



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 10:20 PM EDT

PDB ID : 7MY7
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

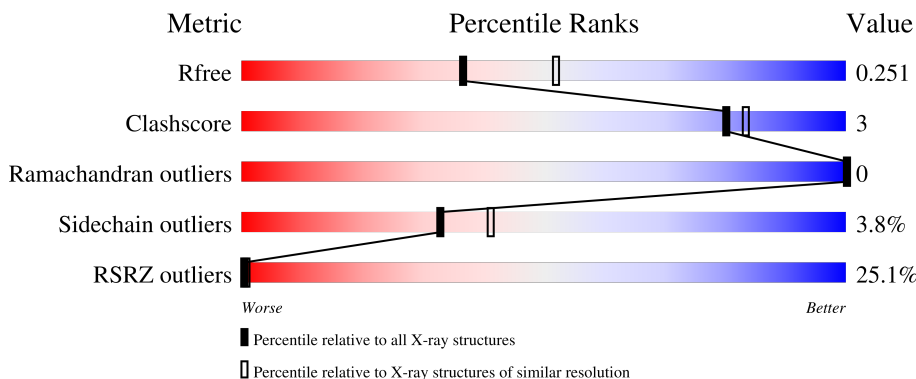
1 Overall quality at a glance i

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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	12% (poor fit) 80% (0 outliers), 5% (1 outlier), 15% (not modelled)
1	BBB	322	5% (poor fit) 79% (0 outliers), 7% (1 outlier), 15% (not modelled)
1	CCC	322	34% (poor fit) 61% (0 outliers), 5% (1 outlier), 34% (not modelled)
1	DDD	322	29% (poor fit) 75% (0 outliers), 5% (1 outlier), 20% (not modelled)

2 Entry composition i

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

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

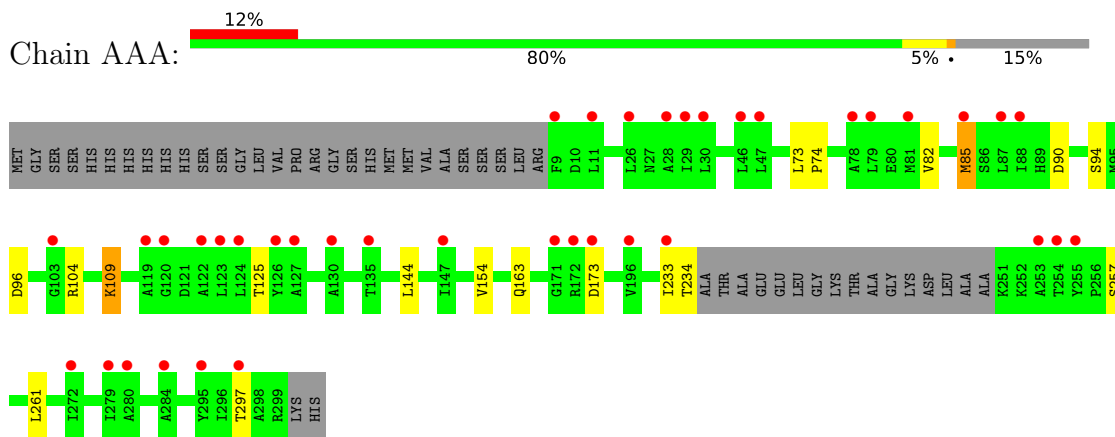
- Molecule 2 is water.

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

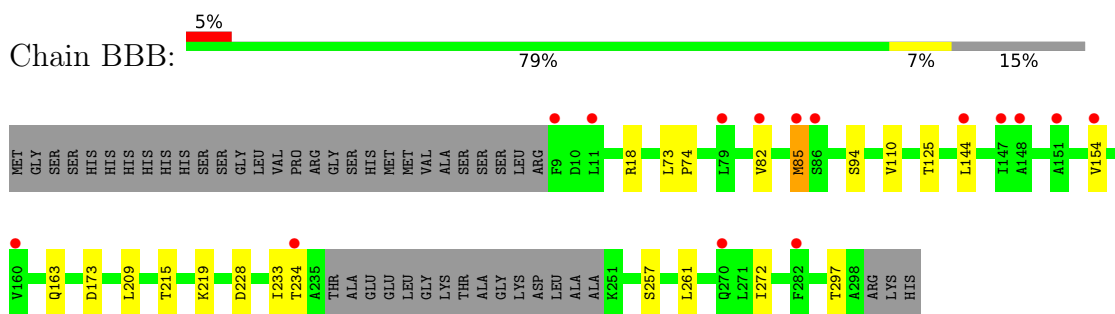
3 Residue-property plots [i](#)

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.

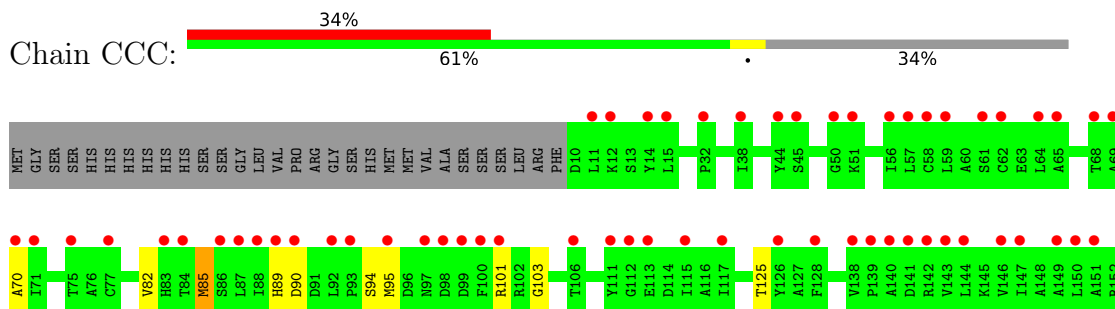
- Molecule 1: Farnesyl-diphosphate synthase

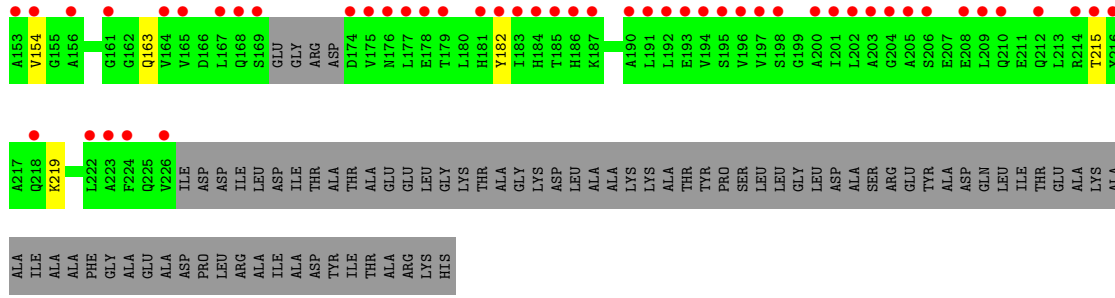


- Molecule 1: Farnesyl-diphosphate synthase

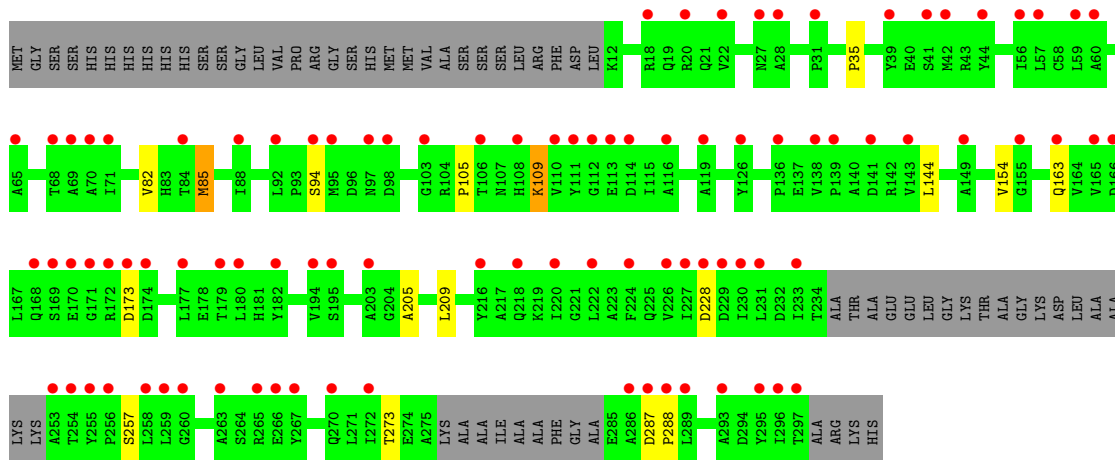
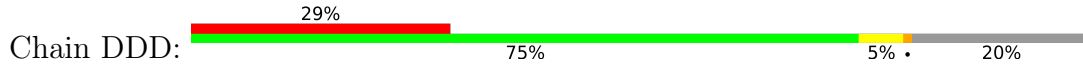


- Molecule 1: Farnesyl-diphosphate synthase





● 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) 99.5 (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)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.218 , 0.247 0.226 , 0.251	Depositor DCC
R_{free} test set	2566 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.70	0/2126	0.80	1/2891 (0.0%)
1	BBB	0.68	0/2087	0.77	0/2844
1	CCC	0.69	0/1535	0.73	0/2100
1	DDD	0.69	0/1873	0.73	0/2562
All	All	0.69	0/7621	0.76	1/10397 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	104	ARG	O-C-N	-5.88	109.93	121.10

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	11	0
1	BBB	2055	0	2034	15	0
1	CCC	1512	0	1430	12	1
1	DDD	1845	0	1741	10	1
2	AAA	41	0	0	0	0
2	BBB	31	0	0	2	0
2	CCC	3	0	0	0	0
All	All	7581	0	7292	40	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 (40) 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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:215:THR:O	1:BBB:219:LYS:HG2	2.21	0.41
1:AAA:90[A]:ASP:CG	1:AAA:96:ASP:OD2	2.59	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 [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	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 [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	215/252 (85%)	207 (96%)	8 (4%)	34	42
1	BBB	208/252 (82%)	198 (95%)	10 (5%)	25	30
1	CCC	143/252 (57%)	140 (98%)	3 (2%)	53	65
1	DDD	174/252 (69%)	167 (96%)	7 (4%)	31	39
All	All	740/1008 (73%)	712 (96%)	28 (4%)	33	41

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
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 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 [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%)	1.11	39 (14%) 2 4	26, 47, 84, 110	0
1	BBB	275/322 (85%)	0.81	15 (5%) 25 36	29, 49, 82, 100	0
1	CCC	213/322 (66%)	2.40	109 (51%) 0 0	68, 97, 124, 146	0
1	DDD	259/322 (80%)	1.83	94 (36%) 0 0	68, 94, 120, 145	0
All	All	1022/1288 (79%)	1.48	257 (25%) 0 1	26, 74, 117, 146	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	203	ALA	12.2
1	DDD	171	GLY	8.7
1	DDD	253	ALA	8.6
1	CCC	11	LEU	8.3
1	CCC	177	LEU	8.2
1	DDD	98	ASP	7.5
1	CCC	181	HIS	7.2
1	CCC	196	VAL	7.0
1	CCC	179	THR	6.8
1	DDD	259	LEU	6.8
1	DDD	288	PRO	6.7
1	CCC	204	GLY	6.6
1	CCC	143	VAL	6.6
1	CCC	185	THR	6.5
1	DDD	226	VAL	6.4
1	DDD	293	ALA	6.3
1	CCC	15	LEU	6.2
1	CCC	202	LEU	6.0
1	DDD	113	GLU	5.9
1	CCC	182	TYR	5.8
1	CCC	175	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	CCC	176	ASN	5.6
1	CCC	169	SER	5.6
1	CCC	139	PRO	5.6
1	CCC	216	TYR	5.4
1	CCC	84	THR	5.4
1	DDD	287	ASP	5.4
1	DDD	222	LEU	5.4
1	CCC	215	THR	5.3
1	DDD	180	LEU	5.3
1	CCC	62	CYS	5.3
1	DDD	297	THR	5.2
1	DDD	165	VAL	5.2
1	DDD	97	ASN	5.2
1	DDD	174	ASP	5.2
1	DDD	172	ARG	5.1
1	DDD	126	TYR	5.0
1	CCC	140	ALA	5.0
1	CCC	156	ALA	5.0
1	CCC	222	LEU	5.0
1	CCC	149	ALA	5.0
1	CCC	64	LEU	4.9
1	CCC	147	ILE	4.9
1	CCC	205	ALA	4.8
1	CCC	59	LEU	4.8
1	CCC	68	THR	4.8
1	DDD	108	HIS	4.7
1	CCC	70	ALA	4.7
1	AAA	9	PHE	4.7
1	CCC	206	SER	4.7
1	DDD	143	VAL	4.7
1	CCC	61	SER	4.6
1	DDD	254	THR	4.5
1	DDD	224	PHE	4.5
1	DDD	70	ALA	4.5
1	CCC	100	PHE	4.5
1	DDD	68	THR	4.4
1	CCC	195	SER	4.4
1	DDD	258	LEU	4.3
1	DDD	138	VAL	4.3
1	DDD	230	ILE	4.3
1	CCC	90	ASP	4.3
1	CCC	141	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	150	LEU	4.2
1	CCC	138	VAL	4.1
1	CCC	99	ASP	4.1
1	AAA	254	THR	4.1
1	CCC	98	ASP	4.1
1	CCC	50	GLY	4.0
1	DDD	103	GLY	4.0
1	DDD	173	ASP	3.9
1	DDD	263	ALA	3.9
1	CCC	93	PRO	3.9
1	CCC	113	GLU	3.9
1	CCC	56	ILE	3.9
1	DDD	44	TYR	3.8
1	CCC	210	GLN	3.8
1	AAA	279	ILE	3.8
1	DDD	22	VAL	3.8
1	CCC	178	GLU	3.8
1	DDD	255	TYR	3.8
1	BBB	282	PHE	3.7
1	CCC	214	ARG	3.7
1	DDD	41	SER	3.7
1	DDD	182	TYR	3.6
1	CCC	191	LEU	3.6
1	CCC	14	TYR	3.6
1	CCC	164	VAL	3.6
1	DDD	69	ALA	3.5
1	AAA	171	GLY	3.5
1	AAA	295	TYR	3.5
1	DDD	295	TYR	3.5
1	DDD	139	PRO	3.5
1	AAA	173	ASP	3.5
1	DDD	296	ILE	3.5
1	CCC	226	VAL	3.4
1	DDD	228	ASP	3.4
1	CCC	57	LEU	3.4
1	CCC	194	VAL	3.4
1	AAA	122	ALA	3.4
1	DDD	88	ILE	3.4
1	AAA	280	ALA	3.4
1	DDD	272	ILE	3.4
1	DDD	266	GLU	3.4
1	DDD	177	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	DDD	92	LEU	3.3
1	DDD	111	TYR	3.3
1	CCC	183	ILE	3.3
1	DDD	231	LEU	3.2
1	CCC	87	LEU	3.2
1	CCC	197	VAL	3.2
1	CCC	186	HIS	3.2
1	DDD	110	VAL	3.2
1	CCC	58	CYS	3.2
1	DDD	195	SER	3.2
1	CCC	75	THR	3.1
1	CCC	224	PHE	3.1
1	CCC	184	HIS	3.1
1	CCC	209	LEU	3.1
1	DDD	94	SER	3.1
1	CCC	154	VAL	3.1
1	DDD	60	ALA	3.1
1	DDD	20	ARG	3.1
1	CCC	198	SER	3.0
1	DDD	95	MET	3.0
1	CCC	201	ILE	3.0
1	CCC	174	ASP	3.0
1	CCC	69	ALA	3.0
1	DDD	56	ILE	3.0
1	DDD	170	GLU	3.0
1	CCC	86	SER	3.0
1	DDD	260	GLY	3.0
1	DDD	286	ALA	3.0
1	CCC	92	LEU	3.0
1	CCC	165	VAL	3.0
1	DDD	216	TYR	2.9
1	DDD	28	ALA	2.9
1	CCC	168	GLN	2.9
1	DDD	270	GLN	2.9
1	CCC	51	LYS	2.9
1	BBB	9	PHE	2.9
1	CCC	223	ALA	2.9
1	DDD	136	PRO	2.8
1	DDD	256	PRO	2.8
1	DDD	114	ASP	2.8
1	CCC	45	SER	2.8
1	DDD	42	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	CCC	71	ILE	2.7
1	DDD	84	THR	2.7
1	DDD	112	GLY	2.7
1	AAA	85	MET	2.7
1	DDD	27	ASN	2.7
1	DDD	31	PRO	2.7
1	CCC	111	TYR	2.7
1	DDD	163	GLN	2.7
1	CCC	88	ILE	2.7
1	AAA	11	LEU	2.7
1	DDD	229	ASP	2.6
1	AAA	284	ALA	2.6
1	CCC	128	PHE	2.6
1	DDD	71	ILE	2.6
1	DDD	119	ALA	2.6
1	CCC	106	THR	2.6
1	AAA	123	LEU	2.6
1	CCC	83	HIS	2.6
1	CCC	200	ALA	2.6
1	CCC	153	ALA	2.6
1	DDD	220	ILE	2.6
1	CCC	101	ARG	2.6
1	CCC	44	TYR	2.6
1	DDD	141	ASP	2.6
1	AAA	29	ILE	2.6
1	AAA	30	LEU	2.5
1	BBB	144	LEU	2.5
1	DDD	227	ILE	2.5
1	AAA	103	GLY	2.5
1	DDD	18	ARG	2.5
1	CCC	208	GLU	2.5
1	DDD	194	VAL	2.5
1	CCC	167	LEU	2.5
1	DDD	203	ALA	2.4
1	AAA	120	GLY	2.4
1	CCC	112	GLY	2.4
1	CCC	38	ILE	2.4
1	CCC	187	LYS	2.4
1	AAA	47	LEU	2.4
1	DDD	218	GLN	2.4
1	CCC	32	PRO	2.4
1	CCC	89	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	88	ILE	2.3
1	AAA	255	TYR	2.3
1	BBB	11	LEU	2.3
1	DDD	166	ASP	2.3
1	DDD	289	LEU	2.3
1	BBB	154	VAL	2.3
1	CCC	142	ARG	2.3
1	DDD	57	LEU	2.3
1	DDD	265	ARG	2.3
1	AAA	81	MET	2.3
1	AAA	135	THR	2.3
1	DDD	179	THR	2.3
1	DDD	168	GLN	2.3
1	AAA	130	ALA	2.3
1	DDD	106	THR	2.3
1	BBB	79	LEU	2.3
1	BBB	85	MET	2.3
1	BBB	82	VAL	2.3
1	AAA	78	ALA	2.3
1	AAA	272	ILE	2.3
1	BBB	148	ALA	2.3
1	AAA	172	ARG	2.2
1	AAA	233	ILE	2.2
1	DDD	149	ALA	2.2
1	DDD	267	TYR	2.2
1	CCC	97	ASN	2.2
1	DDD	39	TYR	2.2
1	DDD	169	SER	2.2
1	CCC	161	GLY	2.2
1	DDD	116	ALA	2.2
1	DDD	59	LEU	2.2
1	CCC	218	GLN	2.2
1	BBB	234	THR	2.2
1	CCC	77	CYS	2.2
1	CCC	117	ILE	2.2
1	DDD	233	ILE	2.2
1	AAA	127	ALA	2.1
1	CCC	193	GLU	2.1
1	AAA	46	LEU	2.1
1	DDD	155	GLY	2.1
1	CCC	12	LYS	2.1
1	CCC	65	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	270	GLN	2.1
1	AAA	297	THR	2.1
1	AAA	126	TYR	2.1
1	AAA	253	ALA	2.1
1	CCC	146	VAL	2.1
1	CCC	190	ALA	2.1
1	AAA	147	ILE	2.1
1	BBB	147	ILE	2.1
1	AAA	79	LEU	2.1
1	CCC	144	LEU	2.1
1	AAA	196	VAL	2.1
1	BBB	160	VAL	2.1
1	CCC	95	MET	2.1
1	AAA	119	ALA	2.1
1	BBB	151	ALA	2.1
1	CCC	212	GLN	2.0
1	AAA	26	LEU	2.0
1	AAA	87	LEU	2.0
1	AAA	28	ALA	2.0
1	CCC	151	ALA	2.0
1	CCC	126	TYR	2.0
1	CCC	115	ILE	2.0
1	BBB	86	SER	2.0
1	DDD	65	ALA	2.0
1	AAA	124	LEU	2.0
1	CCC	192	LEU	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 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.