



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:43 AM UTC

PDB ID : 7A26 / pdb_00007a26
Title : Structure of soluble SmhA crystal form 1 of the tripartite alpha-pore forming toxin, Smh, from *Serratia marcescens*.
Authors : Churchill-Angus, A.M.; Baker, P.J.
Deposited on : 2020-08-16
Resolution : 2.98 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:

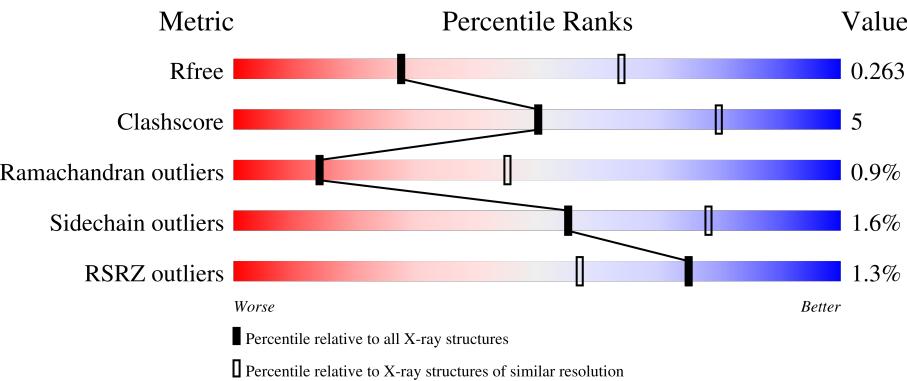
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	373	
1	BBB	373	
1	CCC	373	
1	DDD	373	
1	EEE	373	

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Mol	Chain	Length	Quality of chain
1	FFF	373	
1	GGG	373	
1	HHH	373	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	CCC	403	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41162 atoms, of which 20699 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 SmhA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	344	Total	C	H	N	O	Se	175	0	0
			5195	1620	2622	441	504	8			
1	BBB	341	Total	C	H	N	O	Se	177	0	0
			5176	1614	2613	439	502	8			
1	CCC	348	Total	C	H	N	O	Se	179	0	0
			5256	1639	2650	447	512	8			
1	EEE	346	Total	C	H	N	O	Se	177	0	0
			5225	1629	2635	444	509	8			
1	FFF	345	Total	C	H	N	O	Se	174	0	0
			5208	1625	2627	442	506	8			
1	GGG	345	Total	C	H	N	O	Se	177	0	0
			5218	1627	2632	443	508	8			
1	HHH	347	Total	C	H	N	O	Se	177	0	0
			5237	1633	2641	445	510	8			
1	DDD	327	Total	C	H	N	O	Se	178	0	0
			4604	1459	2279	401	458	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MSE	-	initiating methionine	UNP A0A1Q4NVM5
AAA	366	LEU	-	expression tag	UNP A0A1Q4NVM5
AAA	367	GLU	-	expression tag	UNP A0A1Q4NVM5
AAA	368	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	369	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	370	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	371	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	372	HIS	-	expression tag	UNP A0A1Q4NVM5
AAA	373	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	1	MSE	-	initiating methionine	UNP A0A1Q4NVM5
BBB	366	LEU	-	expression tag	UNP A0A1Q4NVM5
BBB	367	GLU	-	expression tag	UNP A0A1Q4NVM5
BBB	368	HIS	-	expression tag	UNP A0A1Q4NVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	369	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	370	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	371	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	372	HIS	-	expression tag	UNP A0A1Q4NVM5
BBB	373	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	1	MSE	-	initiating methionine	UNP A0A1Q4NVM5
CCC	366	LEU	-	expression tag	UNP A0A1Q4NVM5
CCC	367	GLU	-	expression tag	UNP A0A1Q4NVM5
CCC	368	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	369	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	370	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	371	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	372	HIS	-	expression tag	UNP A0A1Q4NVM5
CCC	373	HIS	-	expression tag	UNP A0A1Q4NVM5
EEE	1	MSE	-	initiating methionine	UNP A0A1Q4NVM5
EEE	366	LEU	-	expression tag	UNP A0A1Q4NVM5
EEE	367	GLU	-	expression tag	UNP A0A1Q4NVM5
EEE	368	HIS	-	expression tag	UNP A0A1Q4NVM5
EEE	369	HIS	-	expression tag	UNP A0A1Q4NVM5
EEE	370	HIS	-	expression tag	UNP A0A1Q4NVM5
EEE	371	HIS	-	expression tag	UNP A0A1Q4NVM5
EEE	372	HIS	-	expression tag	UNP A0A1Q4NVM5
EEE	373	HIS	-	expression tag	UNP A0A1Q4NVM5
FFF	1	MSE	-	initiating methionine	UNP A0A1Q4NVM5
FFF	366	LEU	-	expression tag	UNP A0A1Q4NVM5
FFF	367	GLU	-	expression tag	UNP A0A1Q4NVM5
FFF	368	HIS	-	expression tag	UNP A0A1Q4NVM5
FFF	369	HIS	-	expression tag	UNP A0A1Q4NVM5
FFF	370	HIS	-	expression tag	UNP A0A1Q4NVM5
FFF	371	HIS	-	expression tag	UNP A0A1Q4NVM5
FFF	372	HIS	-	expression tag	UNP A0A1Q4NVM5
FFF	373	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	1	MSE	-	initiating methionine	UNP A0A1Q4NVM5
GGG	366	LEU	-	expression tag	UNP A0A1Q4NVM5
GGG	367	GLU	-	expression tag	UNP A0A1Q4NVM5
GGG	368	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	369	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	370	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	371	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	372	HIS	-	expression tag	UNP A0A1Q4NVM5
GGG	373	HIS	-	expression tag	UNP A0A1Q4NVM5
HHH	1	MSE	-	initiating methionine	UNP A0A1Q4NVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
HHH	366	LEU	-	expression tag	UNP A0A1Q4NVM5
HHH	367	GLU	-	expression tag	UNP A0A1Q4NVM5
HHH	368	HIS	-	expression tag	UNP A0A1Q4NVM5
HHH	369	HIS	-	expression tag	UNP A0A1Q4NVM5
HHH	370	HIS	-	expression tag	UNP A0A1Q4NVM5
HHH	371	HIS	-	expression tag	UNP A0A1Q4NVM5
HHH	372	HIS	-	expression tag	UNP A0A1Q4NVM5
HHH	373	HIS	-	expression tag	UNP A0A1Q4NVM5
DDD	1	MSE	-	initiating methionine	UNP A0A1Q4NVM5
DDD	366	LEU	-	expression tag	UNP A0A1Q4NVM5
DDD	367	GLU	-	expression tag	UNP A0A1Q4NVM5
DDD	368	HIS	-	expression tag	UNP A0A1Q4NVM5
DDD	369	HIS	-	expression tag	UNP A0A1Q4NVM5
DDD	370	HIS	-	expression tag	UNP A0A1Q4NVM5
DDD	371	HIS	-	expression tag	UNP A0A1Q4NVM5
DDD	372	HIS	-	expression tag	UNP A0A1Q4NVM5
DDD	373	HIS	-	expression tag	UNP A0A1Q4NVM5

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total Ca 1 1	0	0
2	CCC	2	Total Ca 2 2	0	0
2	FFF	1	Total Ca 1 1	0	0
2	GGG	1	Total Ca 1 1	0	0
2	HHH	1	Total Ca 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	CCC	1	Total Cl 1 1	0	0
3	FFF	1	Total Cl 1 1	0	0
3	DDD	1	Total Cl 1 1	0	0

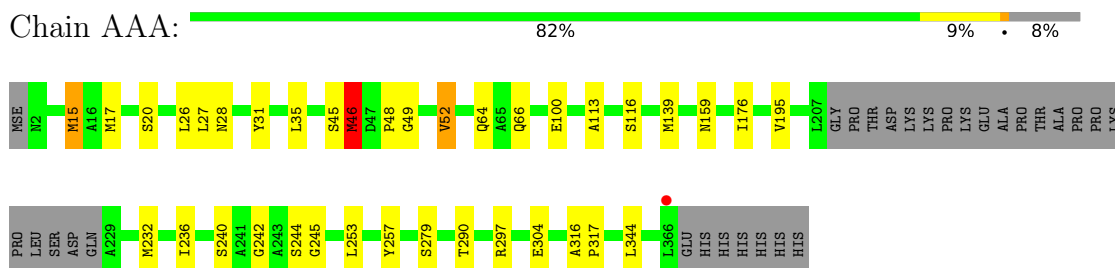
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	6	Total 6	O 6	0	0
4	BBB	10	Total 10	O 10	0	0
4	CCC	2	Total 2	O 2	0	0
4	EEE	3	Total 3	O 3	0	0
4	FFF	3	Total 3	O 3	0	0
4	GGG	5	Total 5	O 5	0	0
4	HHH	3	Total 3	O 3	0	0
4	DDD	2	Total 2	O 2	0	0

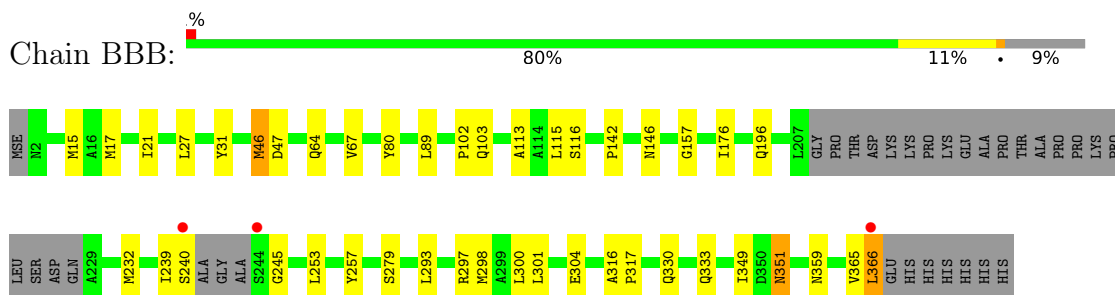
3 Residue-property plots [i](#)

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.

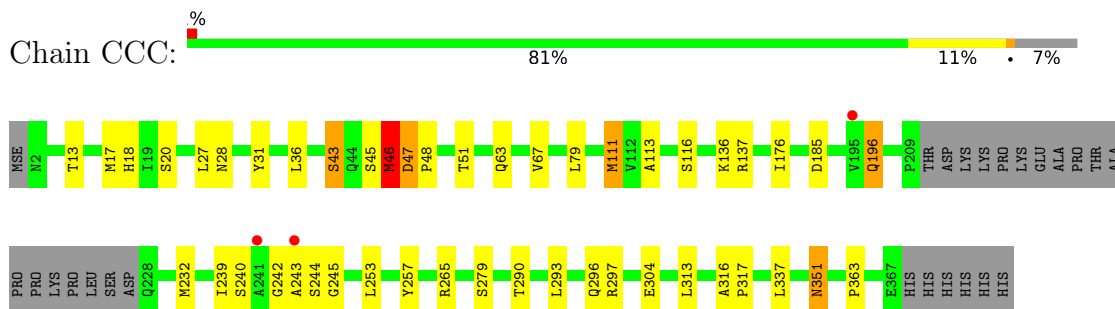
- Molecule 1: SmhA



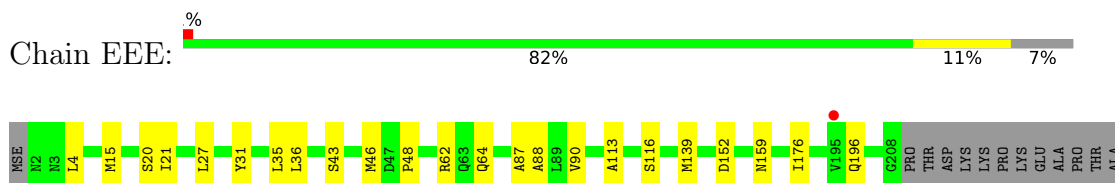
- Molecule 1: SmhA



- Molecule 1: SmhA



- Molecule 1: SmhA





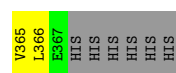
• Molecule 1: SmhA

Chain FFF: 80% 11% 8%



• Molecule 1: SmhA

Chain GGG: 78% 13% 8%



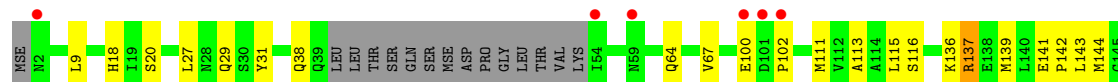
• Molecule 1: SmhA

Chain HHH: 82% 11% 7%



• Molecule 1: SmhA

Chain DDD: 5% 71% 14% 12%





4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	151.36Å 151.36Å 133.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.69 – 2.98 67.69 – 2.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (67.69-2.98) 99.8 (67.69-2.98)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.220 , 0.254 0.227 , 0.263	Depositor DCC
R_{free} test set	3051 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	41162	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9769e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	1.01	0/2595	1.67	7/3510 (0.2%)
1	BBB	1.02	0/2584	1.64	6/3493 (0.2%)
1	CCC	1.04	0/2629	1.62	6/3556 (0.2%)
1	DDD	1.10	0/2344	1.67	6/3181 (0.2%)
1	EEE	1.02	0/2612	1.67	7/3532 (0.2%)
1	FFF	1.04	3/2603 (0.1%)	1.68	10/3521 (0.3%)
1	GGG	1.05	0/2608	1.63	6/3527 (0.2%)
1	HHH	1.02	0/2618	1.66	9/3540 (0.3%)
All	All	1.04	3/20593 (0.0%)	1.65	57/27860 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FFF	298	MSE	SE-CE	-5.80	1.78	1.95
1	FFF	144	MSE	SE-CE	-5.24	1.79	1.95
1	FFF	298	MSE	CG-SE	-5.14	1.80	1.95

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	46	MSE	CG-SE-CE	10.85	122.80	98.92
1	EEE	46	MSE	CG-SE-CE	9.66	120.18	98.92
1	GGG	15	MSE	CG-SE-CE	9.63	120.11	98.92
1	AAA	46	MSE	CG-SE-CE	9.18	119.12	98.92
1	CCC	232	MSE	CG-SE-CE	8.59	117.83	98.92
1	AAA	15	MSE	CG-SE-CE	8.20	116.97	98.92
1	DDD	185	ASP	CA-CB-CG	8.17	120.77	112.60
1	EEE	232	MSE	CG-SE-CE	8.04	116.60	98.92
1	HHH	15	MSE	CG-SE-CE	7.35	115.10	98.92
1	FFF	46	MSE	CG-SE-CE	7.22	114.81	98.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FFF	15	MSE	CG-SE-CE	7.01	114.35	98.92
1	BBB	366	LEU	CA-C-O	7.00	132.71	120.80
1	DDD	281	GLN	CB-CG-CD	-6.93	100.82	112.60
1	BBB	15	MSE	CG-SE-CE	6.92	114.16	98.92
1	FFF	174	GLU	CB-CG-CD	6.86	124.27	112.60
1	FFF	232	MSE	CG-SE-CE	6.86	114.02	98.92
1	GGG	139	MSE	CG-SE-CE	6.64	113.53	98.92
1	DDD	310	GLU	CB-CG-CD	6.59	123.80	112.60
1	EEE	15	MSE	CG-SE-CE	6.57	113.38	98.92
1	CCC	185	ASP	CB-CA-C	6.54	123.24	110.67
1	BBB	46	MSE	CG-SE-CE	6.37	112.93	98.92
1	GGG	101	ASP	CA-CB-CG	6.34	118.94	112.60
1	DDD	139	MSE	CG-SE-CE	6.33	112.86	98.92
1	AAA	232	MSE	CG-SE-CE	6.31	112.80	98.92
1	HHH	139	MSE	CG-SE-CE	6.27	112.71	98.92
1	EEE	139	MSE	CG-SE-CE	6.25	112.68	98.92
1	EEE	152	ASP	CA-CB-CG	6.21	118.81	112.60
1	FFF	239	ILE	CA-C-O	-6.18	113.06	120.78
1	FFF	121	HIS	CA-CB-CG	6.12	119.92	113.80
1	GGG	46	MSE	CG-SE-CE	5.91	111.92	98.92
1	AAA	46	MSE	CA-C-N	5.80	127.39	122.28
1	AAA	46	MSE	C-N-CA	5.80	127.39	122.28
1	HHH	46	MSE	CG-SE-CE	5.79	111.66	98.92
1	AAA	244	SER	CA-C-O	-5.63	115.90	122.37
1	FFF	77	ILE	CA-C-N	5.63	126.23	119.98
1	FFF	77	ILE	C-N-CA	5.63	126.23	119.98
1	GGG	102	PRO	CB-CA-C	5.62	120.84	111.56
1	CCC	196	GLN	CB-CG-CD	5.54	122.02	112.60
1	DDD	232	MSE	CG-SE-CE	5.52	111.07	98.92
1	BBB	232	MSE	CG-SE-CE	5.51	111.05	98.92
1	EEE	196	GLN	CB-CG-CD	5.35	121.70	112.60
1	BBB	351	ASN	CA-CB-CG	-5.34	107.26	112.60
1	EEE	43	SER	CA-C-O	-5.32	113.85	119.97
1	CCC	111	MSE	CG-SE-CE	5.30	110.58	98.92
1	FFF	104	VAL	N-CA-CB	5.28	119.67	110.65
1	GGG	120	GLN	CB-CG-CD	-5.27	103.64	112.60
1	HHH	232	MSE	CG-SE-CE	5.27	110.51	98.92
1	HHH	12	GLN	CB-CA-C	5.24	120.84	110.42
1	HHH	238	ALA	CA-C-O	-5.19	114.48	120.24
1	AAA	139	MSE	CG-SE-CE	5.16	110.27	98.92
1	BBB	47	ASP	CA-CB-CG	5.15	117.75	112.60
1	DDD	152	ASP	CA-CB-CG	5.10	117.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FFF	240	SER	CA-C-O	-5.10	115.02	120.42
1	HHH	174	GLU	CB-CG-CD	5.04	121.18	112.60
1	CCC	351	ASN	CA-CB-CG	5.02	117.62	112.60
1	HHH	107	LYS	CA-C-N	5.01	125.40	119.94
1	HHH	107	LYS	C-N-CA	5.01	125.40	119.94

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	2573	2622	2615	25	0
1	BBB	2563	2613	2607	22	2
1	CCC	2606	2650	2645	26	4
1	DDD	2325	2279	2201	50	1
1	EEE	2590	2635	2630	23	2
1	FFF	2581	2627	2618	27	0
1	GGG	2586	2632	2627	32	1
1	HHH	2596	2641	2634	22	0
2	BBB	1	0	0	0	0
2	CCC	2	0	0	0	0
2	FFF	1	0	0	0	0
2	GGG	1	0	0	0	0
2	HHH	1	0	0	0	0
3	CCC	1	0	0	2	0
3	DDD	1	0	0	1	0
3	FFF	1	0	0	1	0
4	AAA	6	0	0	0	0
4	BBB	10	0	0	1	0
4	CCC	2	0	0	0	0
4	DDD	2	0	0	1	0
4	EEE	3	0	0	0	0
4	FFF	3	0	0	1	0
4	GGG	5	0	0	0	0
4	HHH	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20463	20699	20577	218	5

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 5.

All (218) 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:DDD:196:GLN:O	1:DDD:197:LEU:C	2.09	0.95
1:DDD:38:GLN:HE22	1:DDD:234:SER:H	1.19	0.90
1:DDD:141:GLU:CG	1:DDD:142:PRO:HD3	2.05	0.86
1:DDD:201:ILE:HG21	1:DDD:232:MSE:HE2	1.57	0.85
1:GGG:100:GLU:HB3	1:HHH:142:PRO:HG3	1.63	0.79
1:DDD:141:GLU:HG3	1:DDD:142:PRO:HD3	1.64	0.77
1:GGG:238:ALA:O	1:GGG:239:ILE:HG22	1.85	0.76
1:DDD:205:VAL:HG13	1:DDD:231:TYR:HB3	1.69	0.73
1:DDD:9:LEU:HD13	1:DDD:335:ILE:HD13	1.71	0.72
1:AAA:316:ALA:HB3	1:AAA:317:PRO:HD3	1.71	0.72
1:EEE:316:ALA:HB3	1:EEE:317:PRO:HD3	1.70	0.72
1:DDD:273:LEU:HD23	1:DDD:273:LEU:C	2.15	0.72
1:CCC:316:ALA:HB3	1:CCC:317:PRO:HD3	1.72	0.71
1:BBB:196:GLN:HG3	1:BBB:239:ILE:HD12	1.70	0.71
1:HHH:26:LEU:HD13	1:HHH:195:VAL:HG11	1.73	0.70
1:HHH:316:ALA:HB3	1:HHH:317:PRO:HD3	1.72	0.70
1:DDD:316:ALA:HB3	1:DDD:317:PRO:HD3	1.73	0.70
1:DDD:144:MSE:HE3	1:DDD:281:GLN:OE1	1.91	0.70
1:FFF:316:ALA:HB3	1:FFF:317:PRO:HD3	1.73	0.70
1:DDD:100:GLU:O	1:DDD:102:PRO:HD3	1.91	0.69
1:FFF:18:HIS:NE2	3:FFF:402:CL:CL	2.62	0.69
1:BBB:316:ALA:HB3	1:BBB:317:PRO:HD3	1.73	0.69
1:GGG:316:ALA:HB3	1:GGG:317:PRO:HD3	1.73	0.68
1:DDD:9:LEU:CD1	1:DDD:335:ILE:HD13	2.22	0.68
1:EEE:239:ILE:HD12	1:EEE:239:ILE:O	1.95	0.67
1:AAA:159:ASN:HB2	1:DDD:351:ASN:ND2	2.10	0.67
1:FFF:26:LEU:HD13	1:FFF:195:VAL:HG11	1.77	0.67
1:DDD:141:GLU:HG2	1:DDD:142:PRO:HD3	1.76	0.66
1:GGG:3:ASN:OD1	1:GGG:5:THR:HG22	1.96	0.66
1:GGG:366:LEU:N	1:GGG:366:LEU:HD22	2.11	0.66
1:HHH:17:MSE:HE1	1:HHH:301:LEU:N	2.11	0.66
1:BBB:17:MSE:SE	1:BBB:304:GLU:HG3	2.46	0.65
1:DDD:64:GLN:O	1:DDD:67:VAL:HG12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GGG:17:MSE:SE	1:GGG:304:GLU:HG3	2.48	0.64
1:EEE:242:GLY:O	1:EEE:244:SER:N	2.30	0.63
1:BBB:359:ASN:ND2	4:BBB:501:HOH:O	2.32	0.62
1:GGG:17:MSE:HE1	1:GGG:301:LEU:N	2.14	0.62
1:GGG:337:LEU:O	1:GGG:340:GLU:HG2	1.99	0.62
1:BBB:64:GLN:O	1:BBB:67:VAL:HG12	1.99	0.62
1:FFF:17:MSE:HE1	1:FFF:301:LEU:N	2.14	0.62
1:DDD:206:PRO:C	1:DDD:207:LEU:HD12	2.23	0.62
1:AAA:26:LEU:HD13	1:AAA:195:VAL:HG11	1.81	0.62
1:BBB:17:MSE:HE1	1:BBB:301:LEU:N	2.15	0.62
1:DDD:38:GLN:NE2	1:DDD:234:SER:H	1.97	0.60
1:CCC:18:HIS:NE2	3:CCC:403:CL:CL	2.70	0.60
1:DDD:264:TYR:HD1	1:DDD:275:SER:HG	1.47	0.60
1:DDD:18:HIS:NE2	3:DDD:401:CL:CL	2.69	0.59
1:EEE:31:TYR:O	1:EEE:35:LEU:HD13	2.02	0.59
1:CCC:17:MSE:SE	1:CCC:304:GLU:HG3	2.53	0.58
1:HHH:26:LEU:HD13	1:HHH:195:VAL:CG1	2.33	0.58
1:AAA:17:MSE:SE	1:AAA:304:GLU:HG3	2.54	0.58
1:AAA:159:ASN:HB2	1:DDD:351:ASN:HD21	1.67	0.58
1:FFF:79:LEU:CD1	1:FFF:298:MSE:HE1	2.34	0.58
1:EEE:87:ALA:O	1:EEE:90:VAL:HG22	2.04	0.58
1:DDD:144:MSE:CE	1:DDD:281:GLN:OE1	2.51	0.58
1:AAA:45:SER:O	1:AAA:46:MSE:HB2	2.04	0.57
1:FFF:79:LEU:CD1	1:FFF:298:MSE:CE	2.83	0.57
1:DDD:196:GLN:O	1:DDD:196:GLN:HG2	2.04	0.57
1:AAA:66:GLN:NE2	1:CCC:36:LEU:HD22	2.19	0.57
1:FFF:26:LEU:HD13	1:FFF:195:VAL:CG1	2.35	0.57
1:AAA:31:TYR:O	1:AAA:35:LEU:HD13	2.04	0.56
1:DDD:9:LEU:HD13	1:DDD:335:ILE:CD1	2.35	0.55
1:BBB:102:PRO:O	1:BBB:103:GLN:HG2	2.06	0.55
1:HHH:17:MSE:HE1	1:HHH:301:LEU:CA	2.37	0.55
1:DDD:247:GLN:O	1:DDD:250:VAL:HG23	2.07	0.55
1:FFF:31:TYR:O	1:FFF:35:LEU:HD13	2.05	0.55
1:GGG:333:GLN:OE1	1:GGG:333:GLN:HA	2.06	0.55
1:EEE:330:GLN:O	1:EEE:334:ILE:HG22	2.06	0.55
1:HHH:242:GLY:O	1:HHH:244:SER:N	2.40	0.55
1:AAA:26:LEU:HD13	1:AAA:195:VAL:CG1	2.37	0.54
1:CCC:313:LEU:O	1:CCC:313:LEU:HD23	2.08	0.54
1:FFF:79:LEU:HD12	1:FFF:298:MSE:HE1	1.89	0.54
1:HHH:253:LEU:HD11	1:HHH:257:TYR:CE2	2.43	0.53
1:EEE:253:LEU:HD11	1:EEE:257:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:173:ASN:HA	1:HHH:176:ILE:HG12	1.91	0.53
1:HHH:238:ALA:O	1:HHH:239:ILE:HB	2.09	0.53
1:HHH:132:GLN:HA	1:HHH:132:GLN:OE1	2.08	0.52
1:GGG:17:MSE:HE1	1:GGG:300:LEU:C	2.34	0.52
1:AAA:49:GLY:O	1:AAA:52:VAL:CG2	2.58	0.52
1:GGG:173:ASN:HA	1:GGG:176:ILE:HG12	1.90	0.52
1:AAA:253:LEU:HD11	1:AAA:257:TYR:CE2	2.45	0.52
1:EEE:240:SER:C	1:EEE:242:GLY:H	2.17	0.52
1:DDD:253:LEU:HD11	1:DDD:257:TYR:CE2	2.45	0.52
1:GGG:365:VAL:C	1:GGG:366:LEU:HD22	2.35	0.52
1:DDD:20:SER:HB3	1:DDD:297:ARG:HD3	1.92	0.52
1:AAA:66:GLN:CD	1:CCC:36:LEU:HD22	2.34	0.51
1:CCC:20:SER:HB3	1:CCC:297:ARG:HD3	1.92	0.51
1:CCC:240:SER:C	1:CCC:242:GLY:H	2.19	0.51
1:GGG:253:LEU:HD11	1:GGG:257:TYR:CE2	2.45	0.51
1:AAA:28:ASN:HB2	1:AAA:290:THR:HG22	1.91	0.51
1:BBB:196:GLN:HG3	1:BBB:239:ILE:CD1	2.41	0.51
1:CCC:79:LEU:HG	3:CCC:403:CL:CL	2.48	0.51
1:DDD:196:GLN:HG3	1:DDD:239:ILE:CB	2.41	0.51
1:EEE:87:ALA:O	1:EEE:90:VAL:CG2	2.58	0.50
1:FFF:173:ASN:HA	1:FFF:176:ILE:HG12	1.92	0.50
1:FFF:253:LEU:HD11	1:FFF:257:TYR:CE2	2.45	0.50
1:BBB:17:MSE:HE1	1:BBB:300:LEU:C	2.36	0.50
1:BBB:253:LEU:HD11	1:BBB:257:TYR:CE2	2.46	0.50
1:CCC:253:LEU:HD11	1:CCC:257:TYR:CE2	2.46	0.50
1:FFF:28:ASN:HB2	1:FFF:290:THR:HG22	1.93	0.50
1:DDD:173:ASN:HA	1:DDD:176:ILE:HG12	1.93	0.50
1:AAA:240:SER:C	1:AAA:242:GLY:H	2.19	0.50
1:CCC:28:ASN:HB2	1:CCC:290:THR:HG22	1.93	0.50
1:EEE:113:ALA:O	1:EEE:116:SER:HB3	2.12	0.50
1:DDD:207:LEU:HD12	1:DDD:207:LEU:N	2.26	0.50
1:FFF:101:ASP:HB3	1:FFF:104:VAL:HG13	1.94	0.50
1:GGG:113:ALA:O	1:GGG:116:SER:HB3	2.12	0.49
1:DDD:9:LEU:CD1	1:DDD:335:ILE:CD1	2.89	0.49
1:DDD:244:SER:O	1:DDD:245:GLY:C	2.54	0.49
1:DDD:240:SER:C	1:DDD:242:GLY:H	2.20	0.49
1:CCC:111:MSE:HE2	1:EEE:88:ALA:HB1	1.95	0.49
1:GGG:240:SER:C	1:GGG:242:GLY:H	2.19	0.49
1:AAA:113:ALA:O	1:AAA:116:SER:HB3	2.13	0.49
1:BBB:113:ALA:O	1:BBB:116:SER:HB3	2.13	0.49
1:CCC:113:ALA:O	1:CCC:116:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:49:GLY:O	1:AAA:52:VAL:HG23	2.12	0.49
1:DDD:247:GLN:HA	1:DDD:250:VAL:HG22	1.95	0.49
1:DDD:113:ALA:O	1:DDD:116:SER:HB3	2.13	0.48
1:FFF:17:MSE:HE1	1:FFF:300:LEU:C	2.37	0.48
1:HHH:113:ALA:O	1:HHH:116:SER:HB3	2.13	0.48
1:BBB:333:GLN:OE1	1:BBB:333:GLN:HA	2.12	0.48
1:HHH:240:SER:C	1:HHH:242:GLY:H	2.20	0.48
1:EEE:36:LEU:HD23	1:EEE:62:ARG:HG3	1.96	0.48
1:FFF:17:MSE:HE1	1:FFF:301:LEU:CA	2.43	0.48
1:CCC:313:LEU:HD23	1:CCC:313:LEU:C	2.38	0.48
1:GGG:151:ILE:HD11	1:GGG:277:ALA:HB1	1.95	0.48
1:BBB:142:PRO:O	1:BBB:146:ASN:ND2	2.46	0.48
1:HHH:28:ASN:HB2	1:HHH:290:THR:HG22	1.94	0.47
1:FFF:113:ALA:O	1:FFF:116:SER:HB3	2.14	0.47
1:GGG:238:ALA:O	1:GGG:239:ILE:CG2	2.59	0.47
1:BBB:330:GLN:OE1	1:EEE:48:PRO:HB2	2.15	0.46
1:HHH:242:GLY:C	1:HHH:244:SER:H	2.22	0.46
1:FFF:240:SER:C	1:FFF:242:GLY:H	2.24	0.46
1:HHH:195:VAL:O	1:HHH:195:VAL:HG13	2.16	0.46
1:DDD:147:PHE:HD2	1:DDD:281:GLN:HE22	1.63	0.46
1:EEE:4:LEU:H	1:EEE:4:LEU:HD22	1.79	0.46
1:CCC:293:LEU:O	1:CCC:297:ARG:HG3	2.15	0.46
1:DDD:143:LEU:HA	1:DDD:146:ASN:HD21	1.81	0.46
1:CCC:111:MSE:CE	1:EEE:88:ALA:HB1	2.46	0.46
1:BBB:17:MSE:HE2	1:BBB:17:MSE:HB3	1.77	0.46
1:EEE:90:VAL:HG21	1:EEE:342:TRP:CG	2.51	0.46
1:FFF:142:PRO:O	1:FFF:146:ASN:ND2	2.49	0.46
1:HHH:333:GLN:HA	1:HHH:333:GLN:OE1	2.16	0.46
1:CCC:176:ILE:HG23	1:CCC:253:LEU:CD1	2.46	0.45
1:GGG:321:GLN:OE1	1:GGG:321:GLN:HA	2.16	0.45
1:GGG:103:GLN:HB2	1:GGG:107:LYS:HE2	1.97	0.45
1:FFF:17:MSE:HE2	1:FFF:17:MSE:HB3	1.81	0.45
1:BBB:27:LEU:HG	1:BBB:31:TYR:CE2	2.50	0.45
1:BBB:293:LEU:O	1:BBB:297:ARG:HG3	2.16	0.45
1:DDD:293:LEU:O	1:DDD:297:ARG:HG3	2.15	0.45
1:FFF:196:GLN:HG3	1:FFF:239:ILE:HG13	1.97	0.45
1:CCC:45:SER:O	1:CCC:46:MSE:HB2	2.16	0.45
1:GGG:366:LEU:N	1:GGG:366:LEU:CD2	2.79	0.45
1:FFF:79:LEU:HD12	1:FFF:298:MSE:CE	2.47	0.45
1:CCC:43:SER:HB3	1:CCC:51:THR:HG21	1.98	0.44
1:CCC:242:GLY:O	1:CCC:244:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:27:LEU:HG	1:EEE:31:TYR:CE2	2.51	0.44
1:DDD:337:LEU:C	1:DDD:337:LEU:HD23	2.42	0.44
1:GGG:347:LYS:HD2	1:GGG:347:LYS:HA	1.65	0.44
1:FFF:27:LEU:HG	1:FFF:31:TYR:CE2	2.52	0.44
1:GGG:142:PRO:O	1:GGG:146:ASN:ND2	2.48	0.44
1:FFF:195:VAL:HG13	1:FFF:195:VAL:O	2.18	0.44
1:GGG:27:LEU:HG	1:GGG:31:TYR:CE2	2.52	0.44
1:AAA:195:VAL:HG13	1:AAA:195:VAL:O	2.18	0.43
1:DDD:242:GLY:O	1:DDD:244:SER:N	2.51	0.43
1:AAA:20:SER:HB2	1:AAA:297:ARG:HD2	2.00	0.43
1:AAA:100:GLU:OE2	1:AAA:100:GLU:N	2.51	0.43
4:FFF:501:HOH:O	1:GGG:82:LYS:HE3	2.18	0.43
1:BBB:17:MSE:HE1	1:BBB:301:LEU:CA	2.49	0.43
1:GGG:21:ILE:HG21	1:GGG:298:MSE:HE1	2.01	0.43
1:DDD:29:GLN:CB	4:DDD:502:HOH:O	2.66	0.43
1:CCC:46:MSE:O	1:CCC:47:ASP:C	2.62	0.43
1:DDD:237:GLN:HB2	1:DDD:365:VAL:HG21	2.00	0.43
1:BBB:176:ILE:HG23	1:BBB:253:LEU:CD1	2.48	0.43
1:EEE:176:ILE:HG23	1:EEE:253:LEU:CD1	2.49	0.43
1:AAA:64:GLN:HA	1:AAA:64:GLN:OE1	2.19	0.43
1:GGG:17:MSE:HE2	1:GGG:17:MSE:HB3	1.82	0.43
1:GGG:17:MSE:HE1	1:GGG:301:LEU:CA	2.49	0.43
1:DDD:321:GLN:HA	1:DDD:321:GLN:OE1	2.19	0.43
1:BBB:21:ILE:HG21	1:BBB:298:MSE:HE1	2.01	0.42
1:HHH:17:MSE:HE1	1:HHH:300:LEU:C	2.43	0.42
1:HHH:21:ILE:HG21	1:HHH:298:MSE:HE1	2.00	0.42
1:CCC:239:ILE:HD11	1:CCC:363:PRO:HG2	2.00	0.42
1:FFF:298:MSE:HE3	1:FFF:301:LEU:HD23	2.00	0.42
1:GGG:64:GLN:HA	1:GGG:64:GLN:OE1	2.19	0.42
1:DDD:247:GLN:HA	1:DDD:250:VAL:CG2	2.49	0.42
1:DDD:147:PHE:HD2	1:DDD:281:GLN:NE2	2.17	0.42
1:AAA:27:LEU:HG	1:AAA:31:TYR:CE2	2.53	0.42
1:CCC:47:ASP:HA	1:CCC:48:PRO:HD2	1.93	0.42
1:EEE:4:LEU:HD22	1:EEE:4:LEU:N	2.34	0.42
1:HHH:152:ASP:OD1	1:HHH:156:GLN:NE2	2.53	0.42
1:AAA:15:MSE:HE1	1:AAA:344:LEU:HG	2.02	0.42
1:HHH:17:MSE:HE1	1:HHH:301:LEU:HA	2.01	0.42
1:GGG:329:LYS:C	1:GGG:329:LYS:HD2	2.45	0.42
1:CCC:63:GLN:O	1:CCC:67:VAL:HG23	2.20	0.41
1:CCC:27:LEU:HG	1:CCC:31:TYR:CE2	2.54	0.41
1:FFF:20:SER:HB2	1:FFF:297:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:21:ILE:HG21	1:EEE:298:MSE:HE1	2.02	0.41
1:GGG:20:SER:HB2	1:GGG:297:ARG:HD2	2.02	0.41
1:GGG:79:LEU:HD23	1:GGG:79:LEU:HA	1.90	0.41
1:DDD:143:LEU:HA	1:DDD:146:ASN:ND2	2.35	0.41
1:FFF:239:ILE:HD11	1:FFF:363:PRO:HG2	2.01	0.41
1:DDD:111:MSE:O	1:DDD:115:LEU:HD13	2.21	0.41
1:CCC:293:LEU:HA	1:CCC:296:GLN:HG2	2.01	0.41
1:HHH:27:LEU:HG	1:HHH:31:TYR:CE2	2.55	0.41
1:AAA:48:PRO:HB2	1:GGG:330:GLN:OE1	2.21	0.41
1:EEE:20:SER:HB2	1:EEE:297:ARG:HD2	2.01	0.41
1:BBB:89:LEU:HD13	1:BBB:115:LEU:HD22	2.03	0.41
1:FFF:344:LEU:HD23	1:FFF:344:LEU:HA	1.91	0.41
1:DDD:344:LEU:HD23	1:DDD:344:LEU:HA	1.89	0.41
1:DDD:152:ASP:OD1	1:DDD:156:GLN:NE2	2.53	0.40
1:DDD:207:LEU:N	1:DDD:207:LEU:CD1	2.84	0.40
1:EEE:64:GLN:OE1	1:EEE:64:GLN:HA	2.20	0.40
1:AAA:176:ILE:HG23	1:AAA:253:LEU:CD1	2.51	0.40
1:BBB:80:TYR:HB3	1:BBB:349:ILE:HG23	2.04	0.40
1:AAA:31:TYR:CE1	1:AAA:236:ILE:HD12	2.56	0.40
1:EEE:242:GLY:C	1:EEE:244:SER:H	2.27	0.40
1:DDD:27:LEU:HG	1:DDD:31:TYR:CE2	2.57	0.40

All (5) 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:351:ASN:OD1	1:EEE:159:ASN:HD22[4_565]	1.22	0.38
1:BBB:157:GLY:O	1:CCC:137:ARG:NH2[2_655]	1.96	0.24
1:BBB:157:GLY:O	1:CCC:137:ARG:HH21[2_655]	1.37	0.23
1:CCC:351:ASN:OD1	1:EEE:159:ASN:ND2[4_565]	2.11	0.09
1:GGG:157:GLY:O	1:DDD:137:ARG:NH2[3_645]	2.14	0.06

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	340/373 (91%)	326 (96%)	13 (4%)	1 (0%)	36	67
1	BBB	335/373 (90%)	326 (97%)	7 (2%)	2 (1%)	21	53
1	CCC	344/373 (92%)	328 (95%)	13 (4%)	3 (1%)	14	45
1	DDD	317/373 (85%)	301 (95%)	12 (4%)	4 (1%)	9	36
1	EEE	342/373 (92%)	328 (96%)	12 (4%)	2 (1%)	21	53
1	FFF	341/373 (91%)	327 (96%)	10 (3%)	4 (1%)	10	38
1	GGG	341/373 (91%)	323 (95%)	13 (4%)	5 (2%)	8	33
1	HHH	343/373 (92%)	325 (95%)	14 (4%)	4 (1%)	10	38
All	All	2703/2984 (91%)	2584 (96%)	94 (4%)	25 (1%)	14	45

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	243	ALA
1	EEE	243	ALA
1	FFF	45	SER
1	FFF	246	ALA
1	GGG	239	ILE
1	HHH	43	SER
1	HHH	243	ALA
1	DDD	239	ILE
1	DDD	243	ALA
1	DDD	244	SER
1	DDD	245	GLY
1	AAA	245	GLY
1	BBB	245	GLY
1	CCC	245	GLY
1	EEE	245	GLY
1	GGG	244	SER
1	GGG	245	GLY
1	HHH	245	GLY
1	BBB	365	VAL
1	FFF	43	SER
1	GGG	101	ASP
1	GGG	103	GLN
1	HHH	239	ILE
1	CCC	47	ASP
1	FFF	245	GLY

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	267/285 (94%)	264 (99%)	3 (1%)	65	82
1	BBB	268/285 (94%)	263 (98%)	5 (2%)	50	75
1	CCC	271/285 (95%)	263 (97%)	8 (3%)	36	67
1	DDD	213/285 (75%)	208 (98%)	5 (2%)	44	72
1	EEE	269/285 (94%)	267 (99%)	2 (1%)	76	87
1	FFF	267/285 (94%)	263 (98%)	4 (2%)	57	79
1	GGG	269/285 (94%)	265 (98%)	4 (2%)	57	79
1	HHH	269/285 (94%)	266 (99%)	3 (1%)	65	82
All	All	2093/2280 (92%)	2059 (98%)	34 (2%)	55	78

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	46	MSE
1	AAA	52	VAL
1	AAA	279	SER
1	BBB	46	MSE
1	BBB	240	SER
1	BBB	279	SER
1	BBB	351	ASN
1	BBB	366	LEU
1	CCC	13	THR
1	CCC	43	SER
1	CCC	46	MSE
1	CCC	136	LYS
1	CCC	196	GLN
1	CCC	265	ARG
1	CCC	279	SER
1	CCC	337	LEU
1	EEE	279	SER
1	EEE	337	LEU
1	FFF	46	MSE

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Mol	Chain	Res	Type
1	FFF	63	GLN
1	FFF	163	LYS
1	FFF	279	SER
1	GGG	117	ASP
1	GGG	239	ILE
1	GGG	279	SER
1	GGG	337	LEU
1	HHH	279	SER
1	HHH	337	LEU
1	HHH	367	GLU
1	DDD	136	LYS
1	DDD	137	ARG
1	DDD	205	VAL
1	DDD	250	VAL
1	DDD	273	LEU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	336/373 (90%)	-0.42	1 (0%) 90 82	41, 61, 92, 120	0
1	BBB	333/373 (89%)	-0.42	3 (0%) 81 65	39, 56, 77, 97	0
1	CCC	340/373 (91%)	-0.19	3 (0%) 81 65	43, 67, 104, 136	0
1	DDD	320/373 (85%)	0.39	17 (5%) 32 19	47, 85, 134, 156	0
1	EEE	338/373 (90%)	-0.24	3 (0%) 81 65	49, 66, 99, 127	0
1	FFF	337/373 (90%)	-0.43	1 (0%) 90 82	38, 54, 88, 126	0
1	GGG	337/373 (90%)	-0.28	2 (0%) 85 72	40, 60, 89, 144	0
1	HHH	339/373 (90%)	-0.26	5 (1%) 72 53	46, 64, 103, 132	0
All	All	2680/2984 (89%)	-0.23	35 (1%) 75 57	38, 63, 108, 156	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	366	LEU	3.9
1	DDD	199	GLN	3.8
1	HHH	195	VAL	3.5
1	DDD	2	ASN	3.5
1	DDD	207	LEU	3.4
1	DDD	229	ALA	3.2
1	EEE	195	VAL	3.1
1	DDD	54	ILE	3.0
1	AAA	366	LEU	2.8
1	DDD	102	PRO	2.7
1	HHH	194	VAL	2.7
1	DDD	240	SER	2.6
1	CCC	243	ALA	2.5
1	DDD	204	ALA	2.5
1	FFF	45	SER	2.5
1	CCC	241	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	DDD	59	ASN	2.5
1	DDD	151	ILE	2.4
1	BBB	240	SER	2.4
1	BBB	366	LEU	2.4
1	GGG	101	ASP	2.3
1	EEE	367	GLU	2.3
1	HHH	241	ALA	2.3
1	DDD	242	GLY	2.3
1	HHH	2	ASN	2.2
1	DDD	101	ASP	2.2
1	GGG	195	VAL	2.2
1	DDD	100	GLU	2.2
1	DDD	233	ILE	2.2
1	EEE	241	ALA	2.2
1	DDD	234	SER	2.1
1	HHH	208	GLY	2.1
1	DDD	200	SER	2.1
1	BBB	244	SER	2.0
1	CCC	195	VAL	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](#)

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	HHH	401	1/1	0.87	0.20	130,130,130,130	0
2	CA	CCC	402	1/1	0.88	0.22	122,122,122,122	0
2	CA	GGG	401	1/1	0.89	0.17	93,93,93,93	0
2	CA	BBB	401	1/1	0.95	0.05	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	FFF	401	1/1	0.95	0.24	101,101,101,101	0
3	CL	CCC	403	1/1	0.95	0.33	87,87,87,87	0
3	CL	FFF	402	1/1	0.96	0.28	89,89,89,89	0
3	CL	DDD	401	1/1	0.97	0.26	91,91,91,91	0
2	CA	CCC	401	1/1	0.98	0.04	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.