Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 12:54 pm GMT

PDB ID	:	7A0G
Title	:	Structure of the SmhB pore of the tripartite alpha-pore forming toxin, Smh, from Serratia marcescens.
Authors	:	Churchill-Angus, A.M.; Baker, P.J.
Deposited on	:	2020-08-08
Resolution	:	6.98 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:

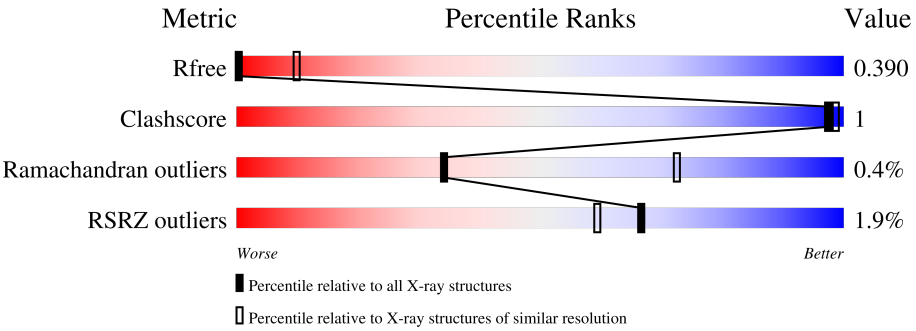
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.98 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}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
RSRZ outliers	127900	1004 (9.50-3.80)

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 <=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	366	3% 89% · 10%
1	BBB	366	% 86% · 13%
1	CCC	366	4% 88% · 10%
1	DDD	366	% 86% · 13%
1	EEE	366	2% 89% · 10%
1	FFF	366	% 83% · 14%

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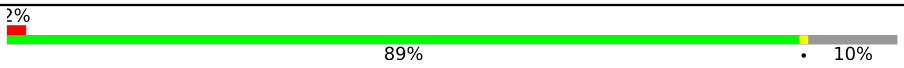
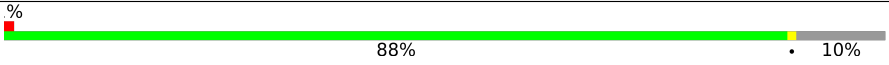
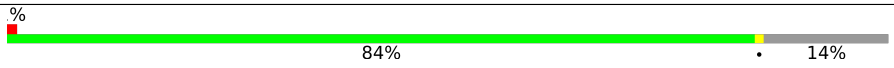
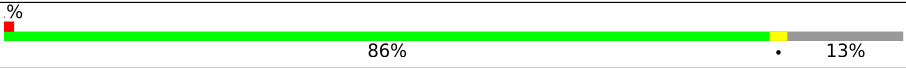
Mol	Chain	Length	Quality of chain
1	GGG	366	
1	HHH	366	
1	III	366	
1	JJJ	366	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 27767 atoms, of which 11987 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 SmhB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	329	Total	C	H	N	O	261	0	0
			2830	950	1222	329	329			
1	BBB	320	Total	C	H	N	O	254	0	0
			2751	924	1187	320	320			
1	CCC	329	Total	C	H	N	O	262	0	0
			2829	950	1221	329	329			
1	DDD	318	Total	C	H	N	O	254	0	0
			2735	919	1180	318	318			
1	EEE	329	Total	C	H	N	O	259	1	0
			2834	951	1225	329	329			
1	FFF	313	Total	C	H	N	O	249	0	0
			2691	904	1161	313	313			
1	GGG	329	Total	C	H	N	O	261	0	0
			2830	950	1222	329	329			
1	HHH	328	Total	C	H	N	O	260	0	0
			2822	947	1219	328	328			
1	III	313	Total	C	H	N	O	250	0	0
			2694	905	1163	313	313			
1	JJJ	320	Total	C	H	N	O	254	0	0
			2751	924	1187	320	320			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	368	LEU	-	expression tag	UNP A0A1Q4NVM7
AAA	369	GLU	-	expression tag	UNP A0A1Q4NVM7
AAA	370	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	371	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	372	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	373	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	374	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	375	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	368	LEU	-	expression tag	UNP A0A1Q4NVM7

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	369	GLU	-	expression tag	UNP A0A1Q4NVM7
BBB	370	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	371	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	372	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	373	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	374	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	375	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	368	LEU	-	expression tag	UNP A0A1Q4NVM7
CCC	369	GLU	-	expression tag	UNP A0A1Q4NVM7
CCC	370	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	371	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	372	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	373	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	374	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	375	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	368	LEU	-	expression tag	UNP A0A1Q4NVM7
DDD	369	GLU	-	expression tag	UNP A0A1Q4NVM7
DDD	370	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	371	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	372	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	373	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	374	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	375	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	368	LEU	-	expression tag	UNP A0A1Q4NVM7
EEE	369	GLU	-	expression tag	UNP A0A1Q4NVM7
EEE	370	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	371	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	372	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	373	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	374	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	375	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	368	LEU	-	expression tag	UNP A0A1Q4NVM7
FFF	369	GLU	-	expression tag	UNP A0A1Q4NVM7
FFF	370	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	371	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	372	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	373	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	374	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	375	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	368	LEU	-	expression tag	UNP A0A1Q4NVM7
GGG	369	GLU	-	expression tag	UNP A0A1Q4NVM7
GGG	370	HIS	-	expression tag	UNP A0A1Q4NVM7

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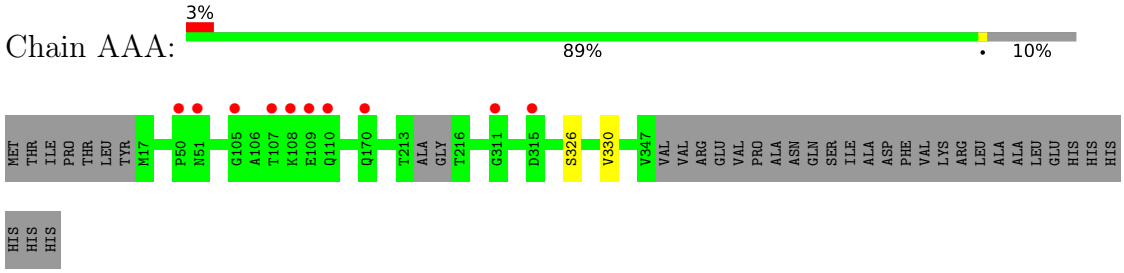
Chain	Residue	Modelled	Actual	Comment	Reference
GGG	371	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	372	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	373	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	374	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	375	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	368	LEU	-	expression tag	UNP A0A1Q4NVM7
HHH	369	GLU	-	expression tag	UNP A0A1Q4NVM7
HHH	370	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	371	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	372	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	373	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	374	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	375	HIS	-	expression tag	UNP A0A1Q4NVM7
III	368	LEU	-	expression tag	UNP A0A1Q4NVM7
III	369	GLU	-	expression tag	UNP A0A1Q4NVM7
III	370	HIS	-	expression tag	UNP A0A1Q4NVM7
III	371	HIS	-	expression tag	UNP A0A1Q4NVM7
III	372	HIS	-	expression tag	UNP A0A1Q4NVM7
III	373	HIS	-	expression tag	UNP A0A1Q4NVM7
III	374	HIS	-	expression tag	UNP A0A1Q4NVM7
III	375	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	368	LEU	-	expression tag	UNP A0A1Q4NVM7
JJJ	369	GLU	-	expression tag	UNP A0A1Q4NVM7
JJJ	370	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	371	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	372	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	373	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	374	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	375	HIS	-	expression tag	UNP A0A1Q4NVM7

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.

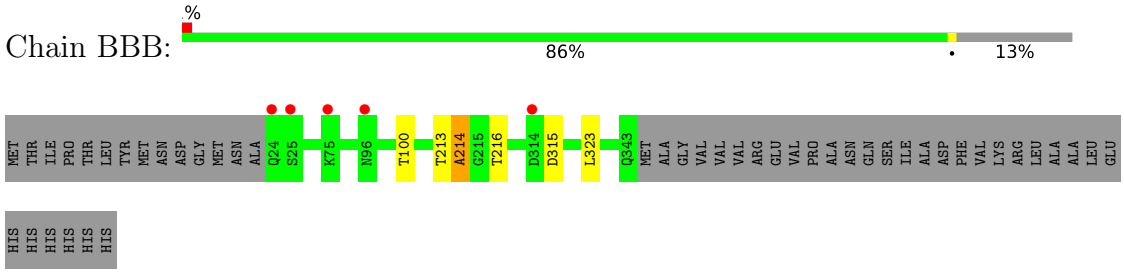
• Molecule 1: SmhB

Chain AAA:



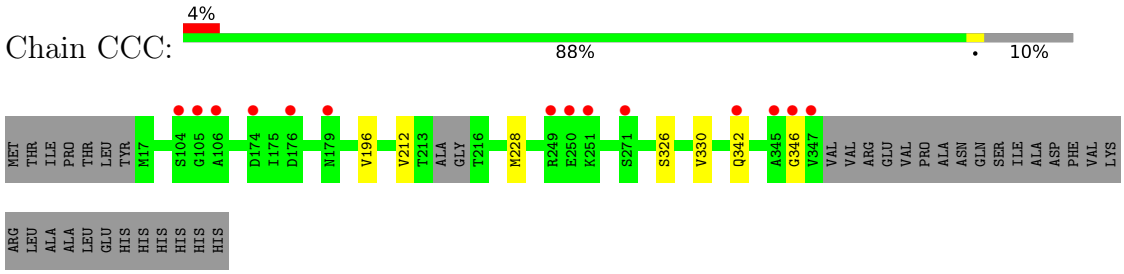
• Molecule 1: SmhB

Chain BBB:



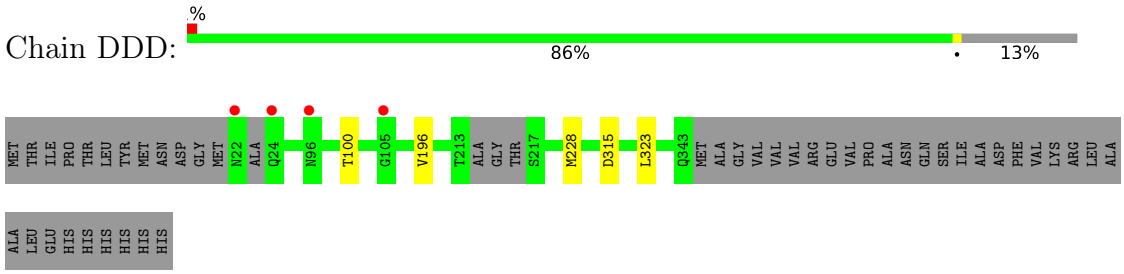
• Molecule 1: SmhB

Chain CCC:



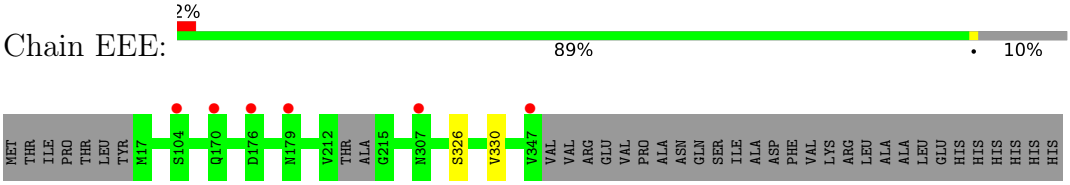
• Molecule 1: SmhB

Chain DDD:



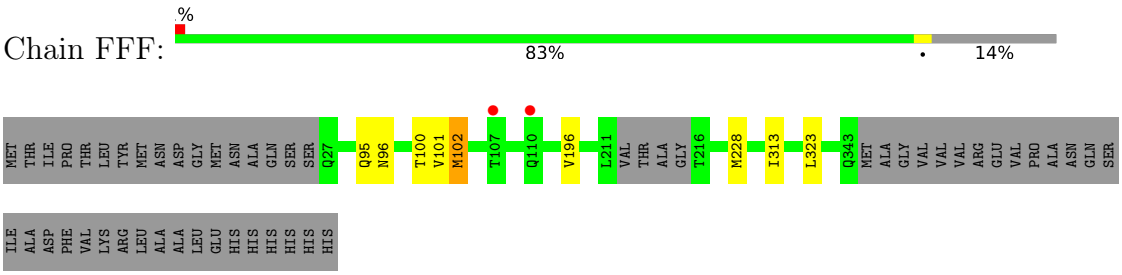
• Molecule 1: SmhB

Chain EEE:



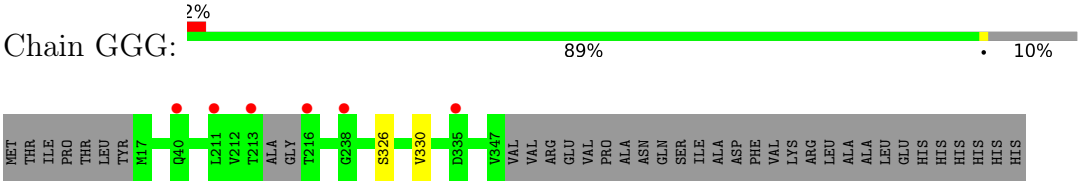
• Molecule 1: SmhB

Chain FFF:



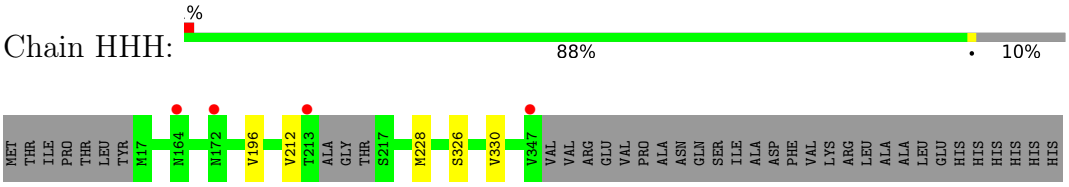
• Molecule 1: SmhB

Chain GGG:



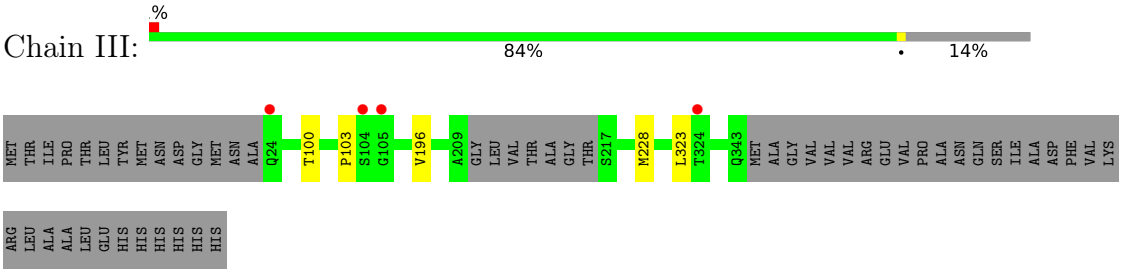
• Molecule 1: SmhB

Chain HHH:



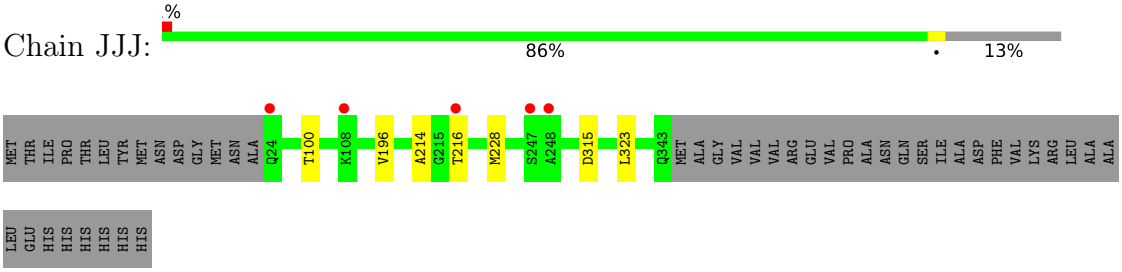
• Molecule 1: SmhB

Chain III:



• Molecule 1: SmhB

Chain JJJ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	224.48Å 118.06Å 209.53Å 90.00° 109.44° 90.00°	Depositor
Resolution (Å)	66.77 – 6.98 66.77 – 6.98	Depositor EDS
% Data completeness (in resolution range)	98.7 (66.77-6.98) 80.5 (66.77-6.98)	Depositor EDS
R_{merge}	2.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.33 (at 6.71Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.334 , 0.335 0.351 , 0.390	Depositor DCC
R_{free} test set	380 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å^2)	-102.2	Xtriage
Anisotropy	-2.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.10 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.65	EDS
Total number of atoms	27767	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.88	0/1606	0.87	0/2223
1	BBB	0.90	0/1563	0.86	0/2165
1	CCC	0.88	0/1606	0.86	0/2223
1	DDD	0.89	0/1552	0.86	0/2147
1	EEE	0.90	0/1610	0.87	0/2228
1	FFF	0.90	0/1528	0.86	0/2115
1	GGG	0.89	0/1606	0.87	0/2223
1	HHH	0.89	0/1601	0.87	0/2216
1	III	0.90	0/1529	0.86	0/2117
1	JJJ	0.89	0/1563	0.86	0/2165
All	All	0.89	0/15764	0.86	0/21822

There are no bond length outliers.

There are no bond angle outliers.

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	1608	1222	769	1	0
1	BBB	1564	1187	748	2	0
1	CCC	1608	1221	766	3	0
1	DDD	1555	1180	738	2	0
1	EEE	1609	1225	772	1	0
1	FFF	1530	1161	729	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GGG	1608	1222	769	1	0
1	HHH	1603	1219	767	2	0
1	III	1531	1163	728	2	0
1	JJJ	1564	1187	748	2	0
All	All	15780	11987	7534	19	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 1.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:III:100:THR:CB	1:III:323:LEU:CB	2.67	0.72
1:FFF:101:VAL:O	1:FFF:102:MET:CB	2.41	0.68
1:BBB:100:THR:HA	1:BBB:323:LEU:CB	2.26	0.64
1:DDD:100:THR:HA	1:DDD:323:LEU:CB	2.28	0.63
1:JJJ:100:THR:HA	1:JJJ:323:LEU:CB	2.29	0.62
1:FFF:100:THR:HA	1:FFF:323:LEU:CB	2.41	0.51
1:GGG:326:SER:HA	1:GGG:330:VAL:CB	2.44	0.47
1:HHH:326:SER:HA	1:HHH:330:VAL:CB	2.45	0.47
1:CCC:326:SER:HA	1:CCC:330:VAL:CB	2.45	0.46
1:AAA:326:SER:HA	1:AAA:330:VAL:CB	2.46	0.45
1:EEE:326:SER:HA	1:EEE:330:VAL:CB	2.46	0.45
1:CCC:342:GLN:O	1:CCC:346:GLY:N	2.50	0.42
1:FFF:196:VAL:HA	1:FFF:228:MET:HA	2.02	0.42
1:HHH:196:VAL:HA	1:HHH:228:MET:HA	2.02	0.42
1:JJJ:196:VAL:HA	1:JJJ:228:MET:HA	2.03	0.41
1:DDD:196:VAL:HA	1:DDD:228:MET:HA	2.02	0.41
1:CCC:196:VAL:HA	1:CCC:228:MET:HA	2.03	0.41
1:III:196:VAL:HA	1:III:228:MET:HA	2.03	0.41
1:BBB:213:THR:O	1:BBB:214:ALA:C	2.59	0.40

There are no symmetry-related clashes.

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	325/366 (89%)	313 (96%)	12 (4%)	0	100	100
1	BBB	318/366 (87%)	303 (95%)	12 (4%)	3 (1%)	17	57
1	CCC	325/366 (89%)	314 (97%)	10 (3%)	1 (0%)	41	77
1	DDD	313/366 (86%)	302 (96%)	10 (3%)	1 (0%)	41	77
1	EEE	326/366 (89%)	315 (97%)	11 (3%)	0	100	100
1	FFF	309/366 (84%)	297 (96%)	8 (3%)	4 (1%)	12	48
1	GGG	325/366 (89%)	313 (96%)	12 (4%)	0	100	100
1	HHH	324/366 (88%)	313 (97%)	10 (3%)	1 (0%)	41	77
1	III	309/366 (84%)	297 (96%)	11 (4%)	1 (0%)	41	77
1	JJJ	318/366 (87%)	304 (96%)	11 (4%)	3 (1%)	17	57
All	All	3192/3660 (87%)	3071 (96%)	107 (3%)	14 (0%)	34	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	214	ALA
1	BBB	216	THR
1	BBB	315	ASP
1	DDD	315	ASP
1	FFF	95	GLN
1	FFF	102	MET
1	JJJ	315	ASP
1	JJJ	216	THR
1	FFF	96	ASN
1	JJJ	214	ALA
1	CCC	212	VAL
1	III	103	PRO
1	HHH	212	VAL
1	FFF	313	ILE

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	329/366 (89%)	0.24	10 (3%) 50 43	0, 0, 0, 0	0
1	BBB	320/366 (87%)	0.21	5 (1%) 72 64	0, 0, 0, 0	0
1	CCC	329/366 (89%)	0.21	14 (4%) 35 32	0, 0, 0, 0	0
1	DDD	318/366 (86%)	0.05	4 (1%) 77 68	0, 0, 0, 0	0
1	EEE	329/366 (89%)	0.28	6 (1%) 68 61	0, 0, 0, 0	0
1	FFF	313/366 (85%)	0.21	2 (0%) 89 83	0, 0, 0, 0	0
1	GGG	329/366 (89%)	0.21	6 (1%) 68 61	0, 0, 0, 0	0
1	HHH	328/366 (89%)	0.15	4 (1%) 79 71	0, 0, 0, 0	0
1	III	313/366 (85%)	0.10	4 (1%) 77 68	0, 0, 0, 0	0
1	JJJ	320/366 (87%)	0.09	5 (1%) 72 64	0, 0, 0, 0	0
All	All	3228/3660 (88%)	0.18	60 (1%) 66 59	0, 0, 0, 0	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	22	ASN	6.2
1	CCC	347	VAL	4.3
1	BBB	24	GLN	4.1
1	CCC	346	GLY	4.0
1	III	105	GLY	3.9
1	III	24	GLN	3.8
1	DDD	24	GLN	3.8
1	EEE	179	ASN	3.7
1	AAA	50	PRO	3.6
1	AAA	108	LYS	3.5
1	EEE	170	GLN	3.5
1	CCC	105	GLY	3.4
1	GGG	216	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	107	THR	3.3
1	GGG	213	THR	3.2
1	HHH	164	ASN	3.0
1	AAA	51	ASN	3.0
1	JJJ	24	GLN	3.0
1	HHH	347	VAL	2.8
1	HHH	213	THR	2.7
1	DDD	96	ASN	2.7
1	BBB	25	SER	2.7
1	EEE	104	SER	2.6
1	CCC	104	SER	2.5
1	CCC	342	GLN	2.5
1	CCC	176	ASP	2.5
1	AAA	110	GLN	2.4
1	AAA	170	GLN	2.4
1	HHH	172	ASN	2.4
1	AAA	109	GLU	2.3
1	CCC	271	SER	2.3
1	AAA	315	ASP	2.3
1	EEE	307	ASN	2.3
1	BBB	96	ASN	2.3
1	III	324	THR	2.3
1	CCC	249	ARG	2.3
1	JJJ	248	ALA	2.3
1	JJJ	108	LYS	2.2
1	FFF	107	THR	2.2
1	GGG	335	ASP	2.2
1	GGG	211	LEU	2.2
1	AAA	311	GLY	2.1
1	GGG	238	GLY	2.1
1	JJJ	216	THR	2.1
1	EEE	347	VAL	2.1
1	CCC	106	ALA	2.1
1	AAA	105	GLY	2.1
1	CCC	250	GLU	2.1
1	FFF	110	GLN	2.1
1	CCC	345	ALA	2.1
1	CCC	174	ASP	2.1
1	EEE	176	ASP	2.0
1	GGG	40	GLN	2.0
1	BBB	75	LYS	2.0
1	DDD	105	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	CCC	179	ASN	2.0
1	BBB	314	ASP	2.0
1	JJJ	247	SER	2.0
1	CCC	251	LYS	2.0
1	III	104	SER	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.