



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:10 AM UTC

PDB ID : 8VDY / pdb_00008vdy
Title : Crystal Structure of Delta 114-117 D-Dopachrome Tautomerase (D-DT)
Authors : Parkins, A.; Pilien, A.; Wolff, A.; Thompson, M.C.; Pantouris, G.
Deposited on : 2023-12-18
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

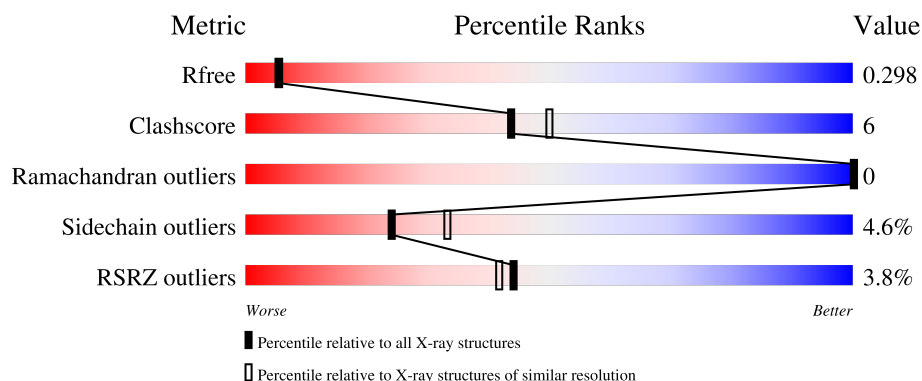
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	113	2% 85% 12% .
1	B	113	% 81% 13% ..
1	C	113	5% 88% 7% ...
1	D	113	5% 81% 12% ..
1	E	113	% 85% 9% ...

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Mol	Chain	Length	Quality of chain
1	F	113	4% 86% 10%
1	G	113	4% 79% 16%
1	H	113	2% 65% 26%
1	I	113	9% 83% 12%
1	J	113	2% 72% 16% 12%
1	K	113	3% 79% 10% 10%
1	L	113	6% 75% 16% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9390 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	A	109	Total	C	N	O	S	0	0	0
			795	504	140	148	3			
1	B	108	Total	C	N	O	S	0	0	0
			792	503	136	150	3			
1	C	109	Total	C	N	O	S	0	0	0
			783	497	139	144	3			
1	D	110	Total	C	N	O	S	0	0	1
			791	500	139	149	3			
1	E	108	Total	C	N	O	S	0	0	0
			795	501	142	149	3			
1	F	109	Total	C	N	O	S	0	1	0
			800	508	140	149	3			
1	G	109	Total	C	N	O	S	0	0	0
			809	510	144	152	3			
1	H	108	Total	C	N	O	S	0	0	0
			789	501	141	144	3			
1	I	108	Total	C	N	O	S	0	0	0
			758	485	130	140	3			
1	J	99	Total	C	N	O	S	0	0	0
			736	470	132	131	3			
1	K	102	Total	C	N	O	S	0	0	0
			759	487	135	134	3			
1	L	106	Total	C	N	O	S	0	0	1
			776	491	137	145	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	3	Total	O	0	0
			3	3		
2	E	2	Total	O	0	0
			2	2		

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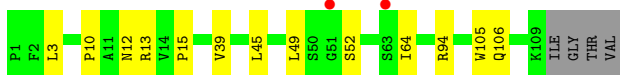
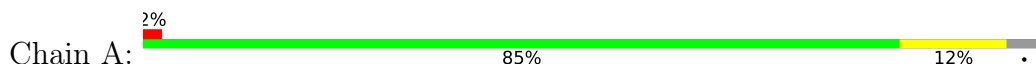
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	O	0	0
			1	1		
2	K	1	Total	O	0	0
			1	1		

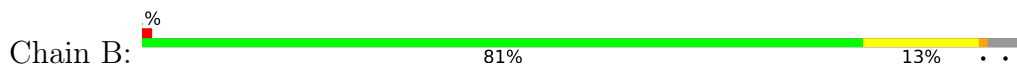
3 Residue-property plots [i](#)

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.

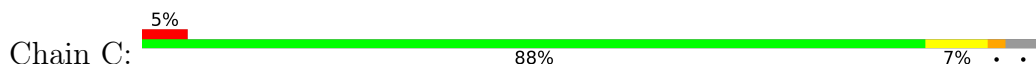
- Molecule 1: D-dopachrome decarboxylase



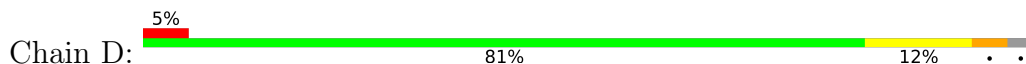
- Molecule 1: D-dopachrome decarboxylase



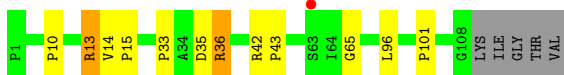
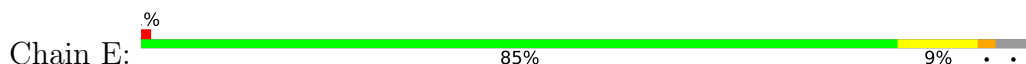
- Molecule 1: D-dopachrome decarboxylase



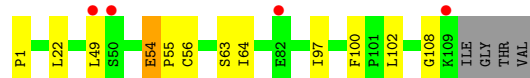
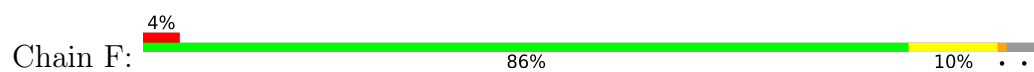
- Molecule 1: D-dopachrome decarboxylase



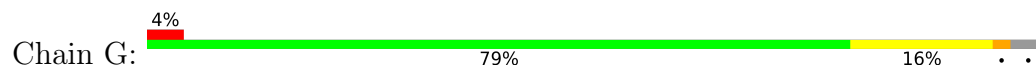
- Molecule 1: D-dopachrome decarboxylase



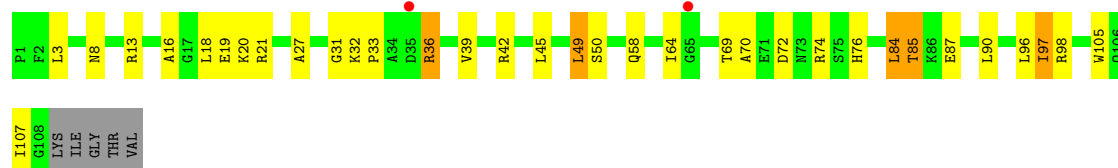
- Molecule 1: D-dopachrome decarboxylase



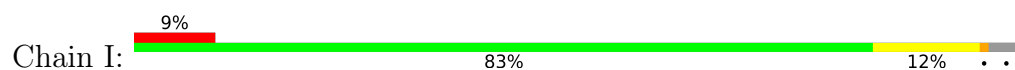
• Molecule 1: D-dopachrome decarboxylase



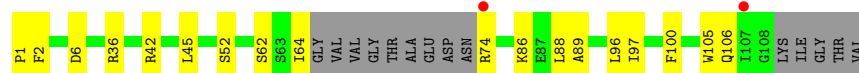
• Molecule 1: D-dopachrome decarboxylase



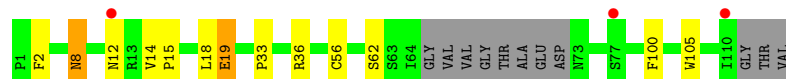
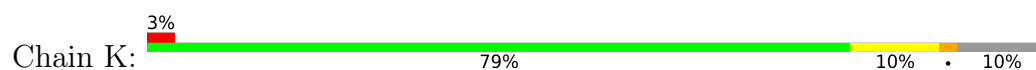
• Molecule 1: D-dopachrome decarboxylase



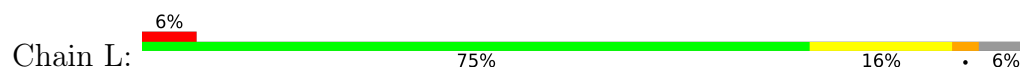
• Molecule 1: D-dopachrome decarboxylase



• Molecule 1: D-dopachrome decarboxylase



• Molecule 1: D-dopachrome decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.53Å 59.53Å 129.98Å 90.00° 107.93° 90.00°	Depositor
Resolution (Å)	89.84 – 2.44 89.84 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.84-2.44) 99.6 (89.84-2.44)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.249 , 0.302 0.252 , 0.298	Depositor DCC
R_{free} test set	2702 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9390	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.44% 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](#)

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	1.09	0/811	1.49	0/1100
1	B	1.06	0/808	1.42	0/1099
1	C	1.14	0/799	1.43	0/1086
1	D	1.07	0/807	1.43	1/1096 (0.1%)
1	E	1.11	0/811	1.44	2/1102 (0.2%)
1	F	1.13	0/819	1.40	4/1113 (0.4%)
1	G	1.16	1/825 (0.1%)	1.47	4/1119 (0.4%)
1	H	1.15	0/805	1.50	5/1094 (0.5%)
1	I	1.06	0/774	1.37	0/1053
1	J	1.10	0/751	1.45	1/1016 (0.1%)
1	K	1.09	0/774	1.46	1/1048 (0.1%)
1	L	1.06	0/791	1.46	1/1075 (0.1%)
All	All	1.10	1/9575 (0.0%)	1.44	19/13001 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	14	VAL	N-CA	5.32	1.50	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	42	ARG	CB-CA-C	6.68	117.15	110.33
1	J	100	PHE	CB-CA-C	6.48	118.85	109.45
1	E	36	ARG	N-CA-C	-6.41	105.43	113.18
1	H	27	ALA	CA-C-N	6.26	128.99	120.54
1	H	27	ALA	C-N-CA	6.26	128.99	120.54
1	G	36	ARG	CA-C-N	-6.20	114.96	122.90
1	G	36	ARG	C-N-CA	-6.20	114.96	122.90
1	G	36	ARG	N-CA-C	-6.19	105.48	113.16
1	F	108	GLY	CA-C-O	-6.12	117.33	122.29
1	F	22	LEU	CA-C-N	5.59	127.71	120.44
1	F	22	LEU	C-N-CA	5.59	127.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	74	ARG	CA-C-N	5.38	127.48	120.28
1	H	74	ARG	C-N-CA	5.38	127.48	120.28
1	F	100	PHE	CB-CA-C	5.33	117.46	109.63
1	D	100	PHE	CB-CA-C	5.26	117.09	109.20
1	H	107	ILE	CA-C-O	-5.13	115.77	121.98
1	G	35	ASP	N-CA-C	-5.10	106.91	113.23
1	L	36	ARG	N-CA-C	-5.09	106.75	113.17
1	K	105	TRP	CA-C-O	-5.08	115.51	121.10

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	795	0	769	12	0
1	B	792	0	777	12	0
1	C	783	0	761	11	0
1	D	791	0	769	10	0
1	E	795	0	774	10	0
1	F	800	0	788	4	0
1	G	809	0	797	11	0
1	H	789	0	775	20	0
1	I	758	0	728	8	0
1	J	736	0	738	9	0
1	K	759	0	760	14	0
1	L	776	0	757	13	0
2	C	3	0	0	0	0
2	E	2	0	0	0	0
2	G	1	0	0	0	0
2	K	1	0	0	0	0
All	All	9390	0	9193	114	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 6.

All (114) 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:K:8:ASN:HD21	1:K:56:CYS:H	1.14	0.95
1:L:54:GLU:HG3	1:L:55:PRO:HD2	1.58	0.85
1:F:54:GLU:HG3	1:F:55:PRO:HD2	1.58	0.84
1:K:8:ASN:H	1:K:8:ASN:HD22	1.35	0.74
1:C:10:PRO:HG2	1:C:13:ARG:HG3	1.71	0.73
1:K:8:ASN:ND2	1:K:56:CYS:H	1.90	0.69
1:G:10:PRO:HG2	1:G:13:ARG:HD3	1.75	0.68
1:B:92:GLN:HG2	1:C:108:GLY:HA3	1.75	0.67
1:A:105:TRP:HE3	1:C:96:LEU:HD11	1.58	0.67
1:I:49:LEU:HD22	1:I:56:CYS:HB2	1.77	0.66
1:A:105:TRP:CE3	1:C:96:LEU:HD11	2.31	0.65
1:G:62:SER:HB3	1:G:102:LEU:HD22	1.81	0.61
1:E:10:PRO:HD2	1:E:13:ARG:HD3	1.83	0.61
1:F:49:LEU:HD12	1:F:56:CYS:HB2	1.83	0.61
1:H:31:GLY:O	1:H:32:LYS:HG2	2.02	0.60
1:B:96:LEU:HD21	1:C:105:TRP:CE3	2.36	0.60
1:L:33:PRO:C	1:L:35:ASP:H	2.09	0.60
1:K:8:ASN:HD21	1:K:56:CYS:N	1.95	0.57
1:L:36:ARG:HH21	1:L:105:TRP:HE1	1.51	0.57
1:C:3:LEU:HD23	1:C:59:LEU:HD11	1.87	0.56
1:G:1:PRO:HD3	1:G:36:ARG:HD3	1.87	0.56
1:K:14:VAL:HG13	1:K:18:LEU:HD23	1.88	0.56
1:F:64:ILE:HA	1:F:102:LEU:O	2.06	0.56
1:L:36:ARG:HG2	1:L:105:TRP:HZ2	1.71	0.55
1:I:9:LEU:HD21	1:I:55:PRO:HB3	1.87	0.55
1:A:106:GLN:O	1:C:96:LEU:HD12	2.07	0.55
1:H:64:ILE:HD11	1:H:105:TRP:CD1	2.43	0.54
1:L:36:ARG:HG2	1:L:105:TRP:CZ2	2.43	0.54
1:J:6:ASP:OD1	1:J:42:ARG:HB2	2.07	0.54
1:K:8:ASN:H	1:K:8:ASN:ND2	2.03	0.53
1:G:2:PHE:HB2	1:G:62:SER:HB2	1.90	0.53
1:H:3:LEU:O	1:H:39:VAL:HA	2.09	0.53
1:A:3:LEU:HB2	1:A:39:VAL:HG22	1.91	0.53
1:B:71:GLU:OE1	1:D:79:HIS:HE1	1.92	0.52
1:L:91:GLY:O	1:L:92:GLN:C	2.52	0.52
1:B:96:LEU:HD21	1:C:105:TRP:HE3	1.75	0.51
1:H:18:LEU:HA	1:H:21:ARG:NH1	2.25	0.51
1:A:10:PRO:HB2	1:A:12:ASN:OD1	2.10	0.51
1:A:49:LEU:HA	1:B:38:ASN:HD22	1.75	0.51
1:A:45:LEU:HD22	1:B:42:ARG:HG2	1.92	0.50
1:D:3:LEU:HD23	1:D:59:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HB3	1:B:95:ILE:HD13	1.95	0.49
1:D:38:ASN:CG	1:E:96:LEU:HD11	2.37	0.49
1:H:42:ARG:HG2	1:I:45:LEU:HD22	1.94	0.49
1:K:15:PRO:HG2	1:K:18:LEU:HB2	1.93	0.49
1:L:58:GLN:HA	1:L:96:LEU:O	2.12	0.49
1:F:1:PRO:HB3	1:F:63:SER:OG	2.13	0.49
1:E:36:ARG:HB2	1:E:36:ARG:HH11	1.78	0.48
1:H:96:LEU:CG	1:J:106:GLN:O	2.62	0.48
1:K:8:ASN:HD22	1:K:8:ASN:N	2.00	0.48
1:I:54:GLU:O	1:I:55:PRO:C	2.55	0.48
1:H:64:ILE:HD11	1:H:105:TRP:NE1	2.28	0.48
1:H:97:ILE:O	1:J:105:TRP:HA	2.14	0.47
1:G:10:PRO:HG2	1:G:13:ARG:CD	2.43	0.47
1:G:10:PRO:CG	1:G:13:ARG:HD3	2.44	0.47
1:B:92:GLN:O	1:C:108:GLY:HA3	2.14	0.47
1:J:96:LEU:HD23	1:J:97:ILE:N	2.29	0.47
1:D:8:ASN:HA	1:D:45:LEU:O	2.15	0.46
1:B:3:LEU:HB3	1:B:59:LEU:HD11	1.98	0.46
1:H:84:LEU:HD12	1:H:84:LEU:HA	1.78	0.46
1:I:42:ARG:HG2	1:J:45:LEU:HD22	1.98	0.46
1:A:52:SER:HB3	1:A:94:ARG:HH12	1.81	0.46
1:G:85:THR:C	1:G:87:GLU:H	2.23	0.46
1:K:19:GLU:H	1:K:19:GLU:CD	2.24	0.46
1:L:33:PRO:C	1:L:35:ASP:N	2.74	0.45
1:G:81:PHE:HB3	1:G:92:GLN:HG2	1.99	0.45
1:H:16:ALA:O	1:H:21:ARG:NH2	2.50	0.45
1:E:33:PRO:HB2	1:E:35:ASP:OD1	2.17	0.45
1:A:106:GLN:HE22	1:C:74:ARG:HA	1.82	0.45
1:E:15:PRO:HG3	1:K:12:ASN:HD21	1.82	0.45
1:E:14:VAL:HG21	1:E:43:PRO:HB3	1.98	0.44
1:D:62:SER:HA	1:D:100:PHE:O	2.18	0.44
1:H:45:LEU:HD22	1:J:42:ARG:HG2	1.99	0.44
1:D:48:ALA:HA	1:D:52:SER:O	2.17	0.44
1:H:49:LEU:O	1:H:50:SER:C	2.60	0.44
1:G:2:PHE:C	1:G:3:LEU:HD12	2.43	0.44
1:G:10:PRO:HB2	1:G:12:ASN:OD1	2.17	0.44
1:H:85:THR:OG1	1:H:90:LEU:O	2.35	0.44
1:K:2:PHE:HB2	1:K:62:SER:HG	1.82	0.44
1:H:69:THR:O	1:H:70:ALA:C	2.62	0.43
1:E:33:PRO:C	1:E:35:ASP:H	2.26	0.43
1:A:13:ARG:O	1:A:13:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:PHE:HB2	1:D:62:SER:OG	2.18	0.43
1:L:84:LEU:HB3	1:L:95:ILE:HD13	2.01	0.43
1:D:54:GLU:HG2	1:D:94:ARG:CZ	2.49	0.43
1:B:92:GLN:HG2	1:C:108:GLY:CA	2.47	0.43
1:I:14:VAL:O	1:I:15:PRO:C	2.62	0.43
1:L:67:VAL:HG11	1:L:99:PHE:HD2	1.84	0.42
1:L:31:GLY:C	1:L:32:LYS:HG2	2.44	0.42
1:A:64:ILE:HD11	1:A:105:TRP:CD1	2.55	0.42
1:K:62:SER:HA	1:K:100:PHE:O	2.19	0.42
1:H:21:ARG:NH1	1:H:87:GLU:OE1	2.53	0.42
1:H:19:GLU:HG2	1:H:20:LYS:N	2.33	0.42
1:K:2:PHE:HB2	1:K:62:SER:OG	2.20	0.42
1:B:59:LEU:O	1:B:97:ILE:HA	2.20	0.41
1:E:65:GLY:O	1:E:101:PRO:HB3	2.20	0.41
1:H:33:PRO:HD2	1:H:36:ARG:HG3	2.02	0.41
1:L:54:GLU:O	1:L:55:PRO:C	2.62	0.41
1:D:84:LEU:HD13	1:D:84:LEU:HA	1.75	0.41
1:J:2:PHE:HB2	1:J:62:SER:OG	2.19	0.41
1:E:10:PRO:HD2	1:E:13:ARG:HG3	2.03	0.41
1:B:61:ILE:O	1:B:99:PHE:HA	2.21	0.41
1:D:8:ASN:HD21	1:D:55:PRO:HA	1.86	0.41
1:H:72:ASP:O	1:H:76:HIS:CG	2.73	0.41
1:J:88:LEU:O	1:J:89:ALA:HB3	2.21	0.41
1:H:8:ASN:HA	1:H:45:LEU:O	2.21	0.41
1:K:33:PRO:HG2	1:K:36:ARG:HG3	2.02	0.41
1:G:59:LEU:O	1:G:97:ILE:HA	2.21	0.41
1:J:1:PRO:N	1:J:36:ARG:O	2.52	0.41
1:I:55:PRO:HB2	1:I:90:LEU:HD21	2.01	0.40
1:I:22:LEU:O	1:I:26:ALA:N	2.55	0.40
1:L:61:ILE:HD12	1:L:99:PHE:CE2	2.56	0.40
1:A:15:PRO:HG3	1:H:13:ARG:HD2	2.03	0.40
1:E:33:PRO:C	1:E:35:ASP:N	2.80	0.40

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	A	107/113 (95%)	106 (99%)	1 (1%)	0	100	100
1	B	106/113 (94%)	100 (94%)	6 (6%)	0	100	100
1	C	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
1	D	108/113 (96%)	104 (96%)	4 (4%)	0	100	100
1	E	106/113 (94%)	101 (95%)	5 (5%)	0	100	100
1	F	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
1	G	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
1	H	106/113 (94%)	101 (95%)	5 (5%)	0	100	100
1	I	106/113 (94%)	100 (94%)	6 (6%)	0	100	100
1	J	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
1	K	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	L	102/113 (90%)	95 (93%)	7 (7%)	0	100	100
All	All	1256/1356 (93%)	1197 (95%)	59 (5%)	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	79/91 (87%)	79 (100%)	0	100	100
1	B	82/91 (90%)	77 (94%)	5 (6%)	17	23
1	C	77/91 (85%)	73 (95%)	4 (5%)	21	28
1	D	81/91 (89%)	75 (93%)	6 (7%)	13	15
1	E	81/91 (89%)	80 (99%)	1 (1%)	63	74
1	F	81/91 (89%)	79 (98%)	2 (2%)	42	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	84/91 (92%)	80 (95%)	4 (5%)	23	32
1	H	79/91 (87%)	72 (91%)	7 (9%)	9	10
1	I	75/91 (82%)	72 (96%)	3 (4%)	28	39
1	J	76/91 (84%)	72 (95%)	4 (5%)	20	28
1	K	76/91 (84%)	74 (97%)	2 (3%)	40	53
1	L	80/91 (88%)	74 (92%)	6 (8%)	12	15
All	All	951/1092 (87%)	907 (95%)	44 (5%)	24	33

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	ASN
1	B	18	LEU
1	B	54	GLU
1	B	84	LEU
1	B	106	GLN
1	C	3	LEU
1	C	13	ARG
1	C	53	THR
1	C	92	GLN
1	D	18	LEU
1	D	54	GLU
1	D	62	SER
1	D	66	VAL
1	D	84	LEU
1	D	95	ILE
1	E	13	ARG
1	F	54	GLU
1	F	97	ILE
1	G	63	SER
1	G	66	VAL
1	G	96	LEU
1	G	102	LEU
1	H	36	ARG
1	H	49	LEU
1	H	58	GLN
1	H	84	LEU
1	H	85	THR
1	H	97	ILE
1	H	98	ARG

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Mol	Chain	Res	Type
1	I	49	LEU
1	I	50	SER
1	I	98	ARG
1	J	52	SER
1	J	64	ILE
1	J	74	ARG
1	J	86	LYS
1	K	8	ASN
1	K	19	GLU
1	L	75	SER
1	L	84	LEU
1	L	92	GLN
1	L	98	ARG
1	L	103	GLU
1	L	106	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	106	GLN
1	B	38	ASN
1	B	92	GLN
1	B	106	GLN
1	C	92	GLN
1	D	38	ASN
1	D	79	HIS
1	E	12	ASN
1	E	79	HIS
1	F	38	ASN
1	I	79	HIS
1	J	12	ASN
1	K	8	ASN
1	K	12	ASN
1	K	38	ASN
1	L	79	HIS

5.3.3 RNA ⓘ

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](#)

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 [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	109/113 (96%)	0.18	2 (1%) 67 68	17, 26, 39, 54	0
1	B	108/113 (95%)	0.15	1 (0%) 81 82	16, 26, 37, 48	0
1	C	109/113 (96%)	0.18	6 (5%) 30 28	15, 25, 37, 47	0
1	D	110/113 (97%)	0.37	6 (5%) 30 28	15, 28, 42, 57	0
1	E	108/113 (95%)	0.13	1 (0%) 81 82	16, 26, 40, 46	0
1	F	109/113 (96%)	0.26	4 (3%) 45 43	16, 29, 42, 68	1 (0%)
1	G	109/113 (96%)	0.55	5 (4%) 37 34	17, 31, 51, 63	0
1	H	108/113 (95%)	0.39	2 (1%) 66 67	19, 29, 45, 53	0
1	I	108/113 (95%)	0.65	10 (9%) 14 11	18, 31, 45, 51	0
1	J	99/113 (87%)	0.35	2 (2%) 65 66	17, 30, 42, 63	0
1	K	102/113 (90%)	0.50	3 (2%) 53 53	18, 30, 48, 69	0
1	L	106/113 (93%)	0.79	7 (6%) 24 21	24, 36, 48, 58	0
All	All	1285/1356 (94%)	0.37	49 (3%) 44 42	15, 29, 44, 69	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	50	SER	5.6
1	K	110	ILE	3.6
1	C	92	GLN	3.5
1	I	108	GLY	3.4
1	L	108	GLY	3.3
1	D	109	LYS	3.2
1	F	49	LEU	3.1
1	I	9	LEU	3.0
1	J	74	ARG	3.0
1	F	50	SER	3.0
1	D	54	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	28	SER	2.9
1	C	28	SER	2.9
1	D	108	GLY	2.7
1	G	105	TRP	2.7
1	A	63	SER	2.6
1	K	77	SER	2.6
1	C	67	VAL	2.5
1	D	51	GLY	2.5
1	I	26	ALA	2.5
1	C	50	SER	2.4
1	G	62	SER	2.4
1	G	107	ILE	2.4
1	A	51	GLY	2.4
1	I	28	SER	2.4
1	G	35	ASP	2.3
1	G	86	LYS	2.3
1	L	56	CYS	2.3
1	L	36	ARG	2.3
1	E	63	SER	2.3
1	L	51	GLY	2.3
1	I	34	ALA	2.2
1	D	110	ILE	2.2
1	L	11	ALA	2.2
1	J	107	ILE	2.2
1	F	109	LYS	2.2
1	K	12	ASN	2.2
1	I	11	ALA	2.1
1	I	12	ASN	2.1
1	B	56	CYS	2.1
1	F	82	GLU	2.1
1	C	35	ASP	2.1
1	H	35	ASP	2.1
1	H	65	GLY	2.1
1	C	96	LEU	2.1
1	I	67	VAL	2.1
1	L	31	GLY	2.1
1	D	84	LEU	2.0
1	I	105	TRP	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.