



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2025 – 08:06 AM EDT

PDB ID : 9NER
Title : cis-CaaD E114D mutant with a covalent acrylate intermediate of the hydration of acetylenecarboxylic acid
Authors : Silva, K.; Geiger, J.H.; Draths, K.
Deposited on : 2025-02-20
Resolution : 2.51 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

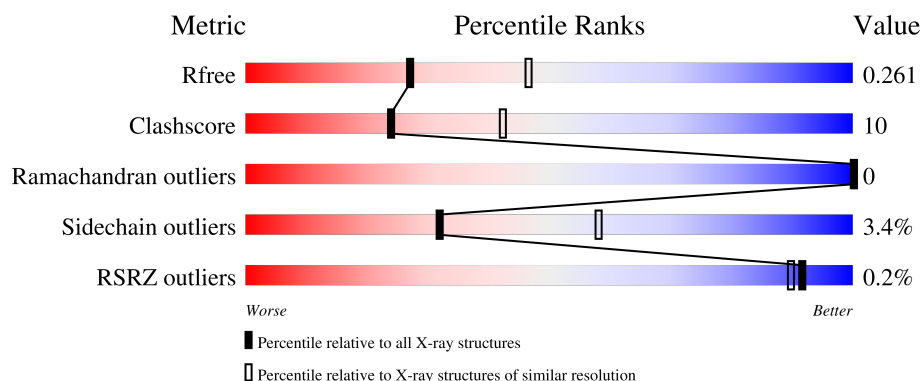
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.51 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	165	
1	B	165	
1	C	165	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A1BXY	C	201	-	-	X	-
3	AKR	B	201	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3534 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 Cis-3-chloroacrylic acid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1141	717	205	215	4			
1	B	145	Total	C	N	O	S	0	0	0
			1141	717	205	215	4			
1	C	145	Total	C	N	O	S	0	0	0
			1141	717	205	215	4			

There are 48 discrepancies between the modelled and reference sequences:

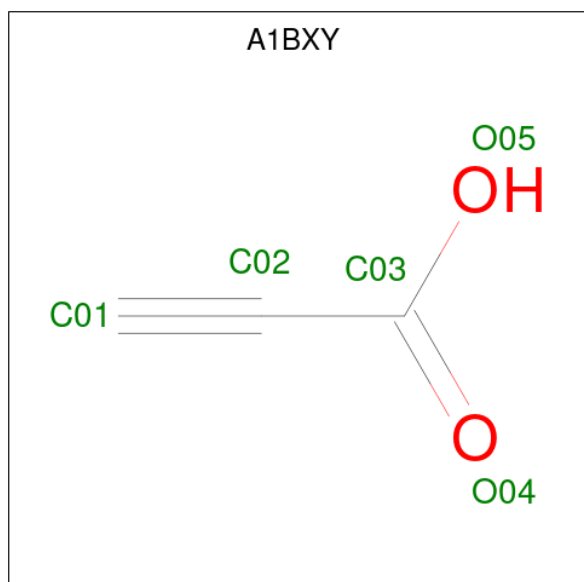
Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ASP	GLU	engineered mutation	UNP Q6VPE5
A	150	GLU	-	expression tag	UNP Q6VPE5
A	151	ASN	-	expression tag	UNP Q6VPE5
A	152	LEU	-	expression tag	UNP Q6VPE5
A	153	TYR	-	expression tag	UNP Q6VPE5
A	154	PHE	-	expression tag	UNP Q6VPE5
A	155	GLN	-	expression tag	UNP Q6VPE5
A	156	GLY	-	expression tag	UNP Q6VPE5
A	157	LEU	-	expression tag	UNP Q6VPE5
A	158	GLU	-	expression tag	UNP Q6VPE5
A	159	HIS	-	expression tag	UNP Q6VPE5
A	160	HIS	-	expression tag	UNP Q6VPE5
A	161	HIS	-	expression tag	UNP Q6VPE5
A	162	HIS	-	expression tag	UNP Q6VPE5
A	163	HIS	-	expression tag	UNP Q6VPE5
A	164	HIS	-	expression tag	UNP Q6VPE5
B	114	ASP	GLU	engineered mutation	UNP Q6VPE5
B	150	GLU	-	expression tag	UNP Q6VPE5
B	151	ASN	-	expression tag	UNP Q6VPE5
B	152	LEU	-	expression tag	UNP Q6VPE5
B	153	TYR	-	expression tag	UNP Q6VPE5
B	154	PHE	-	expression tag	UNP Q6VPE5
B	155	GLN	-	expression tag	UNP Q6VPE5

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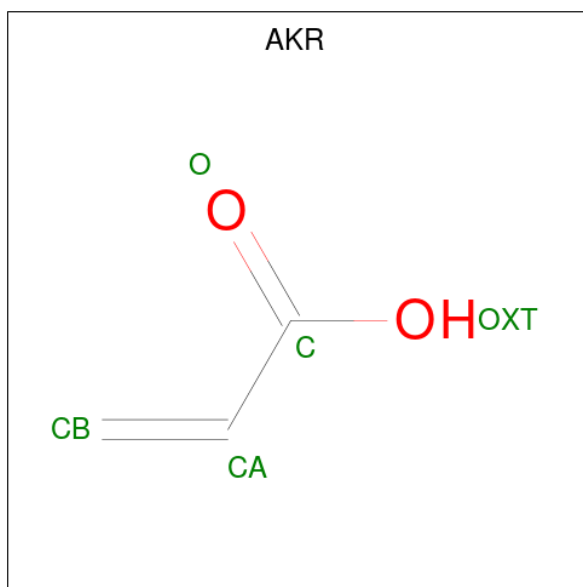
Chain	Residue	Modelled	Actual	Comment	Reference
B	156	GLY	-	expression tag	UNP Q6VPE5
B	157	LEU	-	expression tag	UNP Q6VPE5
B	158	GLU	-	expression tag	UNP Q6VPE5
B	159	HIS	-	expression tag	UNP Q6VPE5
B	160	HIS	-	expression tag	UNP Q6VPE5
B	161	HIS	-	expression tag	UNP Q6VPE5
B	162	HIS	-	expression tag	UNP Q6VPE5
B	163	HIS	-	expression tag	UNP Q6VPE5
B	164	HIS	-	expression tag	UNP Q6VPE5
C	114	ASP	GLU	engineered mutation	UNP Q6VPE5
C	150	GLU	-	expression tag	UNP Q6VPE5
C	151	ASN	-	expression tag	UNP Q6VPE5
C	152	LEU	-	expression tag	UNP Q6VPE5
C	153	TYR	-	expression tag	UNP Q6VPE5
C	154	PHE	-	expression tag	UNP Q6VPE5
C	155	GLN	-	expression tag	UNP Q6VPE5
C	156	GLY	-	expression tag	UNP Q6VPE5
C	157	LEU	-	expression tag	UNP Q6VPE5
C	158	GLU	-	expression tag	UNP Q6VPE5
C	159	HIS	-	expression tag	UNP Q6VPE5
C	160	HIS	-	expression tag	UNP Q6VPE5
C	161	HIS	-	expression tag	UNP Q6VPE5
C	162	HIS	-	expression tag	UNP Q6VPE5
C	163	HIS	-	expression tag	UNP Q6VPE5
C	164	HIS	-	expression tag	UNP Q6VPE5

- Molecule 2 is prop-2-ynoic acid (three-letter code: A1BXY) (formula: $C_3H_2O_2$).



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

- Molecule 3 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



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

- Molecule 4 is water.

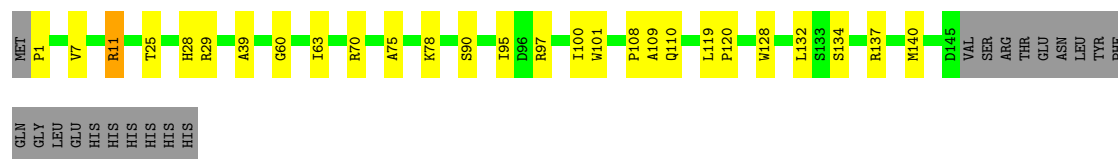
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	29	Total	O	0	0
			29	29		
4	C	32	Total	O	0	0
			32	32		

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.

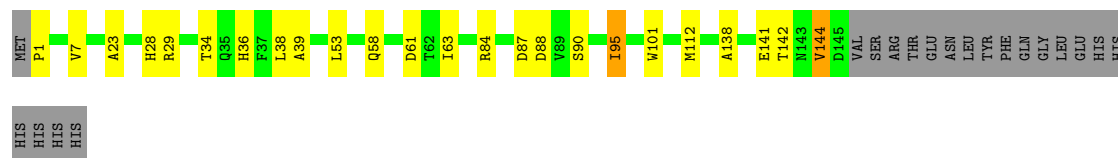
- Molecule 1: Cis-3-chloroacrylic acid dehalogenase

Chain A: 




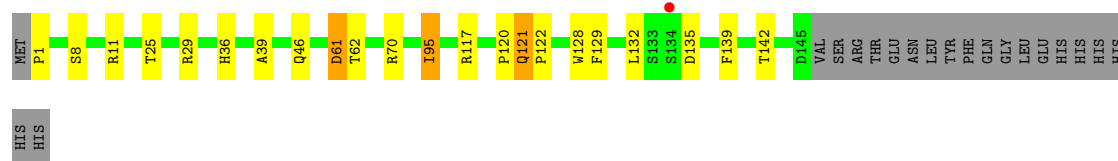
- Molecule 1: Cis-3-chloroacrylic acid dehalogenase

Chain B: 



- Molecule 1: Cis-3-chloroacrylic acid dehalogenase

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.26Å 98.83Å 142.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.60 – 2.51 35.60 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.7 (35.60-2.51) 95.0 (35.60-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.186 , 0.259 0.186 , 0.261	Depositor DCC
R_{free} test set	13476 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.039 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3534	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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: AKR, A1BXY

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	0.40	0/1169	0.56	0/1583
1	B	0.42	0/1169	0.60	0/1583
1	C	0.43	0/1169	0.61	0/1583
All	All	0.42	0/3507	0.59	0/4749

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	1141	0	1084	24	0
1	B	1141	0	1082	20	0
1	C	1141	0	1082	21	0
2	A	5	0	0	1	0
2	C	5	0	0	8	0
3	B	5	0	1	1	0
4	A	35	0	0	0	0
4	B	29	0	0	3	0
4	C	32	0	0	1	0
All	All	3534	0	3249	66	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 10.

The worst 5 of 66 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:B:112:MET:HE1	4:B:322:HOH:O	1.23	1.34
1:B:112:MET:CE	4:B:322:HOH:O	1.93	0.89
1:C:1:PRO:CA	2:C:201:A1BXY:C01	2.52	0.87
1:A:95:ILE:HD13	1:A:100:ILE:HD11	1.59	0.85
1:C:70:ARG:HG2	2:C:201:A1BXY:O04	1.78	0.83

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	143/165 (87%)	140 (98%)	3 (2%)	0	100	100
1	B	143/165 (87%)	141 (99%)	2 (1%)	0	100	100
1	C	143/165 (87%)	136 (95%)	7 (5%)	0	100	100
All	All	429/495 (87%)	417 (97%)	12 (3%)	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	118/137 (86%)	116 (98%)	2 (2%)	56	79
1	B	118/137 (86%)	114 (97%)	4 (3%)	32	58
1	C	118/137 (86%)	112 (95%)	6 (5%)	20	40
All	All	354/411 (86%)	342 (97%)	12 (3%)	32	58

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

Mol	Chain	Res	Type
1	C	62	THR
1	C	95	ILE
1	C	135	ASP
1	C	117	ARG
1	B	84	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	36	HIS
1	B	36	HIS
1	C	36	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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	A1BXY	A	201	-	4,4,4	2.20	1 (25%)	4,4,4	1.85	2 (50%)
2	A1BXY	C	201	-	4,4,4	1.66	1 (25%)	4,4,4	2.00	2 (50%)
3	AKR	B	201	1	4,4,4	2.94	3 (75%)	4,4,4	3.31	2 (50%)

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	A1BXY	A	201	-	-	0/0/2/2	-
2	A1BXY	C	201	-	-	0/0/2/2	-
3	AKR	B	201	1	-	1/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	AKR	CA-C	4.98	1.60	1.46
2	A	201	A1BXY	C02-C03	3.98	1.52	1.46
2	C	201	A1BXY	C02-C03	3.03	1.50	1.46
3	B	201	AKR	CB-CA	2.09	1.40	1.30
3	B	201	AKR	OXT-C	-2.07	1.25	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	AKR	OXT-C-O	-5.40	111.71	122.70
3	B	201	AKR	OXT-C-CA	3.60	123.99	114.19
2	C	201	A1BXY	O05-C03-C02	2.91	122.61	115.67
2	A	201	A1BXY	O05-C03-O04	-2.78	119.13	124.24
2	C	201	A1BXY	O05-C03-O04	-2.48	119.69	124.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	AKR	OXT-C-CA-CB

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	A1BXY	1	0
2	C	201	A1BXY	8	0
3	B	201	AKR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	145/165 (87%)	-0.26	0 100 100	24, 36, 58, 62	0
1	B	145/165 (87%)	-0.38	0 100 100	23, 34, 49, 59	0
1	C	145/165 (87%)	-0.26	1 (0%) 84 81	22, 32, 64, 70	0
All	All	435/495 (87%)	-0.30	1 (0%) 92 90	22, 34, 59, 70	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
3	AKR	B	201	5/5	0.55	0.23	35,38,40,46	0
2	A1BXY	C	201	5/5	0.79	0.15	35,36,45,47	0
2	A1BXY	A	201	5/5	0.87	0.17	25,31,41,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.