



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 09:24 AM EDT

PDB ID : 2ABR
Title : Structure of D280A arginine deiminase with L-arginine forming a S-alkylthiuronium reaction intermediate
Authors : Galkin, A.; Lu, X.; Dunaway-Mariano, D.; Herzberg, O.
Deposited on : 2005-07-15
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

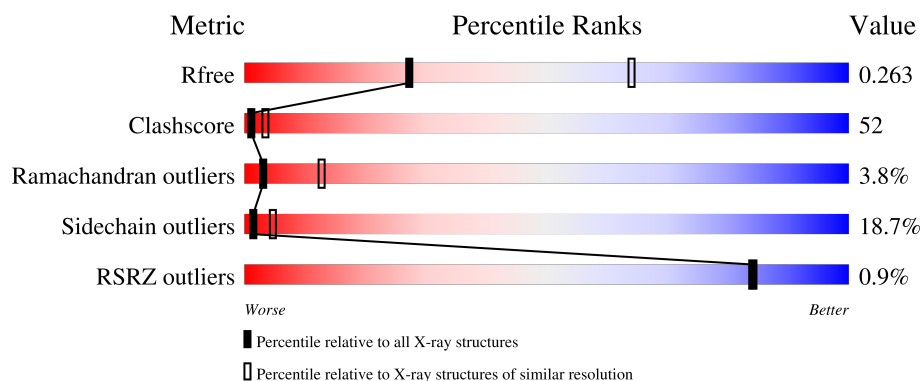
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	418	<div> <div>%</div> <div> <div></div> <div>30%</div> <div>52%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	418	<div> <div></div> <div> <div>32%</div> <div>50%</div> <div>15%</div> <div>•</div> </div> </div>
1	C	418	<div> <div>%</div> <div> <div></div> <div>31%</div> <div>50%</div> <div>14%</div> <div>••</div> </div> </div>
1	D	418	<div> <div>%</div> <div> <div></div> <div>33%</div> <div>49%</div> <div>15%</div> <div>•</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12637 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 Arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3151	1994	549	591	17			
1	B	406	Total	C	N	O	S	0	0	0
			3174	2008	553	596	17			
1	C	403	Total	C	N	O	S	0	0	0
			3158	1998	550	593	17			
1	D	402	Total	C	N	O	S	0	0	0
			3154	1996	552	589	17			

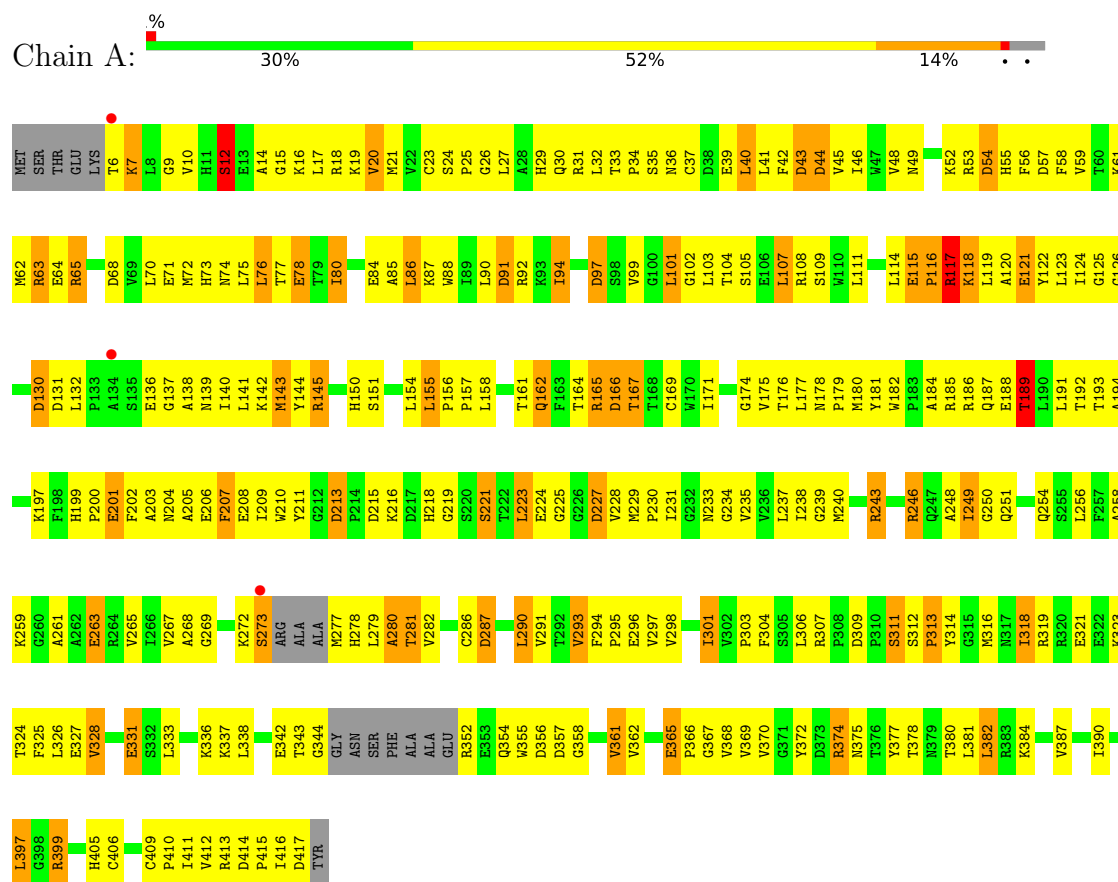
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ALA	ASP	engineered mutation	UNP P13981
A	406	CYR	CYS	modified residue	UNP P13981
B	280	ALA	ASP	engineered mutation	UNP P13981
B	406	CYR	CYS	modified residue	UNP P13981
C	280	ALA	ASP	engineered mutation	UNP P13981
C	406	CYR	CYS	modified residue	UNP P13981
D	280	ALA	ASP	engineered mutation	UNP P13981
D	406	CYR	CYS	modified residue	UNP P13981

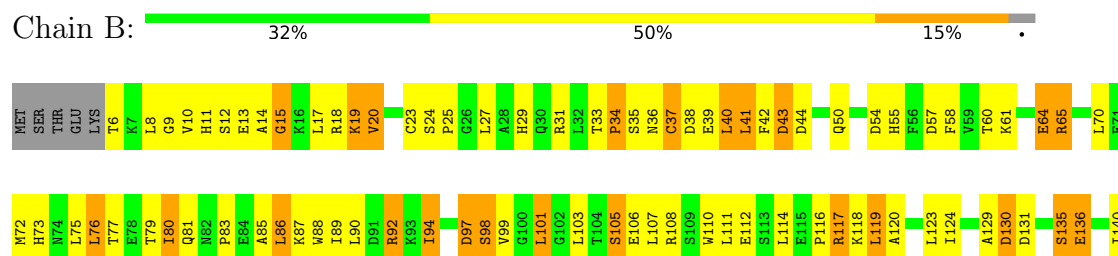
3 Residue-property plots [i](#)

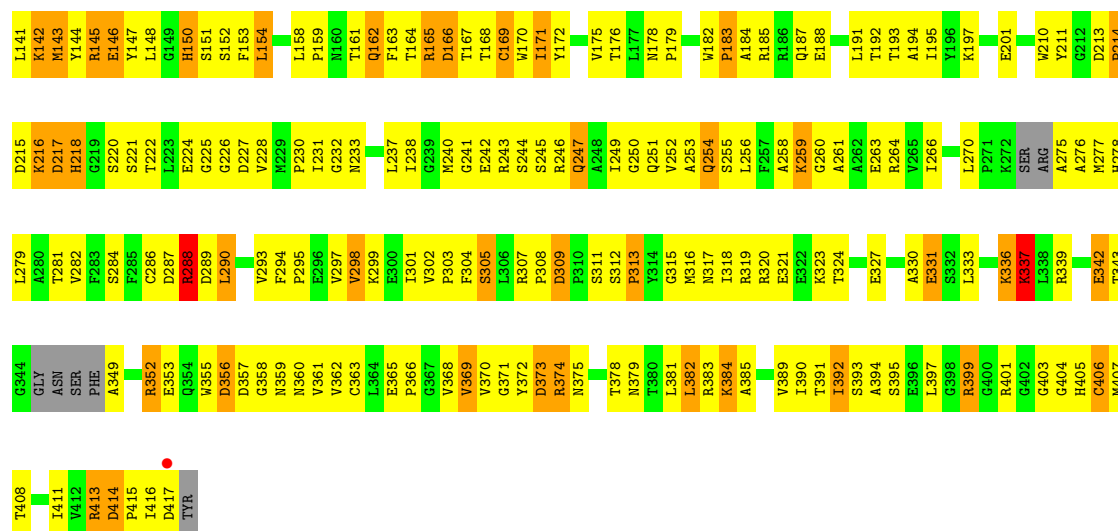
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Arginine deiminase



• Molecule 1: Arginine deiminase



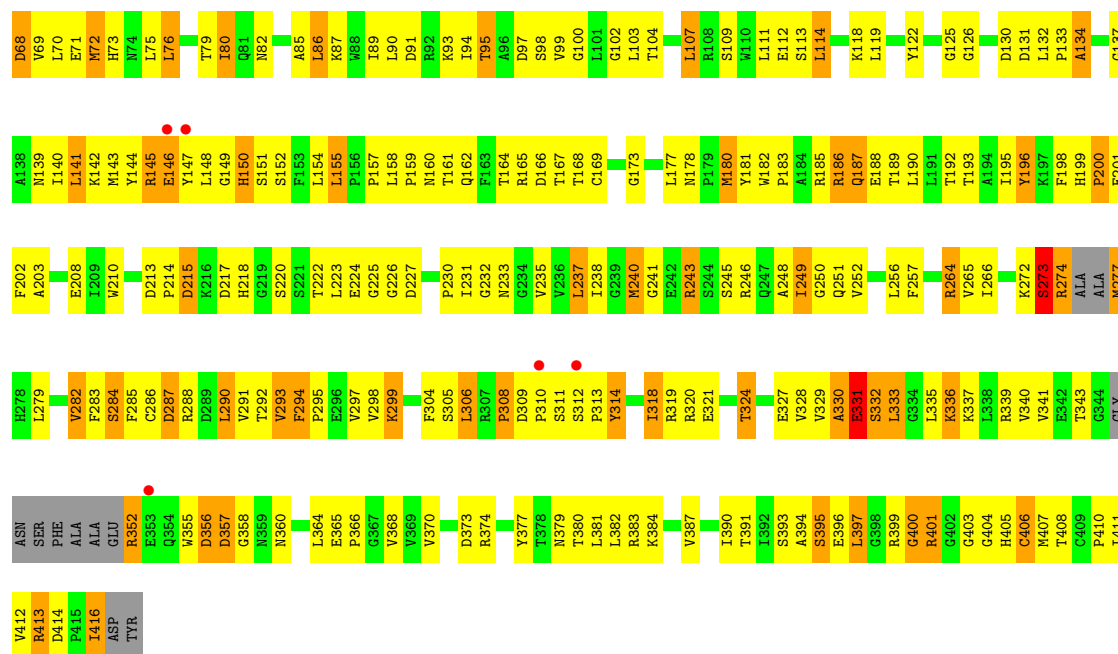


• Molecule 1: Arginine deiminase



• Molecule 1: Arginine deiminase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.60Å 120.60Å 147.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 96.0 (19.92-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.274 0.206 , 0.263	Depositor DCC
R_{free} test set	1715 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12637	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 28.67 % 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 1.7701e-03. 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: CYR

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	0.47	0/3199	0.76	13/4336 (0.3%)
1	B	0.47	0/3222	0.75	11/4368 (0.3%)
1	C	0.46	0/3206	0.78	17/4345 (0.4%)
1	D	0.47	0/3202	0.77	14/4339 (0.3%)
All	All	0.47	0/12829	0.77	55/17388 (0.3%)

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	373	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	227	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	44	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	217	ASP	CB-CG-OD2	5.93	123.64	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3151	0	3139	345	0
1	B	3174	0	3160	298	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3158	0	3143	347	0
1	D	3154	0	3148	388	0
All	All	12637	0	12590	1319	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 52.

The worst 5 of 1319 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:43:ASP:CB	1:D:401:ARG:HH12	1.37	1.36
1:D:43:ASP:HB2	1:D:401:ARG:NH1	1.55	1.20
1:D:14:ALA:O	1:D:366:PRO:HD3	1.39	1.19
1:D:352:ARG:HB3	1:D:352:ARG:NH1	1.59	1.17
1:A:306:LEU:HD13	1:A:318:ILE:HG23	1.21	1.17

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	395/418 (94%)	313 (79%)	65 (16%)	17 (4%)	2	10
1	B	399/418 (96%)	332 (83%)	50 (12%)	17 (4%)	2	10
1	C	396/418 (95%)	323 (82%)	61 (15%)	12 (3%)	4	17
1	D	395/418 (94%)	327 (83%)	54 (14%)	14 (4%)	3	14
All	All	1585/1672 (95%)	1295 (82%)	230 (14%)	60 (4%)	3	13

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	117	ARG
1	A	203	ALA
1	A	221	SER
1	A	249	ILE

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	342/353 (97%)	278 (81%)	64 (19%)	1	5
1	B	342/353 (97%)	279 (82%)	63 (18%)	1	5
1	C	342/353 (97%)	276 (81%)	66 (19%)	1	4
1	D	342/353 (97%)	279 (82%)	63 (18%)	1	5
All	All	1368/1412 (97%)	1112 (81%)	256 (19%)	1	5

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	277	MET
1	D	299	LYS
1	B	169	CYS
1	B	154	LEU
1	D	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	30	GLN
1	C	354	GLN
1	C	199	HIS
1	C	178	ASN
1	C	218	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	CYR	B	406	1	11,16,17	2.29	4 (36%)	6,19,21	1.78	1 (16%)
1	CYR	C	406	1	11,16,17	2.27	2 (18%)	6,19,21	2.41	3 (50%)
1	CYR	A	406	1	11,16,17	2.32	2 (18%)	6,19,21	1.86	2 (33%)
1	CYR	D	406	1	11,16,17	2.31	3 (27%)	6,19,21	2.00	3 (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
1	CYR	B	406	1	-	4/10/18/20	-
1	CYR	C	406	1	-	2/10/18/20	-
1	CYR	A	406	1	-	4/10/18/20	-
1	CYR	D	406	1	-	2/10/18/20	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	CYR	C7-N6	5.45	1.46	1.35
1	D	406	CYR	C7-N6	5.04	1.45	1.35
1	C	406	CYR	C7-N7	4.94	1.46	1.28
1	D	406	CYR	C7-N7	4.88	1.46	1.28
1	C	406	CYR	C7-N6	4.85	1.45	1.35

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	406	CYR	CB-SG-C7	4.03	107.38	102.58
1	B	406	CYR	N6-C7-N7	-3.69	109.51	120.33
1	C	406	CYR	N6-C7-N7	-3.27	110.76	120.33
1	A	406	CYR	CB-SG-C7	2.94	106.09	102.58
1	D	406	CYR	N6-C7-N7	-2.86	111.96	120.33

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	406	CYR	SG-C7-N6-C5
1	A	406	CYR	N6-C7-SG-CB
1	B	406	CYR	C1-C2-C3-C4
1	B	406	CYR	N2-C2-C3-C4
1	B	406	CYR	SG-C7-N6-C5

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	406	CYR	3	0
1	C	406	CYR	3	0
1	D	406	CYR	5	0

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 ⓘ

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	401/418 (95%)	-0.49	3 (0%) 87 87	12, 40, 72, 99	0
1	B	405/418 (96%)	-0.55	1 (0%) 95 95	12, 37, 73, 99	0
1	C	402/418 (96%)	-0.44	6 (1%) 73 73	14, 45, 79, 98	0
1	D	401/418 (95%)	-0.43	5 (1%) 79 79	17, 43, 79, 98	0
All	All	1609/1672 (96%)	-0.48	15 (0%) 84 84	12, 41, 77, 99	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	273	SER	4.1
1	D	147	TYR	3.5
1	A	134	ALA	3.3
1	D	353	GLU	3.1
1	C	313	PRO	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CYR	B	406	17/18	0.93	0.15	22,42,60,63	0
1	CYR	C	406	17/18	0.95	0.12	21,34,46,50	0
1	CYR	A	406	17/18	0.96	0.14	14,45,58,60	0
1	CYR	D	406	17/18	0.97	0.10	15,40,60,62	0

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.