



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2026 – 12:21 PM EDT

PDB ID : 9O3T / pdb_00009o3t
Title : Crystal Structure of S63A Variant of D-Dopachrome Tautomerase (D-DT)
Authors : Pilien, A.V.R.; Argueta, C.; Parkins, A.; Pantouris, G.
Deposited on : 2025-04-07
Resolution : 1.53 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

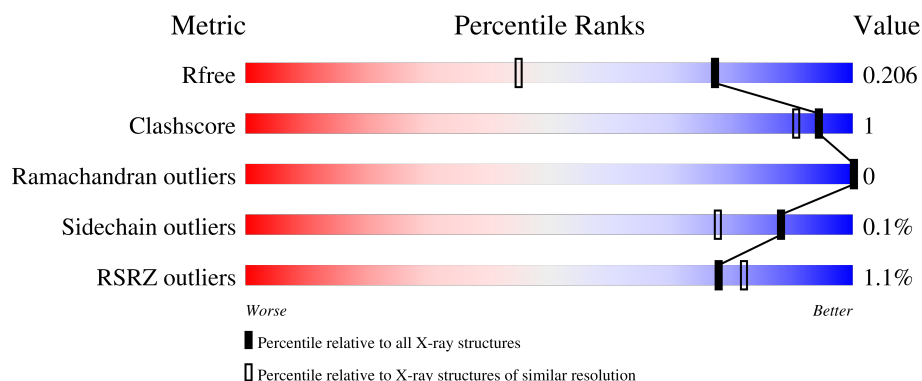
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

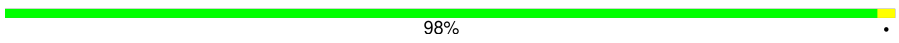
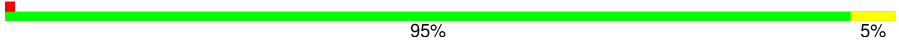
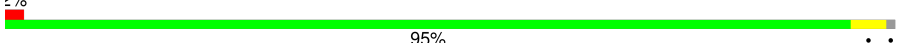
The reported resolution of this entry is 1.53 Å.

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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	AAA	117	 98%
1	BBB	117	 95% 5%
1	CCC	117	 97%
1	DDD	117	 99%
1	EEE	117	 95%

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Mol	Chain	Length	Quality of chain
1	FFF	117	
1	GGG	117	
1	HHH	117	
1	III	117	
1	JJJ	117	
1	KKK	117	
1	LLL	117	

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	TRS	JJJ	201	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11558 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 D-dopachrome decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	III	117	Total	C	N	O	S	0	1	0
			884	565	153	162	4			
1	AAA	117	Total	C	N	O	S	0	1	0
			879	562	150	163	4			
1	BBB	117	Total	C	N	O	S	0	1	0
			879	562	150	162	5			
1	CCC	117	Total	C	N	O	S	0	3	0
			890	569	151	166	4			
1	DDD	117	Total	C	N	O	S	0	3	0
			892	570	154	163	5			
1	EEE	116	Total	C	N	O	S	0	0	0
			868	555	151	158	4			
1	FFF	110	Total	C	N	O	S	0	0	0
			819	522	142	152	3			
1	GGG	114	Total	C	N	O	S	0	0	0
			847	539	149	155	4			
1	HHH	117	Total	C	N	O	S	0	1	0
			886	566	153	162	5			
1	JJJ	117	Total	C	N	O	S	0	0	0
			873	559	150	160	4			
1	KKK	117	Total	C	N	O	S	0	1	0
			869	555	149	161	4			
1	LLL	117	Total	C	N	O	S	0	1	0
			875	560	150	160	5			

There are 12 discrepancies between the modelled and reference sequences:

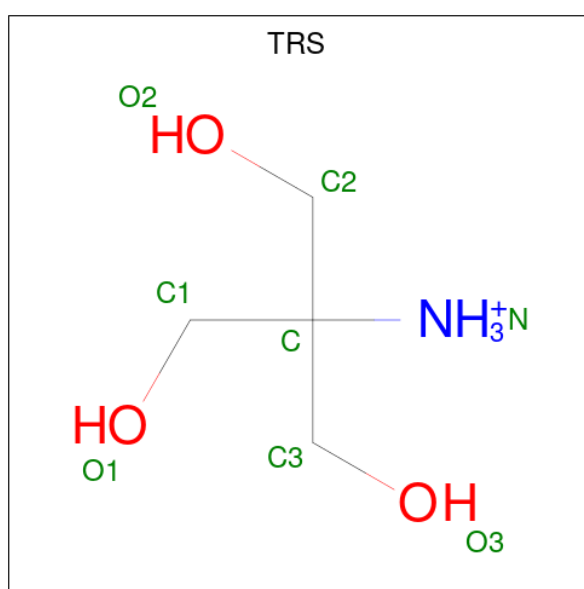
Chain	Residue	Modelled	Actual	Comment	Reference
III	63	ALA	SER	variant	UNP P30046
AAA	63	ALA	SER	variant	UNP P30046
BBB	63	ALA	SER	variant	UNP P30046
CCC	63	ALA	SER	variant	UNP P30046
DDD	63	ALA	SER	variant	UNP P30046

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	63	ALA	SER	variant	UNP P30046
FFF	63	ALA	SER	variant	UNP P30046
GGG	63	ALA	SER	variant	UNP P30046
HHH	63	ALA	SER	variant	UNP P30046
JJJ	63	ALA	SER	variant	UNP P30046
KKK	63	ALA	SER	variant	UNP P30046
LLL	63	ALA	SER	variant	UNP P30046

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			8	4	1	3		
2	BBB	1	Total	C	N	O	0	0
			8	4	1	3		
2	HHH	1	Total	C	N	O	0	0
			8	4	1	3		
2	JJJ	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	III	112	Total	O	0	0
			112	112		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	105	Total 105	O 105	0	0
3	BBB	100	Total 100	O 100	0	0
3	CCC	74	Total 74	O 74	0	0
3	DDD	124	Total 124	O 124	0	0
3	EEE	81	Total 81	O 81	0	0
3	FFF	113	Total 113	O 113	0	0
3	GGG	83	Total 83	O 83	0	0
3	HHH	80	Total 80	O 80	0	0
3	JJJ	81	Total 81	O 81	0	0
3	KKK	57	Total 57	O 57	0	0
3	LLL	55	Total 55	O 55	0	0

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: D-dopachrome decarboxylase

Chain III:  97% .



- Molecule 1: D-dopachrome decarboxylase

Chain AAA:  98% .



- Molecule 1: D-dopachrome decarboxylase

Chain BBB:  95% 5% .



- Molecule 1: D-dopachrome decarboxylase

Chain CCC:  97% .



- Molecule 1: D-dopachrome decarboxylase

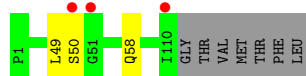
Chain DDD:  99% .



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



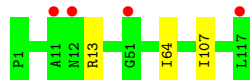
- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.50Å 94.27Å 91.47Å 90.00° 112.39° 90.00°	Depositor
Resolution (Å)	69.90 – 1.53 69.90 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.4 (69.90-1.53) 99.4 (69.90-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.166 , 0.196 0.177 , 0.206	Depositor DCC
R_{free} test set	8792 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11558	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	AAA	1.08	0/899	1.13	0/1219
1	BBB	1.13	0/899	1.17	0/1218
1	CCC	1.04	0/916	1.15	0/1242
1	DDD	1.12	0/922	1.12	0/1248
1	EEE	1.09	0/885	1.22	0/1201
1	FFF	1.11	0/835	1.18	0/1135
1	GGG	1.09	0/863	1.23	0/1172
1	HHH	1.04	0/906	1.18	0/1227
1	III	1.11	0/904	1.13	0/1225
1	JJJ	1.12	0/890	1.19	0/1207
1	KKK	1.06	0/889	1.24	0/1207
1	LLL	1.05	0/895	1.18	0/1214
All	All	1.09	0/10703	1.18	0/14515

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 [i](#)

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	AAA	879	0	893	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	879	0	891	3	0
1	CCC	890	0	905	2	0
1	DDD	892	0	920	1	0
1	EEE	868	0	879	4	0
1	FFF	819	0	822	2	0
1	GGG	847	0	857	3	0
1	HHH	886	0	906	3	0
1	III	884	0	901	3	0
1	JJJ	873	0	886	7	0
1	KKK	869	0	875	1	0
1	LLL	875	0	889	3	0
2	AAA	8	0	12	0	0
2	BBB	8	0	12	0	0
2	HHH	8	0	12	1	0
2	JJJ	8	0	12	1	0
3	AAA	105	0	0	0	0
3	BBB	100	0	0	0	0
3	CCC	74	0	0	0	0
3	DDD	124	0	0	0	0
3	EEE	81	0	0	0	0
3	FFF	113	0	0	0	0
3	GGG	83	0	0	0	0
3	HHH	80	0	0	0	0
3	III	112	0	0	1	0
3	JJJ	81	0	0	0	0
3	KKK	57	0	0	0	0
3	LLL	55	0	0	0	0
All	All	11558	0	10672	28	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 28 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:JJJ:107:ILE:HB	1:JJJ:114:MET:HG3	1.80	0.63
1:BBB:83:PHE:CZ	1:BBB:87:GLU:HG3	2.44	0.53
1:JJJ:64:ILE:HD11	1:JJJ:107:ILE:HD12	1.91	0.53
1:BBB:59:LEU:HD22	1:BBB:84:LEU:HD11	1.91	0.52
1:LLL:18:LEU:O	1:LLL:18:LEU:HD12	2.09	0.52

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	AAA	116/117 (99%)	112 (97%)	4 (3%)	0	100	100
1	BBB	116/117 (99%)	113 (97%)	3 (3%)	0	100	100
1	CCC	118/117 (101%)	114 (97%)	4 (3%)	0	100	100
1	DDD	118/117 (101%)	115 (98%)	3 (2%)	0	100	100
1	EEE	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
1	FFF	108/117 (92%)	106 (98%)	2 (2%)	0	100	100
1	GGG	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
1	HHH	116/117 (99%)	113 (97%)	3 (3%)	0	100	100
1	III	116/117 (99%)	112 (97%)	4 (3%)	0	100	100
1	JJJ	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	KKK	116/117 (99%)	113 (97%)	3 (3%)	0	100	100
1	LLL	116/117 (99%)	112 (97%)	4 (3%)	0	100	100
All	All	1381/1404 (98%)	1343 (97%)	38 (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	AAA	93/94 (99%)	93 (100%)	0	100	100
1	BBB	93/94 (99%)	93 (100%)	0	100	100
1	CCC	95/94 (101%)	95 (100%)	0	100	100
1	DDD	97/94 (103%)	97 (100%)	0	100	100
1	EEE	90/94 (96%)	90 (100%)	0	100	100
1	FFF	85/94 (90%)	85 (100%)	0	100	100
1	GGG	88/94 (94%)	88 (100%)	0	100	100
1	HHH	94/94 (100%)	94 (100%)	0	100	100
1	III	93/94 (99%)	93 (100%)	0	100	100
1	JJJ	91/94 (97%)	91 (100%)	0	100	100
1	KKK	91/94 (97%)	90 (99%)	1 (1%)	65	40
1	LLL	92/94 (98%)	92 (100%)	0	100	100
All	All	1102/1128 (98%)	1101 (100%)	1 (0%)	88	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	KKK	13	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	TRS	JJJ	201	-	7,7,7	1.31	1 (14%)	9,9,9	4.73	8 (88%)
2	TRS	BBB	201	-	7,7,7	0.89	0	9,9,9	1.42	2 (22%)
2	TRS	HHH	201	-	7,7,7	0.68	0	9,9,9	1.03	0
2	TRS	AAA	201	-	7,7,7	1.10	1 (14%)	9,9,9	0.65	0

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	TRS	JJJ	201	-	-	7/9/9/9	-
2	TRS	BBB	201	-	-	0/9/9/9	-
2	TRS	HHH	201	-	-	0/9/9/9	-
2	TRS	AAA	201	-	-	2/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	JJJ	201	TRS	C1-C	2.72	1.60	1.53
2	AAA	201	TRS	C3-C	2.39	1.59	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	JJJ	201	TRS	C2-C-C1	-8.08	89.13	110.66
2	JJJ	201	TRS	C3-C-C1	-7.17	91.56	110.66
2	JJJ	201	TRS	C3-C-N	4.44	119.49	108.17
2	JJJ	201	TRS	C2-C-N	4.40	119.40	108.17
2	JJJ	201	TRS	O3-C3-C	-3.80	100.28	110.88

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	JJJ	201	TRS	N-C-C1-O1
2	JJJ	201	TRS	N-C-C2-O2
2	JJJ	201	TRS	C2-C-C3-O3
2	JJJ	201	TRS	C3-C-C1-O1
2	AAA	201	TRS	N-C-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	JJJ	201	TRS	1	0
2	HHH	201	TRS	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 ⓘ

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	AAA	117/117 (100%)	-0.07	0 100 100	10, 16, 26, 30	1 (0%)
1	BBB	117/117 (100%)	-0.04	1 (0%) 81 84	11, 15, 25, 35	1 (0%)
1	CCC	117/117 (100%)	-0.04	2 (1%) 69 74	10, 17, 31, 39	3 (2%)
1	DDD	117/117 (100%)	-0.10	0 100 100	11, 16, 25, 29	3 (2%)
1	EEE	116/117 (99%)	0.00	2 (1%) 69 74	13, 18, 28, 39	0
1	FFF	110/117 (94%)	0.07	3 (2%) 56 62	13, 18, 29, 40	0
1	GGG	114/117 (97%)	0.06	1 (0%) 81 84	14, 19, 31, 44	0
1	HHH	117/117 (100%)	-0.09	1 (0%) 81 84	10, 18, 29, 37	1 (0%)
1	III	117/117 (100%)	-0.21	0 100 100	10, 16, 24, 36	1 (0%)
1	JJJ	117/117 (100%)	0.35	2 (1%) 69 74	14, 21, 32, 37	0
1	KKK	117/117 (100%)	0.51	4 (3%) 48 55	16, 24, 36, 43	1 (0%)
1	LLL	117/117 (100%)	0.30	0 100 100	15, 22, 32, 41	1 (0%)
All	All	1393/1404 (99%)	0.06	16 (1%) 78 82	10, 18, 30, 44	12 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	16	ALA	4.3
1	EEE	104	SER	3.8
1	JJJ	117	LEU	3.7
1	GGG	114	MET	3.0
1	KKK	11	ALA	2.9

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 [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(\AA^2)	Q<0.9
2	TRS	JJJ	201	8/8	0.83	0.12	31,41,44,44	0
2	TRS	AAA	201	8/8	0.90	0.09	21,27,32,35	0
2	TRS	BBB	201	8/8	0.91	0.09	24,30,36,36	0
2	TRS	HHH	201	8/8	0.97	0.05	17,19,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.