



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2026 – 12:14 PM EDT

PDB ID : 9O3R / pdb_00009o3r
Title : Crystal Structure of I64A Variant of D-Dopachrome Tautomerase (D-DT)
Authors : Pilien, A.V.R.; Argueta, C.; Parkins, A.; Pantouris, G.
Deposited on : 2025-04-07
Resolution : 1.54 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
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

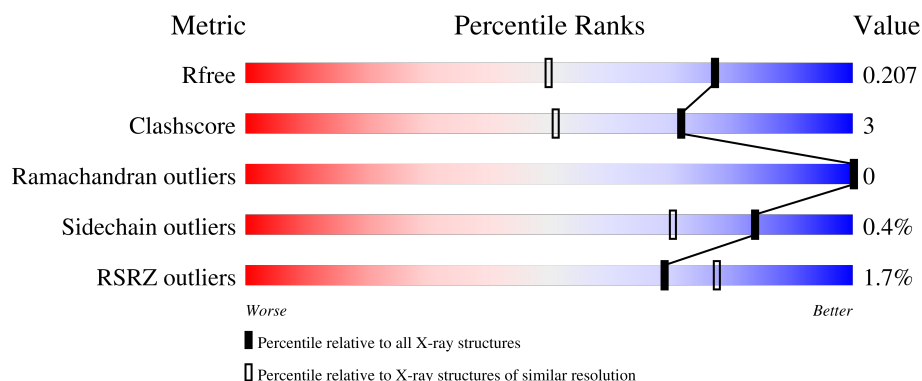
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	<div> <div>8%</div> <div>94%</div> <div>6%</div> </div>
1	BBB	117	<div> <div>95%</div> <div>..</div> </div>
1	CCC	117	<div> <div>89%</div> <div>11%</div> </div>
1	DDD	117	<div> <div>98%</div> <div>.</div> </div>
1	EEE	117	<div> <div>8%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	FFF	117	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	GGG	117	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
1	HHH	117	<div> <div>%</div> <div> <div></div> <div>96%</div> <div></div> </div> </div>
1	III	117	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div></div> </div> </div>
1	JJJ	117	<div> <div></div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	KKK	117	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	LLL	117	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	MMM	117	<div> <div>4%</div> <div> <div></div> <div>98%</div> <div></div> </div> </div>
1	NNN	117	<div> <div>%</div> <div> <div></div> <div>97%</div> <div></div> </div> </div>
1	OOO	117	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	PPP	117	<div> <div>%</div> <div> <div></div> <div>97%</div> <div></div> </div> </div>
1	QQQ	117	<div> <div>%</div> <div> <div></div> <div>96%</div> <div></div> </div> </div>
1	RRR	117	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18907 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	AAA	117	Total	C	N	O	S	0	1	0
			889	565	155	165	4			
1	BBB	117	Total	C	N	O	S	0	1	0
			881	560	155	162	4			
1	CCC	117	Total	C	N	O	S	0	2	0
			894	569	155	166	4			
1	DDD	117	Total	C	N	O	S	0	0	0
			873	556	152	161	4			
1	EEE	114	Total	C	N	O	S	0	1	0
			849	537	149	158	5			
1	FFF	117	Total	C	N	O	S	0	0	0
			874	558	153	159	4			
1	GGG	108	Total	C	N	O	S	0	2	0
			809	514	143	148	4			
1	HHH	117	Total	C	N	O	S	0	2	0
			894	569	156	165	4			
1	III	117	Total	C	N	O	S	0	0	0
			873	556	150	163	4			
1	JJJ	117	Total	C	N	O	S	0	0	0
			869	555	149	161	4			
1	KKK	117	Total	C	N	O	S	0	0	0
			877	558	152	163	4			
1	LLL	117	Total	C	N	O	S	0	1	0
			885	563	154	164	4			
1	MMM	117	Total	C	N	O	S	0	0	0
			868	555	148	161	4			
1	NNN	117	Total	C	N	O	S	0	0	0
			877	558	152	163	4			
1	OOO	117	Total	C	N	O	S	0	0	0
			862	552	147	159	4			
1	PPP	117	Total	C	N	O	S	0	0	0
			876	558	153	161	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QQQ	117	Total	C	N	O	S	0	1	0
			887	564	154	165	4			
1	RRR	117	Total	C	N	O	S	0	3	0
			878	557	152	164	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	64	ALA	ILE	variant	UNP P30046
BBB	64	ALA	ILE	variant	UNP P30046
CCC	64	ALA	ILE	variant	UNP P30046
DDD	64	ALA	ILE	variant	UNP P30046
EEE	64	ALA	ILE	variant	UNP P30046
FFF	64	ALA	ILE	variant	UNP P30046
GGG	64	ALA	ILE	variant	UNP P30046
HHH	64	ALA	ILE	variant	UNP P30046
III	64	ALA	ILE	variant	UNP P30046
JJJ	64	ALA	ILE	variant	UNP P30046
KKK	64	ALA	ILE	variant	UNP P30046
LLL	64	ALA	ILE	variant	UNP P30046
MMM	64	ALA	ILE	variant	UNP P30046
NNN	64	ALA	ILE	variant	UNP P30046
OOO	64	ALA	ILE	variant	UNP P30046
PPP	64	ALA	ILE	variant	UNP P30046
QQQ	64	ALA	ILE	variant	UNP P30046
RRR	64	ALA	ILE	variant	UNP P30046

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Ca	0	0
			1	1		
2	CCC	2	Total	Ca	0	0
			2	2		
2	DDD	1	Total	Ca	0	0
			1	1		
2	FFF	1	Total	Ca	0	0
			1	1		
2	HHH	1	Total	Ca	0	0
			1	1		
2	JJJ	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	KKK	1	Total 1	Ca 1	0	0
2	LLL	1	Total 1	Ca 1	0	0
2	NNN	1	Total 1	Ca 1	0	0
2	OOO	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	211	Total 211	O 211	0	0
3	BBB	172	Total 172	O 172	0	0
3	CCC	197	Total 197	O 197	0	0
3	DDD	206	Total 206	O 206	0	0
3	EEE	168	Total 168	O 168	0	0
3	FFF	144	Total 144	O 144	0	0
3	GGG	161	Total 161	O 161	0	0
3	HHH	201	Total 201	O 201	0	0
3	III	149	Total 149	O 149	0	0
3	JJJ	187	Total 187	O 187	0	0
3	KKK	187	Total 187	O 187	0	0
3	LLL	144	Total 144	O 144	0	0
3	MMM	161	Total 161	O 161	0	0
3	NNN	191	Total 191	O 191	0	0
3	OOO	198	Total 198	O 198	0	0

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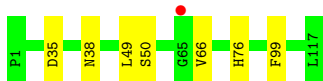
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	PPP	200	Total 200	O 200	0	0
3	QQQ	170	Total 170	O 170	0	0
3	RRR	133	Total 133	O 133	0	0

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



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



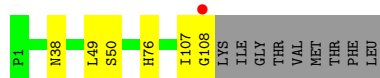
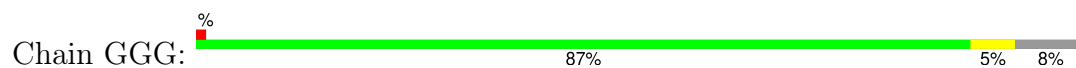
- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



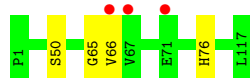
- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



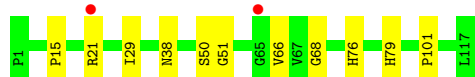
- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase

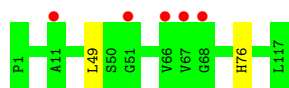


- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase

Chain MMM:  4% 98% .



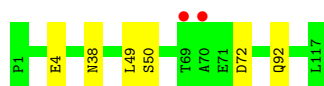
- Molecule 1: D-dopachrome decarboxylase

Chain NNN:  % 97% .



- Molecule 1: D-dopachrome decarboxylase

Chain OOO:  2% 95% 5% .



- Molecule 1: D-dopachrome decarboxylase

Chain PPP:  % 97% .



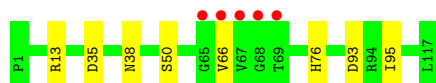
- Molecule 1: D-dopachrome decarboxylase

Chain QQQ:  % 96% .



- Molecule 1: D-dopachrome decarboxylase

Chain RRR:  4% 93% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.52Å 151.77Å 91.49Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	86.51 – 1.54 86.51 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.0 (86.51-1.54) 99.0 (86.51-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.198 0.180 , 0.207	Depositor DCC
R_{free} test set	15097 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18907	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: CA

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	1.09	0/906	1.14	2/1227 (0.2%)
1	BBB	1.11	1/901 (0.1%)	1.17	0/1219
1	CCC	1.08	0/917	1.16	2/1241 (0.2%)
1	DDD	1.10	0/890	1.16	0/1207
1	EEE	1.19	1/868 (0.1%)	1.23	1/1178 (0.1%)
1	FFF	1.08	0/891	1.16	0/1207
1	GGG	1.13	0/831	1.20	0/1128
1	HHH	1.12	1/917 (0.1%)	1.20	0/1241
1	III	1.08	0/890	1.14	0/1207
1	JJJ	1.16	0/886	1.15	0/1202
1	KKK	1.10	0/894	1.17	0/1212
1	LLL	1.08	0/905	1.18	0/1225
1	MMM	1.10	0/885	1.24	0/1200
1	NNN	1.14	0/894	1.19	0/1212
1	OOO	1.13	0/879	1.27	1/1193 (0.1%)
1	PPP	1.08	0/893	1.16	0/1210
1	QQQ	1.13	1/907 (0.1%)	1.14	0/1227
1	RRR	1.09	1/904 (0.1%)	1.21	2/1224 (0.2%)
All	All	1.11	5/16058 (0.0%)	1.18	8/21760 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	RRR	95	ILE	C-O	5.91	1.29	1.24
1	HHH	29	ILE	C-O	5.41	1.30	1.24
1	QQQ	66	VAL	C-O	5.23	1.29	1.24
1	BBB	82	GLU	C-O	5.15	1.30	1.24
1	EEE	107	ILE	C-N	5.13	1.36	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	35	ASP	CA-CB-CG	6.69	119.29	112.60
1	OOO	4	GLU	CB-CG-CD	6.17	123.09	112.60
1	RRR	93	ASP	CA-CB-CG	5.79	118.39	112.60
1	RRR	35	ASP	CA-CB-CG	5.58	118.18	112.60
1	EEE	107	ILE	N-CA-C	5.38	115.60	107.75

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	AAA	889	0	900	8	0
1	BBB	881	0	892	6	0
1	CCC	894	0	914	11	0
1	DDD	873	0	880	2	0
1	EEE	849	0	848	16	0
1	FFF	874	0	889	17	0
1	GGG	809	0	813	10	0
1	HHH	894	0	912	4	0
1	III	873	0	877	7	0
1	JJJ	869	0	873	12	0
1	KKK	877	0	884	10	0
1	LLL	885	0	905	10	0
1	MMM	868	0	874	2	0
1	NNN	877	0	884	4	0
1	OOO	862	0	867	8	0
1	PPP	876	0	889	5	0
1	QQQ	887	0	902	5	0
1	RRR	878	0	878	8	0
2	AAA	1	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	1	0	0	0	0
2	FFF	1	0	0	0	0
2	HHH	1	0	0	0	0
2	JJJ	2	0	0	0	0
2	KKK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	LLL	1	0	0	0	0
2	NNN	1	0	0	0	0
2	OOO	1	0	0	0	0
3	AAA	211	0	0	1	0
3	BBB	172	0	0	4	0
3	CCC	197	0	0	1	0
3	DDD	206	0	0	1	0
3	EEE	168	0	0	5	0
3	FFF	144	0	0	4	0
3	GGG	161	0	0	2	0
3	HHH	201	0	0	2	0
3	III	149	0	0	4	0
3	JJJ	187	0	0	1	0
3	KKK	187	0	0	2	0
3	LLL	144	0	0	0	0
3	MMM	161	0	0	1	0
3	NNN	191	0	0	2	0
3	OOO	198	0	0	3	0
3	PPP	200	0	0	0	0
3	QQQ	170	0	0	0	0
3	RRR	133	0	0	2	0
All	All	18907	0	15881	104	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.

The worst 5 of 104 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:III:65:GLY:HA2	3:III:203:HOH:O	1.47	1.14
1:HHH:66:VAL:HG22	3:HHH:309:HOH:O	1.48	1.11
1:EEE:106:GLN:HB3	3:OOO:346:HOH:O	1.56	1.05
1:CCC:13:ARG:NH1	3:CCC:301:HOH:O	2.24	0.70
1:CCC:66:VAL:O	1:CCC:76:HIS:HE1	1.78	0.67

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	113 (97%)	3 (3%)	0	100	100
1	BBB	116/117 (99%)	114 (98%)	2 (2%)	0	100	100
1	CCC	117/117 (100%)	113 (97%)	4 (3%)	0	100	100
1	DDD	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	EEE	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
1	FFF	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	GGG	108/117 (92%)	107 (99%)	1 (1%)	0	100	100
1	HHH	117/117 (100%)	112 (96%)	5 (4%)	0	100	100
1	III	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	JJJ	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
1	KKK	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	LLL	116/117 (99%)	113 (97%)	3 (3%)	0	100	100
1	MMM	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	NNN	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	OOO	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	PPP	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	QQQ	116/117 (99%)	113 (97%)	3 (3%)	0	100	100
1	RRR	118/117 (101%)	114 (97%)	4 (3%)	0	100	100
All	All	2072/2106 (98%)	2016 (97%)	56 (3%)	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	AAA	94/94 (100%)	94 (100%)	0	100	100
1	BBB	92/94 (98%)	90 (98%)	2 (2%)	45	15
1	CCC	96/94 (102%)	96 (100%)	0	100	100
1	DDD	91/94 (97%)	91 (100%)	0	100	100
1	EEE	88/94 (94%)	85 (97%)	3 (3%)	32	7
1	FFF	91/94 (97%)	91 (100%)	0	100	100
1	GGG	84/94 (89%)	84 (100%)	0	100	100
1	HHH	95/94 (101%)	95 (100%)	0	100	100
1	III	91/94 (97%)	91 (100%)	0	100	100
1	JJJ	90/94 (96%)	90 (100%)	0	100	100
1	KKK	92/94 (98%)	91 (99%)	1 (1%)	65	38
1	LLL	95/94 (101%)	95 (100%)	0	100	100
1	MMM	91/94 (97%)	91 (100%)	0	100	100
1	NNN	92/94 (98%)	92 (100%)	0	100	100
1	OOO	89/94 (95%)	89 (100%)	0	100	100
1	PPP	92/94 (98%)	92 (100%)	0	100	100
1	QQQ	95/94 (101%)	95 (100%)	0	100	100
1	RRR	92/94 (98%)	92 (100%)	0	100	100
All	All	1650/1692 (98%)	1644 (100%)	6 (0%)	84	70

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	101	PRO
1	EEE	104	SER
1	KKK	54	GLU
1	BBB	38	ASN
1	BBB	23	CYS

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

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](#)

Of 12 ligands modelled in this entry, 12 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	AAA	117/117 (100%)	-0.35	1 (0%) 81 86	10, 15, 22, 32	1 (0%)
1	BBB	117/117 (100%)	-0.22	1 (0%) 81 86	12, 17, 27, 33	1 (0%)
1	CCC	117/117 (100%)	-0.35	0 100 100	10, 16, 24, 32	2 (1%)
1	DDD	117/117 (100%)	-0.17	0 100 100	14, 18, 24, 31	0
1	EEE	114/117 (97%)	0.15	9 (7%) 18 23	13, 18, 39, 63	1 (0%)
1	FFF	117/117 (100%)	-0.08	1 (0%) 81 86	14, 18, 27, 38	0
1	GGG	108/117 (92%)	-0.04	1 (0%) 81 86	10, 18, 28, 52	2 (1%)
1	HHH	117/117 (100%)	-0.29	1 (0%) 81 86	11, 16, 24, 30	2 (1%)
1	III	117/117 (100%)	-0.16	3 (2%) 57 66	13, 18, 29, 35	0
1	JJJ	117/117 (100%)	-0.19	0 100 100	12, 17, 27, 37	0
1	KKK	117/117 (100%)	-0.10	1 (0%) 81 86	14, 18, 27, 35	0
1	LLL	117/117 (100%)	-0.12	2 (1%) 69 77	10, 16, 28, 37	1 (0%)
1	MMM	117/117 (100%)	0.13	5 (4%) 40 48	14, 20, 36, 47	0
1	NNN	117/117 (100%)	-0.09	1 (0%) 81 86	13, 19, 30, 47	0
1	OOO	117/117 (100%)	0.09	2 (1%) 69 77	13, 19, 35, 45	0
1	PPP	117/117 (100%)	-0.00	1 (0%) 81 86	14, 19, 30, 37	0
1	QQQ	117/117 (100%)	-0.10	1 (0%) 81 86	12, 17, 32, 36	1 (0%)
1	RRR	117/117 (100%)	0.35	5 (4%) 40 48	11, 22, 41, 50	3 (2%)
All	All	2094/2106 (99%)	-0.09	35 (1%) 69 77	10, 18, 31, 63	14 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	RRR	67	VAL	5.1
1	RRR	65	GLY	5.0
1	RRR	66	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	GGG	108	GLY	4.8
1	EEE	105	TRP	4.3

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 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(Å ²)	Q<0.9
2	CA	JJJ	202	1/1	0.94	0.16	47,47,47,47	0
2	CA	OOO	201	1/1	0.96	0.27	40,40,40,40	0
2	CA	FFF	201	1/1	0.97	0.18	36,36,36,36	0
2	CA	AAA	201	1/1	0.99	0.04	17,17,17,17	0
2	CA	HHH	201	1/1	0.99	0.08	17,17,17,17	0
2	CA	JJJ	201	1/1	0.99	0.04	15,15,15,15	0
2	CA	CCC	202	1/1	0.99	0.07	22,22,22,22	0
2	CA	LLL	201	1/1	0.99	0.04	16,16,16,16	0
2	CA	NNN	201	1/1	0.99	0.06	17,17,17,17	0
2	CA	DDD	201	1/1	0.99	0.06	18,18,18,18	0
2	CA	KKK	201	1/1	1.00	0.04	17,17,17,17	0
2	CA	CCC	201	1/1	1.00	0.08	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.