Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2022 – 03:29 pm GMT

PDB ID	:	6ZJ8
Title	:	Structure of the PAS domain from Bordetella pertussis BvgS
Authors	:	Clantin, B.; Dupre, E.; Jacob-Dubuisson, F.; Villeret, V.
Deposited on	:	2020-06-28
Resolution	:	2.40 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:

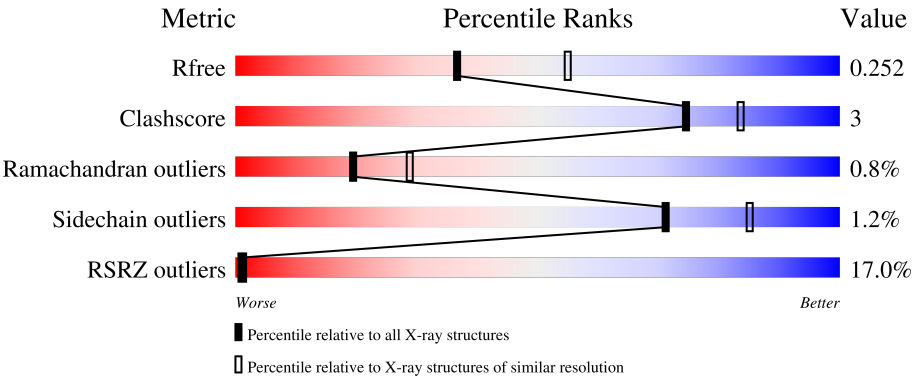
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	162	13% 79% 8% 13%
1	B	162	14% 78% · 18%
1	C	162	10% 64% 10% 27%
1	D	162	21% 59% 12% 29%
1	E	162	9% 78% · 18%

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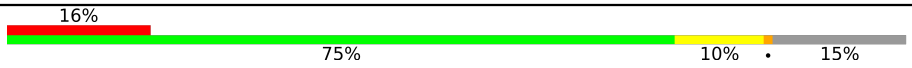
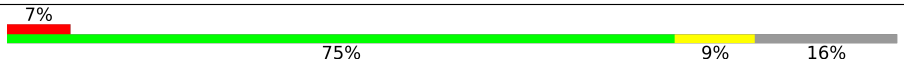
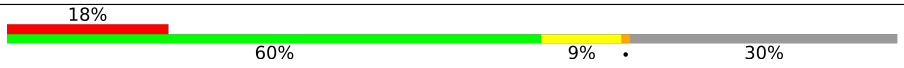
Mol	Chain	Length	Quality of chain
1	F	162	
1	G	162	
1	H	162	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16589 atoms, of which 8229 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 Virulence sensor protein BvgS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	141	Total	C	H	N	O	S	0	0	0
			2253	712	1122	201	214	4			
1	B	133	Total	C	H	N	O	S	0	0	0
			2151	681	1072	193	201	4			
1	C	119	Total	C	H	N	O	S	0	0	0
			1934	616	965	171	178	4			
1	D	115	Total	C	H	N	O	S	0	0	0
			1873	596	931	167	175	4			
1	E	133	Total	C	H	N	O	S	0	0	0
			2123	674	1055	189	201	4			
1	F	138	Total	C	H	N	O	S	0	0	0
			2210	699	1101	198	208	4			
1	G	136	Total	C	H	N	O	S	0	0	0
			2172	688	1082	193	205	4			
1	H	113	Total	C	H	N	O	S	0	0	0
			1825	583	901	162	175	4			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P16575
A	2	ALA	-	expression tag	UNP P16575
A	3	SER	-	expression tag	UNP P16575
A	4	ARG	-	expression tag	UNP P16575
A	5	GLY	-	expression tag	UNP P16575
A	6	SER	-	expression tag	UNP P16575
A	7	HIS	-	expression tag	UNP P16575
A	8	HIS	-	expression tag	UNP P16575
A	9	HIS	-	expression tag	UNP P16575
A	10	HIS	-	expression tag	UNP P16575
A	11	HIS	-	expression tag	UNP P16575
A	12	HIS	-	expression tag	UNP P16575
A	13	GLY	-	expression tag	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ALA	-	expression tag	UNP P16575
A	151	LEU	ALA	conflict	UNP P16575
A	155	LEU	ALA	conflict	UNP P16575
B	1	MET	-	initiating methionine	UNP P16575
B	2	ALA	-	expression tag	UNP P16575
B	3	SER	-	expression tag	UNP P16575
B	4	ARG	-	expression tag	UNP P16575
B	5	GLY	-	expression tag	UNP P16575
B	6	SER	-	expression tag	UNP P16575
B	7	HIS	-	expression tag	UNP P16575
B	8	HIS	-	expression tag	UNP P16575
B	9	HIS	-	expression tag	UNP P16575
B	10	HIS	-	expression tag	UNP P16575
B	11	HIS	-	expression tag	UNP P16575
B	12	HIS	-	expression tag	UNP P16575
B	13	GLY	-	expression tag	UNP P16575
B	14	ALA	-	expression tag	UNP P16575
B	151	LEU	ALA	conflict	UNP P16575
B	155	LEU	ALA	conflict	UNP P16575
C	1	MET	-	initiating methionine	UNP P16575
C	2	ALA	-	expression tag	UNP P16575
C	3	SER	-	expression tag	UNP P16575
C	4	ARG	-	expression tag	UNP P16575
C	5	GLY	-	expression tag	UNP P16575
C	6	SER	-	expression tag	UNP P16575
C	7	HIS	-	expression tag	UNP P16575
C	8	HIS	-	expression tag	UNP P16575
C	9	HIS	-	expression tag	UNP P16575
C	10	HIS	-	expression tag	UNP P16575
C	11	HIS	-	expression tag	UNP P16575
C	12	HIS	-	expression tag	UNP P16575
C	13	GLY	-	expression tag	UNP P16575
C	14	ALA	-	expression tag	UNP P16575
C	151	LEU	ALA	conflict	UNP P16575
C	155	LEU	ALA	conflict	UNP P16575
D	1	MET	-	initiating methionine	UNP P16575
D	2	ALA	-	expression tag	UNP P16575
D	3	SER	-	expression tag	UNP P16575
D	4	ARG	-	expression tag	UNP P16575
D	5	GLY	-	expression tag	UNP P16575
D	6	SER	-	expression tag	UNP P16575
D	7	HIS	-	expression tag	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P16575
D	9	HIS	-	expression tag	UNP P16575
D	10	HIS	-	expression tag	UNP P16575
D	11	HIS	-	expression tag	UNP P16575
D	12	HIS	-	expression tag	UNP P16575
D	13	GLY	-	expression tag	UNP P16575
D	14	ALA	-	expression tag	UNP P16575
D	151	LEU	ALA	conflict	UNP P16575
D	155	LEU	ALA	conflict	UNP P16575
E	1	MET	-	initiating methionine	UNP P16575
E	2	ALA	-	expression tag	UNP P16575
E	3	SER	-	expression tag	UNP P16575
E	4	ARG	-	expression tag	UNP P16575
E	5	GLY	-	expression tag	UNP P16575
E	6	SER	-	expression tag	UNP P16575
E	7	HIS	-	expression tag	UNP P16575
E	8	HIS	-	expression tag	UNP P16575
E	9	HIS	-	expression tag	UNP P16575
E	10	HIS	-	expression tag	UNP P16575
E	11	HIS	-	expression tag	UNP P16575
E	12	HIS	-	expression tag	UNP P16575
E	13	GLY	-	expression tag	UNP P16575
E	14	ALA	-	expression tag	UNP P16575
E	151	LEU	ALA	conflict	UNP P16575
E	155	LEU	ALA	conflict	UNP P16575
F	1	MET	-	initiating methionine	UNP P16575
F	2	ALA	-	expression tag	UNP P16575
F	3	SER	-	expression tag	UNP P16575
F	4	ARG	-	expression tag	UNP P16575
F	5	GLY	-	expression tag	UNP P16575
F	6	SER	-	expression tag	UNP P16575
F	7	HIS	-	expression tag	UNP P16575
F	8	HIS	-	expression tag	UNP P16575
F	9	HIS	-	expression tag	UNP P16575
F	10	HIS	-	expression tag	UNP P16575
F	11	HIS	-	expression tag	UNP P16575
F	12	HIS	-	expression tag	UNP P16575
F	13	GLY	-	expression tag	UNP P16575
F	14	ALA	-	expression tag	UNP P16575
F	151	LEU	ALA	conflict	UNP P16575
F	155	LEU	ALA	conflict	UNP P16575
G	1	MET	-	initiating methionine	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
G	2	ALA	-	expression tag	UNP P16575
G	3	SER	-	expression tag	UNP P16575
G	4	ARG	-	expression tag	UNP P16575
G	5	GLY	-	expression tag	UNP P16575
G	6	SER	-	expression tag	UNP P16575
G	7	HIS	-	expression tag	UNP P16575
G	8	HIS	-	expression tag	UNP P16575
G	9	HIS	-	expression tag	UNP P16575
G	10	HIS	-	expression tag	UNP P16575
G	11	HIS	-	expression tag	UNP P16575
G	12	HIS	-	expression tag	UNP P16575
G	13	GLY	-	expression tag	UNP P16575
G	14	ALA	-	expression tag	UNP P16575
G	151	LEU	ALA	conflict	UNP P16575
G	155	LEU	ALA	conflict	UNP P16575
H	1	MET	-	initiating methionine	UNP P16575
H	2	ALA	-	expression tag	UNP P16575
H	3	SER	-	expression tag	UNP P16575
H	4	ARG	-	expression tag	UNP P16575
H	5	GLY	-	expression tag	UNP P16575
H	6	SER	-	expression tag	UNP P16575
H	7	HIS	-	expression tag	UNP P16575
H	8	HIS	-	expression tag	UNP P16575
H	9	HIS	-	expression tag	UNP P16575
H	10	HIS	-	expression tag	UNP P16575
H	11	HIS	-	expression tag	UNP P16575
H	12	HIS	-	expression tag	UNP P16575
H	13	GLY	-	expression tag	UNP P16575
H	14	ALA	-	expression tag	UNP P16575
H	151	LEU	ALA	conflict	UNP P16575
H	155	LEU	ALA	conflict	UNP P16575

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	6	Total O 6 6	0	0
2	C	5	Total O 5 5	0	0
2	D	5	Total O 5 5	0	0

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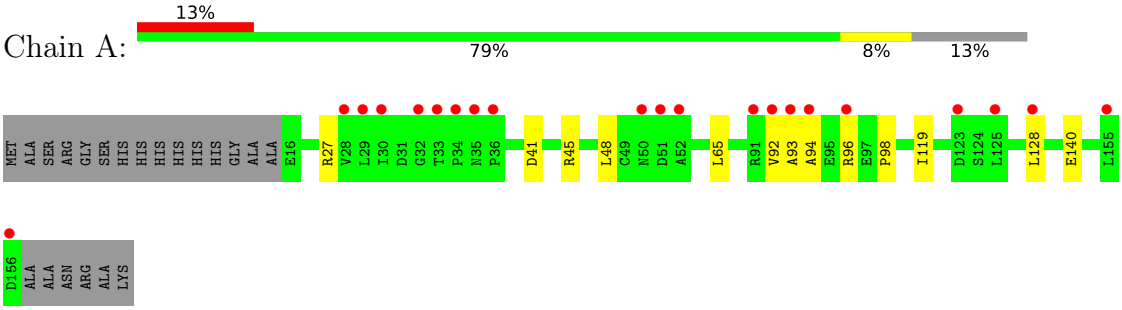
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total O 2 2	0	0
2	F	2	Total O 2 2	0	0
2	G	14	Total O 14 14	0	0
2	H	1	Total O 1 1	0	0

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.

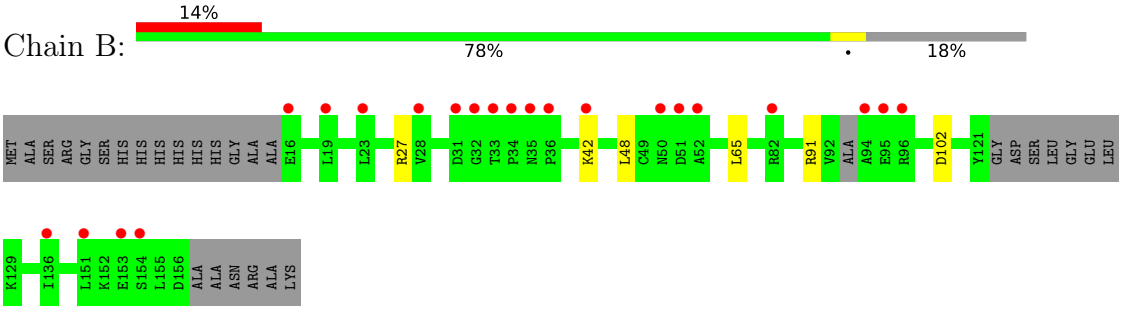
• Molecule 1: Virulence sensor protein BvgS

Chain A:



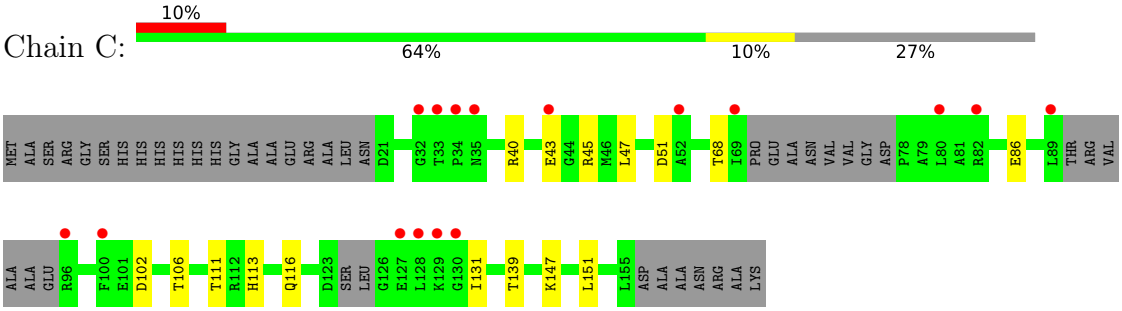
• Molecule 1: Virulence sensor protein BvgS

Chain B:



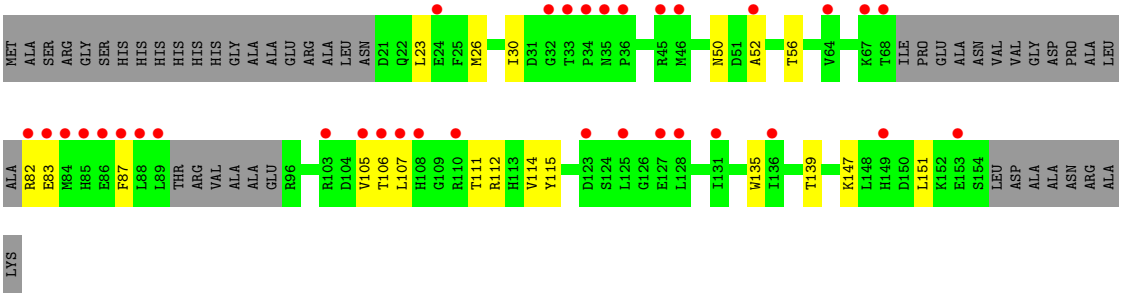
• Molecule 1: Virulence sensor protein BvgS

Chain C:



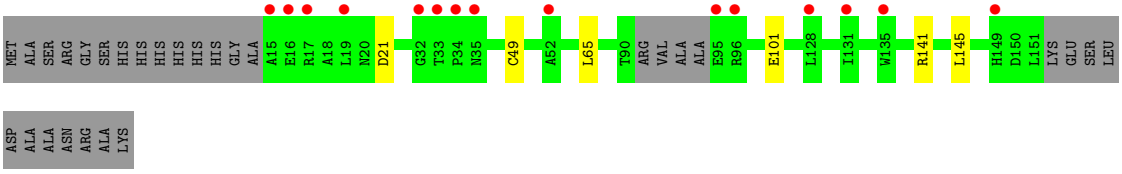
• Molecule 1: Virulence sensor protein BvgS

Chain D:



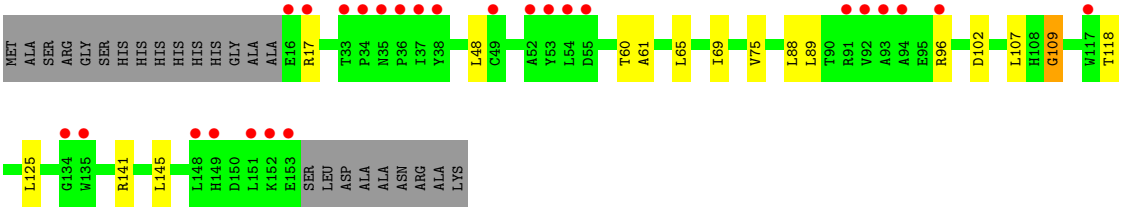
• Molecule 1: Virulence sensor protein BvgS

Chain E:



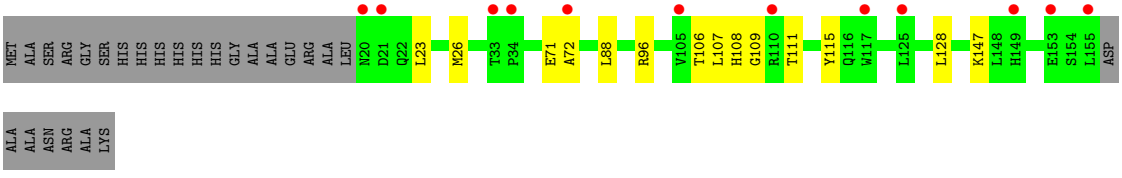
• Molecule 1: Virulence sensor protein BvgS

Chain F:



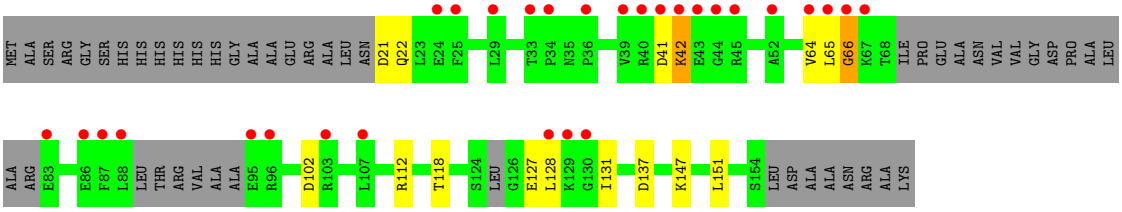
• Molecule 1: Virulence sensor protein BvgS

Chain G:



• Molecule 1: Virulence sensor protein BvgS

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.96Å 122.29Å 105.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.65 – 2.40 44.95 – 2.26	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.65-2.40) 99.9 (44.95-2.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.227 , 0.252 0.227 , 0.252	Depositor DCC
R_{free} test set	3117 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16589	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.93% 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	A	0.24	0/1152	0.43	0/1560
1	B	0.24	0/1098	0.44	0/1484
1	C	0.23	0/986	0.42	0/1327
1	D	0.23	0/959	0.42	0/1291
1	E	0.24	0/1088	0.44	0/1473
1	F	0.24	0/1130	0.44	0/1530
1	G	0.23	0/1111	0.43	0/1505
1	H	0.24	0/940	0.43	0/1264
All	All	0.24	0/8464	0.43	0/11434

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	A	1131	1122	1120	8	0
1	B	1079	1072	1070	4	0
1	C	969	965	963	11	0
1	D	942	931	929	10	0
1	E	1068	1055	1053	7	0
1	F	1109	1101	1100	13	0
1	G	1090	1082	1081	9	0
1	H	924	901	899	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	0	0	0
2	B	6	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	14	0	0	0	0
2	H	1	0	0	0	0
All	All	8360	8229	8215	53	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 3.

All (53) 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:B:65:LEU:HD11	1:D:147:LYS:HE2	1.70	0.74
1:D:106:THR:HG22	1:D:111:THR:HG22	1.68	0.73
1:F:65:LEU:HD11	1:H:147:LYS:HE2	1.71	0.72
1:G:106:THR:OG1	1:G:111:THR:HG22	1.94	0.67
1:H:112:ARG:NH2	1:H:137:ASP:OD1	2.30	0.65
1:G:23:LEU:HD23	1:G:26:MET:HE3	1.77	0.64
1:E:145:LEU:HD12	1:F:145:LEU:HD12	1.79	0.64
1:C:45:ARG:HA	1:C:68:THR:HG22	1.80	0.63
1:B:42:LYS:O	1:B:91:ARG:NH2	2.36	0.59
1:D:23:LEU:HD23	1:D:26:MET:HE3	1.85	0.58
1:E:65:LEU:HD11	1:G:147:LYS:HE2	1.86	0.57
1:F:48:LEU:HD13	1:H:151:LEU:HD11	1.88	0.55
1:A:96:ARG:HG2	1:A:128:LEU:HD11	1.90	0.54
1:E:145:LEU:CD1	1:F:145:LEU:HD12	2.38	0.54
1:D:87:PHE:CZ	1:D:105:VAL:HG21	2.44	0.53
1:A:92:VAL:O	1:A:94:ALA:N	2.42	0.53
1:F:69:ILE:HD13	1:F:88:LEU:HD11	1.92	0.52
1:B:27:ARG:NH1	1:D:139:THR:O	2.40	0.52
1:D:112:ARG:NH1	2:D:201:HOH:O	2.43	0.51
1:A:48:LEU:HD13	1:C:151:LEU:HD11	1.92	0.51
1:G:23:LEU:HD23	1:G:26:MET:CE	2.40	0.51
1:H:64:VAL:O	1:H:66:GLY:N	2.44	0.50
1:D:30:ILE:HG22	1:D:50:ASN:HB3	1.93	0.50
1:F:89:LEU:HD12	1:F:118:THR:HG23	1.92	0.50
1:F:107:LEU:O	1:F:109:GLY:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:ASP:O	1:H:42:LYS:HB2	2.12	0.50
1:B:48:LEU:HD13	1:D:151:LEU:HD11	1.92	0.50
1:C:106:THR:HG22	1:C:111:THR:HG22	1.93	0.49
1:C:47:LEU:HA	1:F:125:LEU:HD21	1.95	0.49
1:C:86:GLU:O	1:C:116:GLN:NE2	2.45	0.49
1:D:52:ALA:O	1:D:56:THR:HG23	2.13	0.49
1:G:96:ARG:HG2	1:G:128:LEU:HD21	1.95	0.48
1:H:21:ASP:OD1	1:H:22:GLN:N	2.48	0.47
1:A:27:ARG:NH1	1:C:139:THR:O	2.44	0.47
1:G:71:GLU:O	1:G:72:ALA:HB3	2.14	0.47
1:A:98:PRO:HB3	1:A:119:ILE:HD13	1.97	0.47
1:C:43:GLU:N	1:C:43:GLU:OE1	2.48	0.46
1:A:41:ASP:OD1	1:A:45:ARG:N	2.50	0.45
1:F:60:THR:HG22	1:F:61:ALA:N	2.32	0.44
1:G:88:LEU:C	1:G:88:LEU:HD23	2.39	0.43
1:G:107:LEU:O	1:G:109:GLY:N	2.52	0.43
1:H:118:THR:HB	1:H:131:ILE:HD11	1.99	0.43
1:C:40:ARG:O	1:C:131:ILE:N	2.48	0.43
1:E:21:ASP:OD2	1:H:102:ASP:OD2	2.37	0.42
1:E:145:LEU:HD12	1:F:145:LEU:CD1	2.48	0.42
1:C:102:ASP:OD1	1:C:113:HIS:NE2	2.43	0.42
1:F:48:LEU:CD1	1:H:151:LEU:HD11	2.49	0.42
1:A:65:LEU:HD11	1:C:147:LYS:HE2	2.02	0.41
1:D:114:VAL:CG1	1:D:135:TRP:HB2	2.50	0.41
1:F:69:ILE:HD13	1:F:88:LEU:CD1	2.51	0.41
1:E:141:ARG:HG3	1:F:141:ARG:HG3	2.03	0.40
1:A:140:GLU:OE1	1:C:51:ASP:OD2	2.39	0.40
1:E:49:CYS:O	1:G:147:LYS:NZ	2.55	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	A	139/162 (86%)	133 (96%)	5 (4%)	1 (1%)	22 32
1	B	127/162 (78%)	125 (98%)	2 (2%)	0	100 100
1	C	111/162 (68%)	110 (99%)	1 (1%)	0	100 100
1	D	109/162 (67%)	108 (99%)	1 (1%)	0	100 100
1	E	129/162 (80%)	126 (98%)	3 (2%)	0	100 100
1	F	136/162 (84%)	130 (96%)	4 (3%)	2 (2%)	10 14
1	G	134/162 (83%)	129 (96%)	4 (3%)	1 (1%)	22 32
1	H	105/162 (65%)	97 (92%)	4 (4%)	4 (4%)	3 2
All	All	990/1296 (76%)	958 (97%)	24 (2%)	8 (1%)	19 29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	128	LEU
1	A	93	ALA
1	G	108	HIS
1	H	42	LYS
1	H	65	LEU
1	F	109	GLY
1	F	96	ARG
1	H	66	GLY

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	A	120/133 (90%)	120 (100%)	0	100 100
1	B	115/133 (86%)	114 (99%)	1 (1%)	78 90
1	C	103/133 (77%)	103 (100%)	0	100 100
1	D	101/133 (76%)	97 (96%)	4 (4%)	31 49
1	E	113/133 (85%)	112 (99%)	1 (1%)	78 90
1	F	117/133 (88%)	114 (97%)	3 (3%)	46 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	116/133 (87%)	115 (99%)	1 (1%)	78 90
1	H	99/133 (74%)	98 (99%)	1 (1%)	76 88
All	All	884/1064 (83%)	873 (99%)	11 (1%)	71 85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	ASP
1	D	82	ARG
1	D	83	GLU
1	D	107	LEU
1	D	115	TYR
1	E	101	GLU
1	F	17	ARG
1	F	75	VAL
1	F	102	ASP
1	G	115	TYR
1	H	127	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	ASN

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, 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	A	141/162 (87%)	0.78	21 (14%)	2 2	52, 67, 123, 135	0
1	B	133/162 (82%)	0.83	22 (16%)	1 1	52, 72, 102, 133	0
1	C	119/162 (73%)	0.90	16 (13%)	3 2	52, 81, 112, 122	0
1	D	115/162 (70%)	1.36	34 (29%)	0 0	62, 88, 121, 138	0
1	E	133/162 (82%)	0.54	15 (11%)	5 4	58, 73, 102, 135	0
1	F	138/162 (85%)	0.97	26 (18%)	1 1	58, 72, 115, 142	0
1	G	136/162 (83%)	0.61	12 (8%)	10 9	54, 69, 104, 127	0
1	H	113/162 (69%)	1.31	29 (25%)	0 0	71, 90, 122, 141	0
All	All	1028/1296 (79%)	0.89	175 (17%)	1 1	52, 75, 118, 142	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	43	GLU	6.2
1	F	17	ARG	5.4
1	A	91	ARG	5.4
1	H	25	PHE	5.3
1	A	93	ALA	4.6
1	C	32	GLY	4.6
1	D	45	ARG	4.6
1	F	152	LYS	4.6
1	F	93	ALA	4.5
1	H	41	ASP	4.4
1	D	84	MET	4.4
1	D	82	ARG	4.4
1	D	103	ARG	4.3
1	C	82	ARG	4.3
1	G	153	GLU	4.3
1	F	149	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	106	THR	4.3
1	G	110	ARG	4.2
1	D	89	LEU	4.2
1	F	52	ALA	4.1
1	G	155	LEU	4.0
1	C	96	ARG	4.0
1	E	17	ARG	3.9
1	H	34	PRO	3.9
1	A	33	THR	3.9
1	A	156	ASP	3.9
1	H	42	LYS	3.8
1	D	34	PRO	3.8
1	D	35	ASN	3.8
1	D	83	GLU	3.8
1	B	34	PRO	3.8
1	F	151	LEU	3.7
1	B	52	ALA	3.7
1	F	91	ARG	3.7
1	E	19	LEU	3.6
1	F	153	GLU	3.6
1	G	34	PRO	3.6
1	D	125	LEU	3.6
1	A	32	GLY	3.6
1	A	34	PRO	3.6
1	A	96	ARG	3.6
1	B	32	GLY	3.6
1	F	36	PRO	3.5
1	F	34	PRO	3.5
1	D	67	LYS	3.5
1	F	35	ASN	3.5
1	D	149	HIS	3.4
1	D	128	LEU	3.4
1	B	23	LEU	3.4
1	B	82	ARG	3.4
1	H	45	ARG	3.4
1	B	36	PRO	3.3
1	B	16	GLU	3.3
1	H	40	ARG	3.3
1	B	33	THR	3.3
1	C	34	PRO	3.2
1	B	94	ALA	3.2
1	E	16	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	85	HIS	3.2
1	E	15	ALA	3.2
1	B	153	GLU	3.1
1	H	67	LYS	3.1
1	H	39	VAL	3.1
1	D	88	LEU	3.1
1	H	107	LEU	3.1
1	D	123	ASP	3.1
1	D	33	THR	3.1
1	E	128	LEU	3.1
1	G	125	LEU	3.0
1	C	129	LYS	3.0
1	C	89	LEU	3.0
1	H	87	PHE	3.0
1	F	33	THR	3.0
1	H	65	LEU	3.0
1	C	80	LEU	2.9
1	A	52	ALA	2.9
1	D	105	VAL	2.9
1	A	35	ASN	2.9
1	D	36	PRO	2.9
1	H	128	LEU	2.9
1	F	37	ILE	2.9
1	D	68	THR	2.9
1	H	88	LEU	2.9
1	H	83	GLU	2.8
1	C	69	ILE	2.8
1	F	53	TYR	2.8
1	D	24	GLU	2.8
1	D	52	ALA	2.8
1	G	20	ASN	2.8
1	A	28	VAL	2.8
1	G	105	VAL	2.8
1	C	128	LEU	2.7
1	D	32	GLY	2.7
1	H	33	THR	2.7
1	D	107	LEU	2.7
1	H	36	PRO	2.7
1	H	86	GLU	2.7
1	E	149	HIS	2.7
1	H	44	GLY	2.7
1	G	33	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	151	LEU	2.6
1	F	92	VAL	2.6
1	H	96	ARG	2.6
1	G	21	ASP	2.6
1	G	72	ALA	2.6
1	E	131	ILE	2.6
1	B	154	SER	2.6
1	H	52	ALA	2.5
1	E	34	PRO	2.5
1	D	86	GLU	2.5
1	E	33	THR	2.5
1	E	95	GLU	2.5
1	F	16	GLU	2.5
1	A	128	LEU	2.5
1	B	35	ASN	2.5
1	H	64	VAL	2.5
1	H	130	GLY	2.4
1	A	29	LEU	2.4
1	D	87	PHE	2.4
1	D	131	ILE	2.4
1	F	94	ALA	2.4
1	A	92	VAL	2.4
1	A	36	PRO	2.4
1	G	149	HIS	2.4
1	E	96	ARG	2.4
1	C	52	ALA	2.4
1	A	155	LEU	2.4
1	C	35	ASN	2.3
1	D	110	ARG	2.3
1	B	95	GLU	2.3
1	F	117	TRP	2.3
1	D	64	VAL	2.3
1	A	94	ALA	2.3
1	E	52	ALA	2.3
1	C	43	GLU	2.3
1	A	51	ASP	2.3
1	D	108	HIS	2.3
1	F	135	TRP	2.3
1	B	50	ASN	2.3
1	F	49	CYS	2.3
1	D	127	GLU	2.3
1	F	134	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	123	ASP	2.3
1	C	33	THR	2.3
1	A	125	LEU	2.3
1	H	103	ARG	2.2
1	H	66	GLY	2.2
1	F	55	ASP	2.2
1	H	24	GLU	2.2
1	E	32	GLY	2.2
1	B	28	VAL	2.2
1	D	46	MET	2.2
1	A	30	ILE	2.2
1	B	136	ILE	2.2
1	D	136	ILE	2.2
1	B	31	ASP	2.2
1	F	148	LEU	2.2
1	B	51	ASP	2.2
1	C	130	GLY	2.2
1	C	127	GLU	2.2
1	A	50	ASN	2.1
1	F	96	ARG	2.1
1	B	42	LYS	2.1
1	F	38	TYR	2.1
1	B	96	ARG	2.1
1	C	100	PHE	2.1
1	H	95	GLU	2.1
1	B	19	LEU	2.1
1	D	153	GLU	2.1
1	F	54	LEU	2.1
1	G	117	TRP	2.1
1	E	35	ASN	2.1
1	E	135	TRP	2.1
1	H	129	LYS	2.0
1	H	29	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.