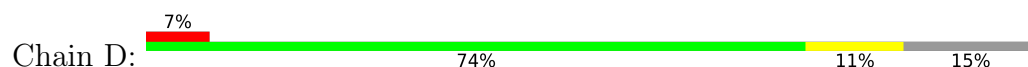
#### • Molecule 1: NEQ131



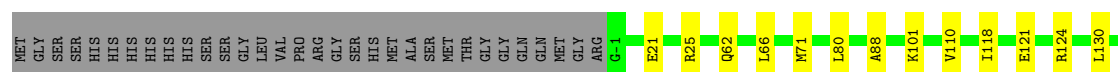
#### • Molecule 2: NEQ131



#### • Molecule 2: NEQ131



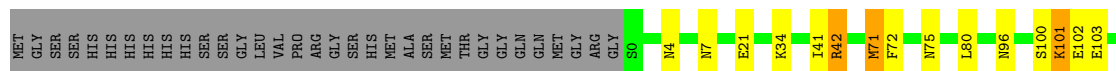
#### • Molecule 2: NEQ131





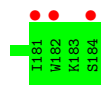
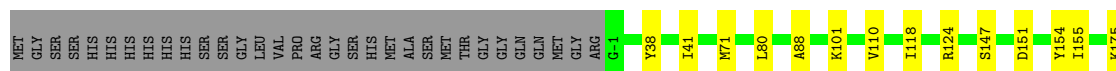
• Molecule 2: NEQ131

Chain F: 73% 11% 15%



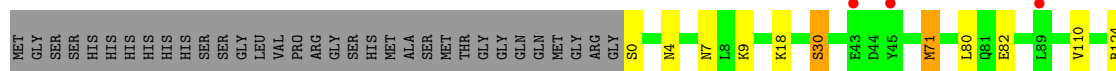
• Molecule 2: NEQ131

Chain G: 79% 6% 15%



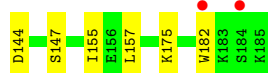
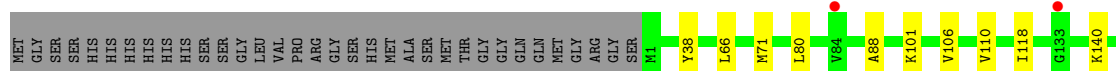
• Molecule 2: NEQ131

Chain H: 75% 9% 15%



• Molecule 3: NEQ131

Chain C: 77% 7% 16%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.44Å 92.71Å 92.75Å 114.29° 113.39° 95.76°	Depositor
Resolution (Å)	30.00 – 2.40 30.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-2.40) 95.2 (30.06-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.229 , 0.252 0.230 , 0.248	Depositor DCC
$R_{free}$ test set	4260 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.49	0/1574	0.67	2/2113 (0.1%)
2	B	0.50	0/1560	0.67	1/2096 (0.0%)
2	D	0.47	0/1514	0.71	4/2043 (0.2%)
2	E	0.50	1/1569 (0.1%)	0.67	3/2106 (0.1%)
2	F	0.49	1/1562 (0.1%)	0.68	2/2098 (0.1%)
2	G	0.47	0/1570	0.65	0/2107
2	H	0.49	0/1541	0.75	5/2074 (0.2%)
3	C	0.46	0/1552	0.64	1/2086 (0.0%)
All	All	0.48	2/12442 (0.0%)	0.68	18/16723 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	21	GLU	CD-OE2	-5.13	1.20	1.25
2	E	21	GLU	CD-OE2	-5.08	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	71	MET	CG-SD-CE	-9.52	84.98	100.20
2	H	71	MET	CG-SD-CE	-9.12	85.61	100.20
2	H	124	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	66	LEU	CA-CB-CG	7.48	132.51	115.30
2	E	140	LYS	CD-CE-NZ	6.22	126.02	111.70
1	A	66	LEU	CB-CG-CD1	-6.10	100.64	111.00
2	H	18	LYS	CD-CE-NZ	6.00	125.51	111.70
2	B	182	TRP	CA-CB-CG	-5.99	102.32	113.70
2	D	66	LEU	CA-CB-CG	5.93	128.94	115.30
2	H	140	LYS	CD-CE-NZ	5.92	125.31	111.70
2	D	136	GLU	CG-CD-OE1	-5.85	106.59	118.30
2	E	66	LEU	CA-CB-CG	5.82	128.70	115.30
3	C	66	LEU	CA-CB-CG	5.81	128.66	115.30
2	D	136	GLU	CG-CD-OE2	5.63	129.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	21	GLU	CB-CA-C	5.31	121.02	110.40
2	F	21	GLU	CB-CA-C	5.23	120.86	110.40
2	D	21	GLU	CB-CA-C	5.06	120.52	110.40
2	H	124	ARG	CD-NE-CZ	5.00	130.61	123.60

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	A	1548	0	1563	14	0
2	B	1534	0	1541	19	0
2	D	1488	0	1426	14	0
2	E	1543	0	1567	15	0
2	F	1536	0	1549	16	0
2	G	1544	0	1566	7	0
2	H	1515	0	1510	10	0
3	C	1526	0	1515	8	0
4	A	13	0	0	0	0
4	B	6	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	12	0	0	1	0
4	F	7	0	0	0	0
4	G	7	0	0	0	0
4	H	2	0	0	0	0
All	All	12286	0	12237	84	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 3.

All (84) 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:E:130:LEU:HD11	2:E:135:ILE:HD12	1.46	0.95
2:H:30:SER:OG	2:H:82:GLU:OE2	1.93	0.86
2:B:182:TRP:CD2	2:D:182:TRP:HZ3	2.03	0.77
2:B:182:TRP:CG	2:D:182:TRP:CZ3	2.84	0.65
2:E:130:LEU:HD11	2:E:135:ILE:CD1	2.27	0.62
2:F:96:ASN:OD1	2:F:140:LYS:NZ	2.32	0.62
1:A:7:ASN:OD1	1:A:11:GLU:OE2	2.19	0.60
1:A:182:TRP:CZ3	3:C:182:TRP:HD1	2.22	0.58
2:B:66:LEU:HG	2:B:73:TYR:HA	1.86	0.57
2:B:100:SER:OG	2:B:103:GLU:HG3	2.06	0.56
2:B:182:TRP:CD2	2:D:182:TRP:CZ3	2.90	0.55
2:B:31:LYS:O	2:B:31:LYS:HD2	2.07	0.55
2:B:182:TRP:CG	2:D:182:TRP:HZ3	2.23	0.54
2:D:96:ASN:OD1	2:D:140:LYS:NZ	2.42	0.53
2:F:42:ARG:CG	2:F:42:ARG:HH11	2.21	0.53
2:F:100:SER:OG	2:F:103:GLU:HG3	2.09	0.53
2:G:151:ASP:OD1	2:H:0:SER:HB2	2.07	0.53
2:E:25:ARG:HH11	2:E:62:GLN:NE2	2.08	0.52
2:B:25:ARG:NH1	2:B:62:GLN:OE1	2.43	0.51
2:F:101:LYS:HE2	2:F:102:GLU:OE2	2.10	0.51
1:A:25:ARG:NH1	1:A:62:GLN:OE1	2.43	0.50
3:C:140:LYS:NZ	3:C:144:ASP:OD2	2.44	0.50
1:A:182:TRP:CE3	3:C:182:TRP:CD1	2.99	0.50
1:A:66:LEU:HG	1:A:73:TYR:HA	1.94	0.49
2:E:135:ILE:HD11	2:E:180:ILE:HA	1.93	0.49
2:F:42:ARG:HH11	2:F:42:ARG:HG2	1.77	0.49
2:G:41:ILE:HD13	2:G:124:ARG:HG3	1.94	0.49
2:D:41:ILE:HD13	2:D:124:ARG:HG3	1.95	0.49
2:F:130:LEU:HB3	2:H:181:ILE:CD1	2.43	0.48
2:F:41:ILE:HD13	2:F:124:ARG:HG3	1.95	0.48
1:A:41:ILE:HD13	1:A:124:ARG:HG3	1.95	0.48
2:B:41:ILE:HD13	2:B:124:ARG:HG3	1.94	0.48
2:F:42:ARG:CG	2:F:42:ARG:NH1	2.74	0.48
1:A:101:LYS:HB3	1:A:111:TYR:CD1	2.49	0.47
2:B:182:TRP:CZ2	2:E:182:TRP:CD1	3.03	0.47
1:A:62:GLN:O	1:A:66:LEU:HD13	2.15	0.47
2:B:182:TRP:HZ2	2:E:182:TRP:CD1	2.32	0.47
2:E:25:ARG:NH1	2:E:62:GLN:NE2	2.64	0.46
2:F:124:ARG:HD3	2:H:174:ASN:ND2	2.31	0.46
1:A:155:ILE:HD11	1:A:157:LEU:HD21	1.98	0.45
3:C:155:ILE:HD11	3:C:157:LEU:HD21	1.98	0.45
2:H:159:ASN:HD22	2:H:162:LEU:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD11	3:C:38:TYR:CE1	2.52	0.45
1:A:80:LEU:HB3	1:A:110:VAL:HG11	1.99	0.45
2:E:155:ILE:HD11	2:E:157:LEU:HD21	1.99	0.45
2:B:38:TYR:OH	2:D:146:GLU:HB3	2.17	0.45
2:E:138:ALA:HB2	4:E:210:HOH:O	2.16	0.44
2:H:155:ILE:HD11	2:H:157:LEU:HD21	1.99	0.44
2:B:174:ASN:HD21	2:E:124:ARG:HD3	1.82	0.44
2:D:155:ILE:HD11	2:D:157:LEU:HD21	1.99	0.44
2:E:80:LEU:HB3	2:E:110:VAL:HG11	2.01	0.43
2:B:34:LYS:HE2	2:D:167:ASP:OD1	2.18	0.43
2:B:155:ILE:HD11	2:B:157:LEU:HD21	2.00	0.43
2:D:80:LEU:HB3	2:D:110:VAL:HG11	2.00	0.43
2:F:155:ILE:HD11	2:F:157:LEU:HD21	1.99	0.43
2:G:154:TYR:O	2:H:9:LYS:HE3	2.19	0.43
2:F:34:LYS:HE2	2:H:167:ASP:OD1	2.17	0.43
2:G:155:ILE:O	2:G:155:ILE:HG22	2.18	0.43
2:E:150:LEU:HD11	2:G:38:TYR:CE1	2.54	0.43
2:D:63:ILE:HG23	2:D:80:LEU:HD21	2.01	0.42
2:F:80:LEU:HB3	2:F:110:VAL:HG11	2.01	0.42
3:C:88:ALA:CB	3:C:118:ILE:HD12	2.49	0.42
1:A:101:LYS:HB3	1:A:111:TYR:CG	2.54	0.42
3:C:80:LEU:HB3	3:C:110:VAL:HG11	2.00	0.42
2:E:130:LEU:CD2	2:E:179:PHE:HB3	2.50	0.42
2:H:80:LEU:HB3	2:H:110:VAL:HG11	2.01	0.42
3:C:101:LYS:HG3	3:C:106:VAL:O	2.19	0.42
2:B:124:ARG:HD3	2:D:174:ASN:ND2	2.35	0.42
1:A:159:ASN:HD22	1:A:162:LEU:H	1.68	0.42
2:B:80:LEU:HB3	2:B:110:VAL:HG11	2.00	0.42
2:D:159:ASN:HD22	2:D:162:LEU:H	1.68	0.41
2:G:88:ALA:CB	2:G:118:ILE:HD12	2.50	0.41
2:E:88:ALA:CB	2:E:118:ILE:HD12	2.50	0.41
2:F:4:ASN:HB3	2:F:7:ASN:HB3	2.03	0.41
2:H:4:ASN:HB3	2:H:7:ASN:HB3	2.03	0.41
2:B:4:ASN:HB3	2:B:7:ASN:HB3	2.02	0.41
2:F:72:PHE:HA	2:F:75:ASN:HD22	1.86	0.41
2:D:88:ALA:CB	2:D:118:ILE:HD12	2.51	0.40
2:E:159:ASN:HD22	2:E:162:LEU:H	1.68	0.40
1:A:130:LEU:CD2	1:A:179:PHE:HB3	2.51	0.40
2:B:159:ASN:HD22	2:B:162:LEU:H	1.69	0.40
2:G:80:LEU:HB3	2:G:110:VAL:HG11	2.02	0.40
2:F:130:LEU:CD2	2:F:179:PHE:HB3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:159:ASN:HD22	2:F:162:LEU:H	1.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	186/219 (85%)	185 (100%)	1 (0%)	0	100	100
2	B	184/218 (84%)	183 (100%)	1 (0%)	0	100	100
2	D	183/218 (84%)	182 (100%)	1 (0%)	0	100	100
2	E	184/218 (84%)	183 (100%)	1 (0%)	0	100	100
2	F	183/218 (84%)	182 (100%)	1 (0%)	0	100	100
2	G	184/218 (84%)	183 (100%)	1 (0%)	0	100	100
2	H	183/218 (84%)	182 (100%)	1 (0%)	0	100	100
3	C	183/219 (84%)	182 (100%)	1 (0%)	0	100	100
All	All	1470/1746 (84%)	1462 (100%)	8 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/196 (85%)	161 (97%)	5 (3%)	41	61
2	B	163/196 (83%)	159 (98%)	4 (2%)	47	67
2	D	150/196 (76%)	147 (98%)	3 (2%)	55	74
2	E	168/196 (86%)	163 (97%)	5 (3%)	41	61
2	F	165/196 (84%)	160 (97%)	5 (3%)	41	61
2	G	167/196 (85%)	163 (98%)	4 (2%)	49	68
2	H	160/196 (82%)	156 (98%)	4 (2%)	47	67
3	C	160/197 (81%)	157 (98%)	3 (2%)	57	75
All	All	1299/1569 (83%)	1266 (98%)	33 (2%)	47	67

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	MET
1	A	101	LYS
1	A	121	GLU
1	A	147	SER
1	A	175	LYS
2	B	71	MET
2	B	121	GLU
2	B	147	SER
2	B	182	TRP
3	C	71	MET
3	C	147	SER
3	C	175	LYS
2	D	71	MET
2	D	83	TYR
2	D	147	SER
2	E	71	MET
2	E	101	LYS
2	E	121	GLU
2	E	147	SER
2	E	175	LYS
2	F	42	ARG
2	F	71	MET
2	F	101	LYS
2	F	147	SER
2	F	175	LYS
2	G	71	MET
2	G	101	LYS

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Mol	Chain	Res	Type
2	G	147	SER
2	G	175	LYS
2	H	30	SER
2	H	71	MET
2	H	147	SER
2	H	175	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	159	ASN
1	A	174	ASN
2	B	75	ASN
2	B	159	ASN
2	B	174	ASN
3	C	75	ASN
3	C	159	ASN
2	D	75	ASN
2	D	159	ASN
2	D	174	ASN
2	E	62	GLN
2	E	75	ASN
2	E	159	ASN
2	F	75	ASN
2	F	159	ASN
2	F	174	ASN
2	G	75	ASN
2	G	159	ASN
2	G	174	ASN
2	H	75	ASN
2	H	159	ASN
2	H	174	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	188/219 (85%)	-0.39	3 (1%) 72 70	37, 54, 90, 116	0
2	B	186/218 (85%)	-0.35	2 (1%) 80 79	41, 59, 85, 110	0
2	D	185/218 (84%)	0.33	16 (8%) 10 9	56, 88, 129, 144	0
2	E	186/218 (85%)	-0.38	1 (0%) 91 89	39, 56, 83, 109	0
2	F	185/218 (84%)	-0.37	0 100 100	38, 57, 79, 95	0
2	G	186/218 (85%)	-0.37	3 (1%) 72 70	41, 59, 86, 109	0
2	H	185/218 (84%)	-0.19	6 (3%) 47 46	41, 63, 101, 151	0
3	C	185/219 (84%)	-0.24	4 (2%) 62 60	42, 64, 101, 131	0
All	All	1486/1746 (85%)	-0.25	35 (2%) 59 57	37, 61, 102, 151	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	46	LYS	6.5
2	D	48	ALA	6.5
2	H	45	TYR	5.2
2	G	182	TRP	4.8
2	H	43	GLU	4.8
1	A	185	ALA	4.7
3	C	184	SER	3.8
2	D	41	ILE	3.4
2	D	45	TYR	3.3
2	D	38	TYR	3.3
2	D	50	LYS	3.3
2	H	131	ILE	3.2
2	D	134	ASN	3.0
2	H	135	ILE	3.0
2	D	115	ILE	2.9
2	E	179	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	89	LEU	2.7
2	B	-1	GLY	2.7
1	A	183	LYS	2.7
2	D	42	ARG	2.7
2	D	137	TYR	2.6
2	B	182	TRP	2.6
2	G	184	SER	2.5
2	D	90	TYR	2.5
3	C	133	GLY	2.5
1	A	179	PHE	2.4
2	D	131	ILE	2.3
2	D	39	SER	2.2
3	C	84	VAL	2.2
2	H	134	ASN	2.2
2	D	97	ARG	2.2
2	G	181	ILE	2.2
3	C	182	TRP	2.1
2	D	51	TYR	2.0
2	D	53	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.