



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 06:30 AM UTC

PDB ID : 6ZWK / pdb_00006zwk
Title : Crystal structure of the phosphorylated C-terminal tail of histone H2AX in complex with a specific nanobody (C6 gammaXbody)
Authors : McEwen, A.G.; Moeglin, E.; Desplancq, D.; Weiss, E.; Poterszman, A.
Deposited on : 2020-07-28
Resolution : 1.55 Å(reported)

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

We welcome your comments at 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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

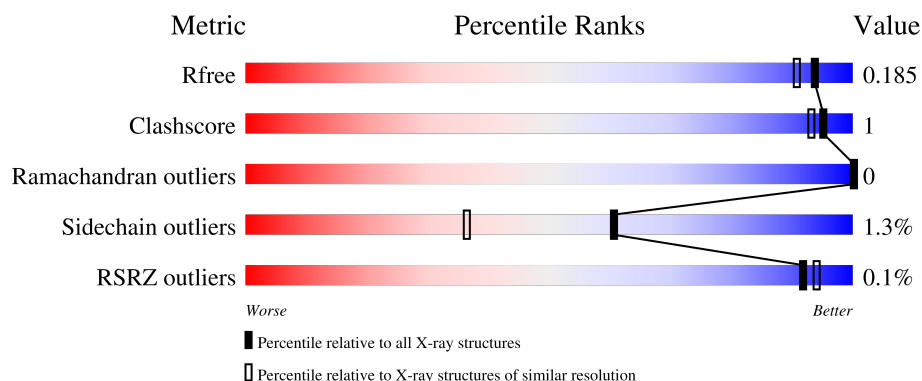
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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.



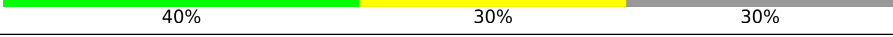
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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 ≥ 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	150	
1	B	150	
1	C	150	
1	D	150	
1	E	150	

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Mol	Chain	Length	Quality of chain
1	F	150	
2	G	10	
2	H	10	
2	I	10	
2	J	10	
2	K	10	
2	L	10	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14070 atoms, of which 6449 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 gammaXbody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	127	Total	C	H	N	O	S	0	7	0
			2041	635	1018	187	197	4			
1	B	127	Total	C	H	N	O	S	0	6	1
			2004	628	992	180	200	4			
1	C	128	Total	C	H	N	O	S	0	15	0
			2111	661	1040	193	213	4			
1	D	127	Total	C	H	N	O	S	0	13	0
			2141	664	1076	194	203	4			
1	E	129	Total	C	H	N	O	S	0	9	1
			2055	643	1018	187	203	4			
1	F	129	Total	C	H	N	O	S	0	10	0
			2089	651	1039	189	206	4			

- Molecule 2 is a protein called Histone H2AX.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	6	Total	C	H	N	O	P	0	1	0
			95	31	40	7	16	1			
2	H	7	Total	C	H	N	O	P	0	1	0
			115	37	49	10	18	1			
2	I	6	Total	C	H	N	O	P	0	1	0
			95	31	40	7	16	1			
2	J	7	Total	C	H	N	O	P	0	0	0
			101	33	41	9	17	1			
2	K	7	Total	C	H	N	O	P	0	1	0
			115	37	49	10	18	1			
2	L	6	Total	C	H	N	O	P	0	1	0
			108	34	47	9	17	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	133	CYS	LYS	engineered mutation	UNP P16104

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Chain	Residue	Modelled	Actual	Comment	Reference
H	133	CYS	LYS	engineered mutation	UNP P16104
I	133	CYS	LYS	engineered mutation	UNP P16104
J	133	CYS	LYS	engineered mutation	UNP P16104
K	133	CYS	LYS	engineered mutation	UNP P16104
L	133	CYS	LYS	engineered mutation	UNP P16104

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	2	Total Na 2 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

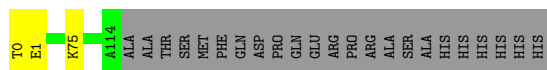
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	149	Total O 151 151	0	4
5	B	145	Total O 146 146	0	4
5	C	153	Total O 156 156	0	6
5	D	149	Total O 150 150	0	7
5	E	167	Total O 169 169	0	7

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	151	Total 154	O 154	0	9
5	G	11	Total 11	O 11	0	0
5	H	12	Total 12	O 12	0	0
5	I	11	Total 11	O 11	0	0
5	J	11	Total 11	O 11	0	0
5	K	9	Total 9	O 9	0	0
5	L	12	Total 12	O 12	0	0

- Molecule 1: gammaXbody



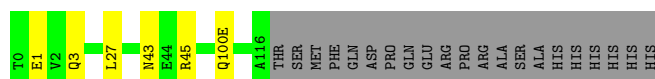
- | | | | | | | |
|----|----|-----|------|-----|------|------|
| TO | Q3 | R66 | Q82A | S99 | E101 | A114 | ALA | THR | SER | MET | PHE | GLN | ASP | PRO | GLN | GLU | ARG | PRO | ARG | ALA | SER | ALA | ALA | HIS | HIS | HIS | HIS | HIS | HIS |
|----|----|-----|------|-----|------|------|

- | | | | | | |
|----|-----|-----|-----|------|------|
| TO | Q13 | D16 | L27 | E101 | A115 | ALA | THR | SER | MET | PHE | GLN | ASP | PRO | PRO | GLU | ARG | PRO | ARG | ALA | SER | ALA | HIS | HIS | HIS | HIS | HIS |
|----|-----|-----|-----|------|------|

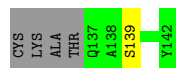
- | Position | Residue | Score |
|----------|---------|-------|
| TO | ALA | 0.00 |
| V12 | ALA | 0.00 |
| L18 | ALA | 0.00 |
| R31 | ALA | 0.00 |
| Y96 | ALA | 0.00 |
| S113 | ALA | 0.00 |
| A114 | ALA | 0.00 |
| ALA | ALA | 0.00 |
| THR | THR | 0.00 |
| SER | SER | 0.00 |
| MET | MET | 0.00 |
| PHE | PHE | 0.00 |
| GLN | GLN | 0.00 |
| ASP | ASP | 0.00 |
| PRO | PRO | 0.00 |
| GLN | GLN | 0.00 |
| GLU | GLU | 0.00 |
| ARG | ARG | 0.00 |
| PRO | PRO | 0.00 |
| ARG | ARG | 0.00 |
| ALA | ALA | 0.00 |
| SER | SER | 0.00 |
| ALA | ALA | 0.00 |
| HIS | HIS | 0.00 |
| HIS | HIS | 0.00 |
| HIS | HIS | 0.00 |
| HIS | HIS | 0.00 |
| HIS | HIS | 0.00 |

- | | | | | | | | | | | | | |
|----|--|--|-----|--|-----|--|------|--|-----|--|------|------|
| T0 | | | R31 | | R66 | | Q82A | | Y96 | | E101 | A116 | THR | SER | MET | PHE | GLN | ASP | PRO | GLN | GLU | ARG | PRO | ARG | ALA | SER | ALA | HIS | HIS | HIS | HIS | HIS | HIS |
|----|--|--|-----|--|-----|--|------|--|-----|--|------|------|

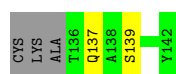
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



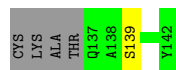
● Molecule 2: Histone H2AX



● Molecule 2: Histone H2AX



● Molecule 2: Histone H2AX



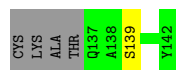
● Molecule 2: Histone H2AX



● Molecule 2: Histone H2AX



● Molecule 2: Histone H2AX



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	87.41Å 87.41Å 105.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.49 – 1.55 61.49 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.49-1.55) 99.9 (61.49-1.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.55Å)	Xtriage
Refinement program	PHENIX dev_3915	Depositor
R, R_{free}	0.149 , 0.184 0.150 , 0.185	Depositor DCC
R_{free} test set	6418 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.034 for h,-h-k,-l 0.145 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	14070	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 40.56 % 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 2.6886e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SEP, NA

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	0.25	0/1061	0.49	0/1431
1	B	0.25	0/1047	0.51	0/1415
1	C	0.23	0/1120	0.47	0/1514
1	D	0.25	0/1121	0.48	0/1511
1	E	0.24	0/1081	0.50	0/1461
1	F	0.26	0/1097	0.53	0/1481
2	G	0.17	0/47	0.33	0/59
2	H	0.20	0/58	0.37	0/74
2	I	0.19	0/47	0.28	0/59
2	J	0.18	0/49	0.49	0/62
2	K	0.20	0/58	0.35	0/74
2	L	0.25	0/53	0.40	0/67
All	All	0.25	0/6839	0.49	0/9208

There are no bond length outliers.

There are no bond angle outliers.

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	1023	1018	1018	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1012	992	992	2	0
1	C	1071	1040	1029	1	0
1	D	1065	1076	1076	4	0
1	E	1037	1018	1020	2	0
1	F	1050	1039	1039	2	0
2	G	55	40	40	0	0
2	H	66	49	49	1	0
2	I	55	40	40	0	0
2	J	60	41	41	1	0
2	K	66	49	49	1	0
2	L	61	47	47	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
4	D	1	0	0	0	0
5	A	151	0	0	1	0
5	B	146	0	0	1	0
5	C	156	0	0	0	0
5	D	150	0	0	2	0
5	E	169	0	0	0	0
5	F	154	0	0	1	0
5	G	11	0	0	0	0
5	H	12	0	0	1	0
5	I	11	0	0	0	0
5	J	11	0	0	0	0
5	K	9	0	0	0	0
5	L	12	0	0	0	0
All	All	7621	6449	6440	16	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 1.

The worst 5 of 16 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:D:31[B]:ARG:NH2	1:D:96:TYR:OH	2.21	0.74
1:F:43:ASN:OD1	5:F:301[A]:HOH:O	2.08	0.70
1:E:31[B]:ARG:NH2	1:E:96:TYR:OH	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:GLN:NE2	5:H:201:HOH:O	2.34	0.59
1:A:75[B]:LYS:NZ	5:A:302:HOH:O	2.23	0.58

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	132/150 (88%)	131 (99%)	1 (1%)	0	100	100
1	B	131/150 (87%)	130 (99%)	1 (1%)	0	100	100
1	C	141/150 (94%)	140 (99%)	1 (1%)	0	100	100
1	D	138/150 (92%)	137 (99%)	1 (1%)	0	100	100
1	E	136/150 (91%)	135 (99%)	1 (1%)	0	100	100
1	F	137/150 (91%)	136 (99%)	1 (1%)	0	100	100
2	G	4/10 (40%)	4 (100%)	0	0	100	100
2	H	5/10 (50%)	5 (100%)	0	0	100	100
2	I	4/10 (40%)	4 (100%)	0	0	100	100
2	J	4/10 (40%)	3 (75%)	1 (25%)	0	100	100
2	K	5/10 (50%)	4 (80%)	1 (20%)	0	100	100
2	L	4/10 (40%)	4 (100%)	0	0	100	100
All	All	841/960 (88%)	833 (99%)	8 (1%)	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	A	108/120 (90%)	108 (100%)	0	100	100
1	B	107/120 (89%)	104 (97%)	3 (3%)	38	11
1	C	112/120 (93%)	109 (97%)	3 (3%)	39	12
1	D	114/120 (95%)	114 (100%)	0	100	100
1	E	109/120 (91%)	107 (98%)	2 (2%)	51	24
1	F	111/120 (92%)	107 (96%)	4 (4%)	31	6
2	G	4/7 (57%)	4 (100%)	0	100	100
2	H	5/7 (71%)	5 (100%)	0	100	100
2	I	4/7 (57%)	4 (100%)	0	100	100
2	J	4/7 (57%)	4 (100%)	0	100	100
2	K	5/7 (71%)	5 (100%)	0	100	100
2	L	5/7 (71%)	5 (100%)	0	100	100
All	All	688/762 (90%)	676 (98%)	12 (2%)	61	25

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	101[B]	GLU
1	F	1[A]	GLU
1	F	27	LEU
1	F	1[B]	GLU
1	C	27	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	76	ASN
1	F	81	GLN
1	F	82(A)	GLN
1	D	43	ASN

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Mol	Chain	Res	Type
1	D	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	SEP	G	139	2	8,9,10	1.50	1 (12%)	7,12,14	1.00	0
2	SEP	J	139	2	8,9,10	1.56	1 (12%)	7,12,14	1.08	0
2	SEP	I	139	2	8,9,10	1.58	1 (12%)	7,12,14	1.08	1 (14%)
2	SEP	L	139	2	8,9,10	1.57	1 (12%)	7,12,14	1.15	0
2	SEP	K	139	2	8,9,10	1.60	1 (12%)	7,12,14	0.79	0
2	SEP	H	139	2	8,9,10	1.58	1 (12%)	7,12,14	1.34	2 (28%)

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	SEP	G	139	2	-	1/6/8/10	-
2	SEP	J	139	2	-	1/6/8/10	-
2	SEP	I	139	2	-	1/6/8/10	-
2	SEP	L	139	2	-	1/6/8/10	-
2	SEP	K	139	2	-	1/6/8/10	-
2	SEP	H	139	2	-	1/6/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	139	SEP	P-O1P	3.54	1.61	1.50
2	I	139	SEP	P-O1P	3.48	1.61	1.50
2	L	139	SEP	P-O1P	3.48	1.61	1.50
2	H	139	SEP	P-O1P	3.44	1.61	1.50
2	J	139	SEP	P-O1P	3.43	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	139	SEP	OG-CB-CA	2.55	110.63	108.14
2	H	139	SEP	O3P-P-OG	2.16	112.31	106.67
2	I	139	SEP	O3P-P-OG	2.01	111.90	106.67

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	139	SEP	CA-CB-OG-P
2	H	139	SEP	CA-CB-OG-P
2	I	139	SEP	CA-CB-OG-P
2	J	139	SEP	CA-CB-OG-P
2	K	139	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [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	127/150 (84%)	-1.21	0	100	100	15, 30, 51, 70	7 (5%)
1	B	127/150 (84%)	-1.22	0	100	100	16, 31, 51, 66	6 (4%)
1	C	128/150 (85%)	-1.19	0	100	100	17, 28, 43, 78	13 (10%)
1	D	127/150 (84%)	-1.22	1 (0%)	82	87	17, 29, 54, 86	13 (10%)
1	E	129/150 (86%)	-1.20	0	100	100	16, 30, 51, 71	9 (6%)
1	F	129/150 (86%)	-1.22	0	100	100	16, 29, 54, 75	10 (7%)
2	G	5/10 (50%)	-0.86	0	100	100	22, 33, 48, 50	1 (20%)
2	H	6/10 (60%)	-0.72	0	100	100	21, 33, 74, 75	1 (16%)
2	I	5/10 (50%)	-0.93	0	100	100	23, 31, 50, 52	1 (20%)
2	J	6/10 (60%)	-0.58	0	100	100	36, 48, 77, 81	0
2	K	6/10 (60%)	-0.94	0	100	100	22, 32, 77, 78	1 (16%)
2	L	5/10 (50%)	-1.16	0	100	100	20, 28, 49, 70	1 (20%)
All	All	800/960 (83%)	-1.20	1 (0%)	92	94	15, 30, 55, 86	63 (7%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	ALA	2.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SEP	G	139	10/11	1.00	0.02	25,31,37,41	0
2	SEP	H	139	10/11	1.00	0.02	25,30,36,41	0
2	SEP	I	139	10/11	1.00	0.02	28,33,40,43	0
2	SEP	J	139	10/11	1.00	0.02	27,34,41,46	0
2	SEP	K	139	10/11	1.00	0.02	26,30,37,42	0
2	SEP	L	139	10/11	1.00	0.02	22,27,33,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	F	202	1/1	0.99	0.07	26,26,26,26	1
3	NA	B	201	1/1	1.00	0.02	37,37,37,37	0
3	NA	C	201	1/1	1.00	0.04	32,32,32,32	0
3	NA	D	201	1/1	1.00	0.01	33,33,33,33	0
3	NA	E	201	1/1	1.00	0.03	45,45,45,45	0
3	NA	F	201	1/1	1.00	0.02	32,32,32,32	0
3	NA	A	201	1/1	1.00	0.01	33,33,33,33	0
4	CL	D	202	1/1	1.00	0.06	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.