



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:03 AM UTC

PDB ID : 7MY7 / pdb_00007my7
Title : Se-CrtE N-term His-tag structure
Authors : Peat, T.S.; Newman, J.
Deposited on : 2021-05-20
Resolution : 2.36 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

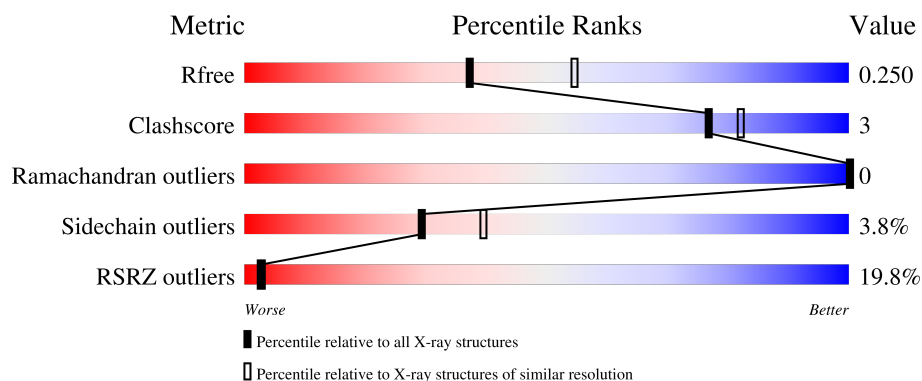
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	322	4% 79% 6% 15%
1	BBB	322	4% 78% 7% 15%
1	CCC	322	26% 61% • 34%
1	DDD	322	28% 75% 5% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7581 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 Farnesyl-diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	275	Total	C	N	O	S	0	2	0
			2094	1320	358	409	7			
1	BBB	275	Total	C	N	O	S	0	0	0
			2055	1297	350	401	7			
1	CCC	213	Total	C	N	O	S	0	0	0
			1512	947	265	293	7			
1	DDD	259	Total	C	N	O	S	0	0	0
			1845	1161	317	360	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-20	MET	-	expression tag	UNP Q31Q61
AAA	-19	GLY	-	expression tag	UNP Q31Q61
AAA	-18	SER	-	expression tag	UNP Q31Q61
AAA	-17	SER	-	expression tag	UNP Q31Q61
AAA	-16	HIS	-	expression tag	UNP Q31Q61
AAA	-15	HIS	-	expression tag	UNP Q31Q61
AAA	-14	HIS	-	expression tag	UNP Q31Q61
AAA	-13	HIS	-	expression tag	UNP Q31Q61
AAA	-12	HIS	-	expression tag	UNP Q31Q61
AAA	-11	HIS	-	expression tag	UNP Q31Q61
AAA	-10	SER	-	expression tag	UNP Q31Q61
AAA	-9	SER	-	expression tag	UNP Q31Q61
AAA	-8	GLY	-	expression tag	UNP Q31Q61
AAA	-7	LEU	-	expression tag	UNP Q31Q61
AAA	-6	VAL	-	expression tag	UNP Q31Q61
AAA	-5	PRO	-	expression tag	UNP Q31Q61
AAA	-4	ARG	-	expression tag	UNP Q31Q61
AAA	-3	GLY	-	expression tag	UNP Q31Q61
AAA	-2	SER	-	expression tag	UNP Q31Q61
AAA	-1	HIS	-	expression tag	UNP Q31Q61
AAA	0	MET	-	expression tag	UNP Q31Q61

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-20	MET	-	expression tag	UNP Q31Q61
BBB	-19	GLY	-	expression tag	UNP Q31Q61
BBB	-18	SER	-	expression tag	UNP Q31Q61
BBB	-17	SER	-	expression tag	UNP Q31Q61
BBB	-16	HIS	-	expression tag	UNP Q31Q61
BBB	-15	HIS	-	expression tag	UNP Q31Q61
BBB	-14	HIS	-	expression tag	UNP Q31Q61
BBB	-13	HIS	-	expression tag	UNP Q31Q61
BBB	-12	HIS	-	expression tag	UNP Q31Q61
BBB	-11	HIS	-	expression tag	UNP Q31Q61
BBB	-10	SER	-	expression tag	UNP Q31Q61
BBB	-9	SER	-	expression tag	UNP Q31Q61
BBB	-8	GLY	-	expression tag	UNP Q31Q61
BBB	-7	LEU	-	expression tag	UNP Q31Q61
BBB	-6	VAL	-	expression tag	UNP Q31Q61
BBB	-5	PRO	-	expression tag	UNP Q31Q61
BBB	-4	ARG	-	expression tag	UNP Q31Q61
BBB	-3	GLY	-	expression tag	UNP Q31Q61
BBB	-2	SER	-	expression tag	UNP Q31Q61
BBB	-1	HIS	-	expression tag	UNP Q31Q61
BBB	0	MET	-	expression tag	UNP Q31Q61
CCC	-20	MET	-	expression tag	UNP Q31Q61
CCC	-19	GLY	-	expression tag	UNP Q31Q61
CCC	-18	SER	-	expression tag	UNP Q31Q61
CCC	-17	SER	-	expression tag	UNP Q31Q61
CCC	-16	HIS	-	expression tag	UNP Q31Q61
CCC	-15	HIS	-	expression tag	UNP Q31Q61
CCC	-14	HIS	-	expression tag	UNP Q31Q61
CCC	-13	HIS	-	expression tag	UNP Q31Q61
CCC	-12	HIS	-	expression tag	UNP Q31Q61
CCC	-11	HIS	-	expression tag	UNP Q31Q61
CCC	-10	SER	-	expression tag	UNP Q31Q61
CCC	-9	SER	-	expression tag	UNP Q31Q61
CCC	-8	GLY	-	expression tag	UNP Q31Q61
CCC	-7	LEU	-	expression tag	UNP Q31Q61
CCC	-6	VAL	-	expression tag	UNP Q31Q61
CCC	-5	PRO	-	expression tag	UNP Q31Q61
CCC	-4	ARG	-	expression tag	UNP Q31Q61
CCC	-3	GLY	-	expression tag	UNP Q31Q61
CCC	-2	SER	-	expression tag	UNP Q31Q61
CCC	-1	HIS	-	expression tag	UNP Q31Q61
CCC	0	MET	-	expression tag	UNP Q31Q61

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-20	MET	-	expression tag	UNP Q31Q61
DDD	-19	GLY	-	expression tag	UNP Q31Q61
DDD	-18	SER	-	expression tag	UNP Q31Q61
DDD	-17	SER	-	expression tag	UNP Q31Q61
DDD	-16	HIS	-	expression tag	UNP Q31Q61
DDD	-15	HIS	-	expression tag	UNP Q31Q61
DDD	-14	HIS	-	expression tag	UNP Q31Q61
DDD	-13	HIS	-	expression tag	UNP Q31Q61
DDD	-12	HIS	-	expression tag	UNP Q31Q61
DDD	-11	HIS	-	expression tag	UNP Q31Q61
DDD	-10	SER	-	expression tag	UNP Q31Q61
DDD	-9	SER	-	expression tag	UNP Q31Q61
DDD	-8	GLY	-	expression tag	UNP Q31Q61
DDD	-7	LEU	-	expression tag	UNP Q31Q61
DDD	-6	VAL	-	expression tag	UNP Q31Q61
DDD	-5	PRO	-	expression tag	UNP Q31Q61
DDD	-4	ARG	-	expression tag	UNP Q31Q61
DDD	-3	GLY	-	expression tag	UNP Q31Q61
DDD	-2	SER	-	expression tag	UNP Q31Q61
DDD	-1	HIS	-	expression tag	UNP Q31Q61
DDD	0	MET	-	expression tag	UNP Q31Q61

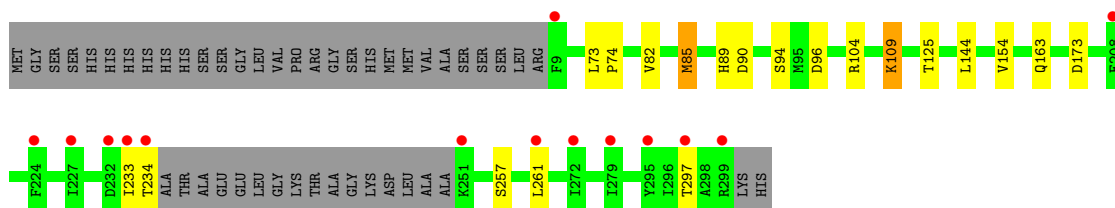
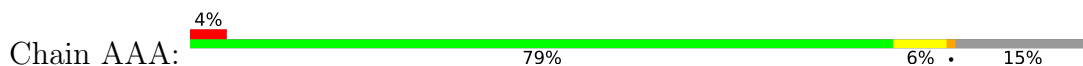
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	41	Total O 41 41	0	0
2	BBB	31	Total O 31 31	0	0
2	CCC	3	Total O 3 3	0	0

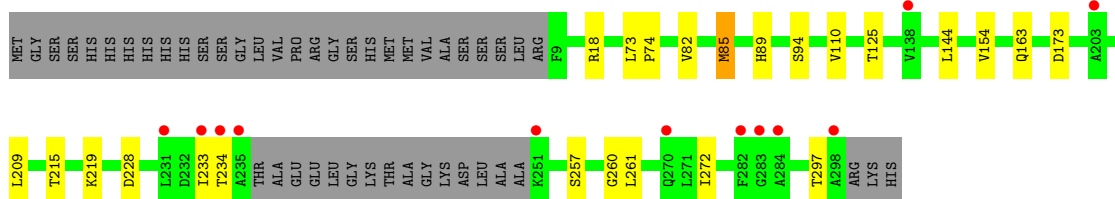
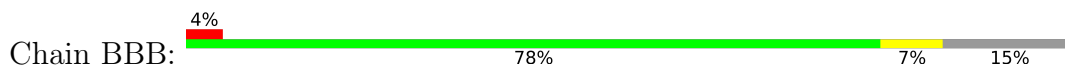
3 Residue-property plots [i](#)

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.

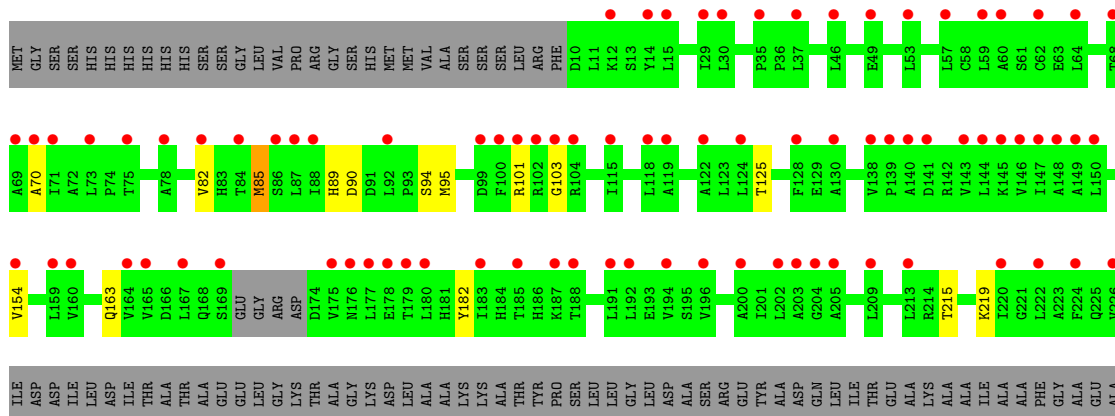
- Molecule 1: Farnesyl-diphosphate synthase



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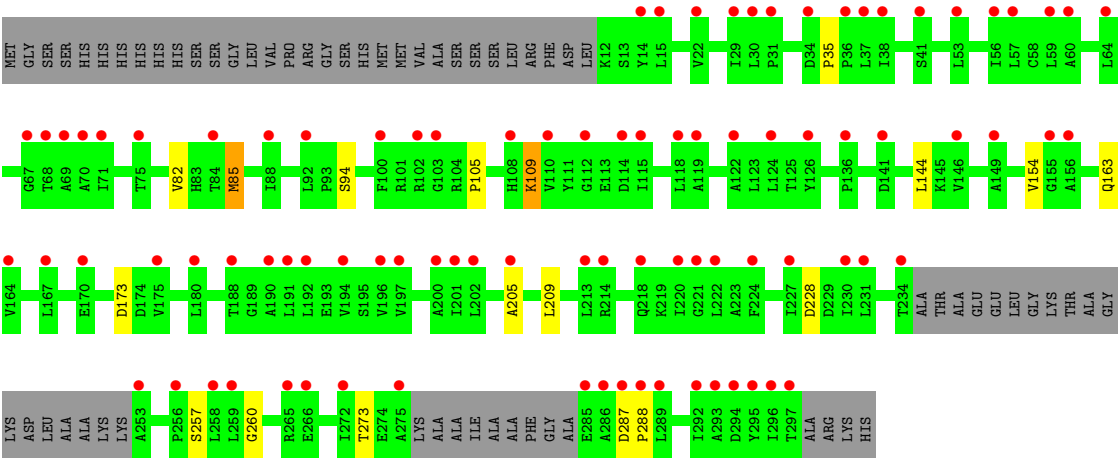
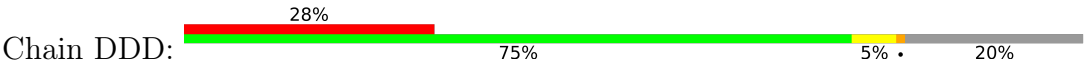


- Molecule 1: Farnesyl-diphosphate synthase



ASP
PRO
LEU
SER
ARG
ALA
TLE
TLE
ALA
ASP
TYR
THR
TLE
ALA
ARG
LYS
HIS

● Molecule 1: Farnesyl-diphosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.51Å 56.44Å 144.81Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	48.65 – 2.36 48.65 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.65-2.36) 99.9 (48.65-2.36)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.218 , 0.247 0.226 , 0.250	Depositor DCC
R_{free} test set	2566 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7581	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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	AAA	1.03	0/2126	1.50	2/2891 (0.1%)
1	BBB	1.03	0/2087	1.46	1/2844 (0.0%)
1	CCC	1.05	0/1535	1.51	0/2100
1	DDD	1.06	0/1873	1.50	1/2562 (0.0%)
All	All	1.04	0/7621	1.49	4/10397 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	104	ARG	O-C-N	-11.44	109.93	121.94
1	DDD	260	GLY	CA-C-O	-6.14	116.90	122.24
1	BBB	260	GLY	CA-C-O	-5.78	117.37	121.88
1	AAA	104	ARG	CA-C-O	5.07	125.51	120.03

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	2094	0	2087	12	0
1	BBB	2055	0	2034	16	0
1	CCC	1512	0	1430	12	1
1	DDD	1845	0	1741	11	1
2	AAA	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	31	0	0	2	0
2	CCC	3	0	0	0	0
All	All	7581	0	7292	43	1

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.

All (43) 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:BBB:272:ILE:HG13	1:BBB:297:THR:HG23	1.52	0.92
1:AAA:90[A]:ASP:OD2	1:AAA:96:ASP:OD2	1.88	0.91
1:BBB:272:ILE:HG13	1:BBB:297:THR:CG2	2.02	0.89
1:BBB:110:VAL:CG1	1:CCC:70:ALA:HB2	2.05	0.84
1:BBB:110:VAL:HG13	1:CCC:70:ALA:HB2	1.63	0.81
1:CCC:90:ASP:OD1	1:CCC:163:GLN:NE2	2.22	0.72
1:BBB:110:VAL:HG11	1:CCC:70:ALA:HB2	1.77	0.67
1:BBB:110:VAL:HG11	1:CCC:70:ALA:CB	2.35	0.57
1:BBB:163:GLN:NE2	2:BBB:401:HOH:O	2.38	0.56
1:DDD:205:ALA:HB1	1:DDD:209:LEU:HD23	1.90	0.53
1:AAA:233:ILE:HD11	1:AAA:261:LEU:HD13	1.91	0.53
1:AAA:82:VAL:O	1:AAA:85:MET:HG3	2.10	0.52
1:BBB:82:VAL:O	1:BBB:85:MET:HG3	2.10	0.52
1:DDD:82:VAL:O	1:DDD:85:MET:HG3	2.10	0.52
1:DDD:105:PRO:HB3	1:DDD:109:LYS:HG2	1.95	0.48
1:BBB:82:VAL:HG11	1:BBB:154:VAL:HG22	1.99	0.46
1:AAA:90[A]:ASP:CG	1:AAA:96:ASP:OD2	2.59	0.45
1:AAA:109:LYS:HA	1:AAA:109:LYS:HD2	1.64	0.45
1:BBB:18:ARG:HD2	2:BBB:411:HOH:O	2.15	0.45
1:CCC:82:VAL:O	1:CCC:85:MET:HG3	2.17	0.45
1:AAA:73:LEU:HB3	1:AAA:74:PRO:HD3	1.98	0.44
1:AAA:125:THR:HG21	1:BBB:154:VAL:HG12	1.98	0.44
1:DDD:82:VAL:HG11	1:DDD:154:VAL:HG22	2.00	0.44
1:CCC:82:VAL:HG11	1:CCC:154:VAL:HG22	2.00	0.44
1:AAA:82:VAL:HG11	1:AAA:154:VAL:CG2	2.48	0.44
1:CCC:89:HIS:O	1:CCC:95:MET:HG3	2.18	0.44
1:CCC:82:VAL:HG11	1:CCC:154:VAL:CG2	2.48	0.43
1:DDD:287:ASP:N	1:DDD:288:PRO:HD3	2.34	0.43
1:DDD:144:LEU:HD12	1:DDD:144:LEU:HA	1.86	0.43
1:DDD:82:VAL:HG11	1:DDD:154:VAL:CG2	2.49	0.43
1:AAA:85:MET:HE1	1:AAA:89:HIS:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:154:VAL:HG12	1:BBB:125:THR:HG21	2.01	0.42
1:CCC:215:THR:O	1:CCC:219:LYS:HG2	2.20	0.42
1:AAA:90[B]:ASP:OD1	1:AAA:163:GLN:NE2	2.44	0.42
1:BBB:73:LEU:HB3	1:BBB:74:PRO:HD3	2.02	0.42
1:AAA:82:VAL:HG11	1:AAA:154:VAL:HG22	2.02	0.41
1:BBB:85:MET:HE1	1:BBB:89:HIS:CE1	2.56	0.41
1:CCC:182:TYR:OH	1:DDD:35:PRO:HD3	2.20	0.41
1:DDD:205:ALA:CB	1:DDD:209:LEU:HD23	2.51	0.41
1:BBB:82:VAL:HG11	1:BBB:154:VAL:CG2	2.50	0.41
1:BBB:215:THR:O	1:BBB:219:LYS:HG2	2.21	0.41
1:DDD:85:MET:HE2	1:DDD:85:MET:HB2	1.93	0.40
1:CCC:125:THR:HG21	1:DDD:154:VAL:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:103:GLY:O	1:DDD:273:THR:O[1_565]	1.91	0.29

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	273/322 (85%)	270 (99%)	3 (1%)	0	100	100
1	BBB	271/322 (84%)	265 (98%)	6 (2%)	0	100	100
1	CCC	209/322 (65%)	206 (99%)	3 (1%)	0	100	100
1	DDD	253/322 (79%)	248 (98%)	5 (2%)	0	100	100
All	All	1006/1288 (78%)	989 (98%)	17 (2%)	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	215/252 (85%)	207 (96%)	8 (4%)	30	40
1	BBB	208/252 (82%)	198 (95%)	10 (5%)	23	29
1	CCC	143/252 (57%)	140 (98%)	3 (2%)	47	61
1	DDD	174/252 (69%)	167 (96%)	7 (4%)	28	37
All	All	740/1008 (73%)	712 (96%)	28 (4%)	29	39

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	85	MET
1	AAA	94	SER
1	AAA	109	LYS
1	AAA	144	LEU
1	AAA	173	ASP
1	AAA	234	THR
1	AAA	257	SER
1	AAA	297	THR
1	BBB	85	MET
1	BBB	94	SER
1	BBB	144	LEU
1	BBB	173	ASP
1	BBB	209	LEU
1	BBB	228	ASP
1	BBB	233	ILE
1	BBB	234	THR
1	BBB	257	SER
1	BBB	261	LEU
1	CCC	85	MET
1	CCC	94	SER
1	CCC	101	ARG
1	DDD	85	MET
1	DDD	94	SER
1	DDD	109	LYS

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Mol	Chain	Res	Type
1	DDD	163	GLN
1	DDD	173	ASP
1	DDD	228	ASP
1	DDD	257	SER

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](#)

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	AAA	275/322 (85%)	0.38	14 (5%) 33 39	21, 46, 84, 110	2 (0%)
1	BBB	275/322 (85%)	0.41	12 (4%) 39 45	29, 49, 82, 100	0
1	CCC	213/322 (66%)	1.84	85 (39%) 1 0	68, 97, 124, 146	0
1	DDD	259/322 (80%)	1.72	91 (35%) 1 0	68, 94, 120, 145	0
All	All	1022/1288 (79%)	1.03	202 (19%) 3 3	21, 74, 117, 146	2 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	69	ALA	6.4
1	CCC	102	ARG	5.2
1	DDD	59	LEU	4.9
1	DDD	286	ALA	4.9
1	CCC	53	LEU	4.8
1	CCC	69	ALA	4.8
1	CCC	203	ALA	4.8
1	CCC	100	PHE	4.4
1	CCC	147	ILE	4.4
1	DDD	14	TYR	4.2
1	CCC	150	LEU	4.1
1	CCC	49	GLU	4.1
1	CCC	68	THR	4.0
1	CCC	143	VAL	3.9
1	DDD	297	THR	3.9
1	AAA	299	ARG	3.8
1	DDD	296	ILE	3.8
1	DDD	202	LEU	3.7
1	CCC	226	VAL	3.7
1	AAA	233	ILE	3.6
1	CCC	103	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	9	PHE	3.6
1	DDD	289	LEU	3.6
1	DDD	294	ASP	3.6
1	CCC	70	ALA	3.6
1	CCC	139	PRO	3.6
1	DDD	234	THR	3.5
1	CCC	194	VAL	3.5
1	DDD	253	ALA	3.5
1	BBB	233	ILE	3.5
1	DDD	231	LEU	3.5
1	CCC	183	ILE	3.5
1	CCC	154	VAL	3.4
1	CCC	175	VAL	3.4
1	DDD	68	THR	3.4
1	CCC	130	ALA	3.4
1	DDD	275	ALA	3.4
1	CCC	222	LEU	3.4
1	CCC	148	ALA	3.4
1	CCC	149	ALA	3.4
1	AAA	251	LYS	3.4
1	CCC	88	ILE	3.3
1	DDD	272	ILE	3.3
1	DDD	285	GLU	3.3
1	CCC	140	ALA	3.3
1	DDD	103	GLY	3.3
1	AAA	232	ASP	3.3
1	AAA	234	THR	3.3
1	CCC	146	VAL	3.3
1	DDD	288	PRO	3.2
1	DDD	190	ALA	3.2
1	CCC	59	LEU	3.2
1	CCC	87	LEU	3.2
1	DDD	287	ASP	3.2
1	CCC	180	LEU	3.2
1	CCC	29	ILE	3.2
1	CCC	224	PHE	3.1
1	DDD	293	ALA	3.1
1	AAA	272	ILE	3.1
1	BBB	235	ALA	3.1
1	CCC	196	VAL	3.1
1	CCC	213	LEU	3.1
1	CCC	176	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	DDD	149	ALA	3.1
1	CCC	191	LEU	3.1
1	AAA	297	THR	3.0
1	DDD	213	LEU	3.0
1	AAA	295	TYR	3.0
1	DDD	164	VAL	3.0
1	BBB	282	PHE	3.0
1	CCC	192	LEU	3.0
1	DDD	108	HIS	2.9
1	BBB	251	LYS	2.9
1	DDD	29	ILE	2.9
1	CCC	144	LEU	2.9
1	DDD	75	THR	2.9
1	BBB	284	ALA	2.9
1	CCC	177	LEU	2.9
1	DDD	197	VAL	2.9
1	CCC	101	ARG	2.9
1	DDD	70	ALA	2.9
1	DDD	222	LEU	2.8
1	CCC	104	ARG	2.8
1	DDD	220	ILE	2.8
1	AAA	208[A]	GLU	2.8
1	DDD	180	LEU	2.8
1	DDD	194	VAL	2.8
1	DDD	88	ILE	2.7
1	DDD	218	GLN	2.7
1	CCC	187	LYS	2.7
1	DDD	57	LEU	2.7
1	CCC	15	LEU	2.7
1	CCC	167	LEU	2.7
1	DDD	191	LEU	2.7
1	DDD	196	VAL	2.7
1	CCC	75	THR	2.7
1	CCC	160	VAL	2.6
1	CCC	188	THR	2.6
1	DDD	71	ILE	2.6
1	DDD	227	ILE	2.6
1	CCC	64	LEU	2.6
1	CCC	145	LYS	2.6
1	DDD	102	ARG	2.6
1	AAA	224	PHE	2.6
1	DDD	84	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	DDD	188	THR	2.6
1	CCC	209	LEU	2.6
1	DDD	119	ALA	2.6
1	BBB	283	GLY	2.6
1	DDD	41	SER	2.5
1	DDD	175	VAL	2.5
1	CCC	71	ILE	2.5
1	DDD	192	LEU	2.5
1	CCC	205	ALA	2.5
1	DDD	156	ALA	2.5
1	CCC	84	THR	2.5
1	DDD	224	PHE	2.5
1	CCC	220	ILE	2.5
1	DDD	118	LEU	2.5
1	BBB	270	GLN	2.5
1	CCC	164	VAL	2.5
1	DDD	259	LEU	2.5
1	CCC	179	THR	2.4
1	DDD	64	LEU	2.4
1	DDD	124	LEU	2.4
1	DDD	295	TYR	2.4
1	CCC	204	GLY	2.4
1	BBB	138	VAL	2.4
1	DDD	30	LEU	2.4
1	DDD	37	LEU	2.4
1	DDD	53	LEU	2.4
1	DDD	266	GLU	2.4
1	CCC	86	SER	2.4
1	CCC	128	PHE	2.4
1	DDD	110	VAL	2.4
1	DDD	146	VAL	2.4
1	DDD	92	LEU	2.4
1	DDD	167	LEU	2.4
1	CCC	60	ALA	2.4
1	CCC	169	SER	2.4
1	CCC	46	LEU	2.4
1	DDD	112	GLY	2.3
1	DDD	230	ILE	2.3
1	CCC	178	GLU	2.3
1	CCC	141	ASP	2.3
1	DDD	126	TYR	2.3
1	CCC	200	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	DDD	38	ILE	2.3
1	CCC	124	LEU	2.3
1	BBB	234	THR	2.3
1	CCC	57	LEU	2.2
1	DDD	31	PRO	2.2
1	DDD	60	ALA	2.2
1	DDD	115	ILE	2.2
1	DDD	201	ILE	2.2
1	BBB	231	LEU	2.2
1	CCC	92	LEU	2.2
1	CCC	202	LEU	2.2
1	DDD	214	ARG	2.2
1	CCC	12	LYS	2.2
1	CCC	119	ALA	2.2
1	AAA	279	ILE	2.2
1	CCC	115	ILE	2.2
1	AAA	261	LEU	2.2
1	CCC	138	VAL	2.2
1	DDD	141	ASP	2.2
1	DDD	136	PRO	2.2
1	DDD	256	PRO	2.2
1	BBB	203	ALA	2.2
1	CCC	159	LEU	2.2
1	DDD	22	VAL	2.2
1	DDD	265	ARG	2.1
1	CCC	73	LEU	2.1
1	DDD	15	LEU	2.1
1	CCC	165	VAL	2.1
1	CCC	14	TYR	2.1
1	DDD	292	ILE	2.1
1	DDD	170	GLU	2.1
1	DDD	155	GLY	2.1
1	CCC	37	LEU	2.1
1	DDD	67	GLY	2.1
1	CCC	78	ALA	2.1
1	CCC	122	ALA	2.1
1	DDD	122	ALA	2.1
1	CCC	30	LEU	2.1
1	AAA	227	ILE	2.1
1	CCC	99	ASP	2.1
1	DDD	34	ASP	2.1
1	DDD	56	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	DDD	114	ASP	2.1
1	CCC	118	LEU	2.0
1	DDD	258	LEU	2.0
1	CCC	35	PRO	2.0
1	CCC	82	VAL	2.0
1	DDD	221	GLY	2.0
1	DDD	100	PHE	2.0
1	CCC	185	THR	2.0
1	BBB	298	ALA	2.0
1	DDD	200	ALA	2.0
1	DDD	205	ALA	2.0
1	CCC	62	CYS	2.0
1	DDD	36	PRO	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.