Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:21 AM GMT

PDB ID	:	2GR8
Title	:	Hia 1022-1098
Authors	:	Meng, G.; Waksman, G.
Deposited on	:	2006-04-23
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

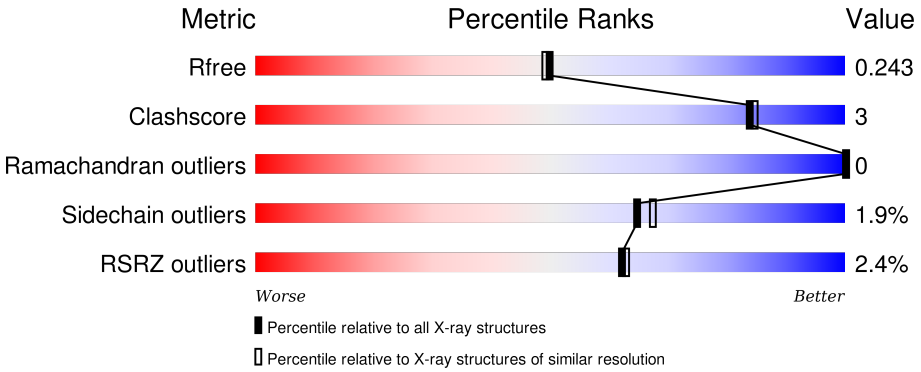
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	99	2% 72% 6% 21%
1	B	99	2% 74% 5% 21%
1	C	99	2% 73% 5% 21%
1	D	99	% 73% 5% 21%
1	E	99	3% 71% 7% 21%

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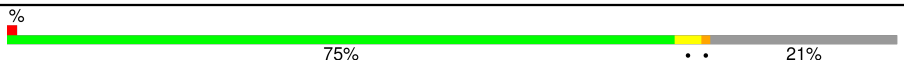
Mol	Chain	Length	Quality of chain
1	F	99	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3432 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 Adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			535	327	98	108	2			
1	B	78	Total	C	N	O	S	0	0	0
			527	320	97	108	2			
1	C	78	Total	C	N	O	S	0	0	0
			536	328	98	108	2			
1	D	78	Total	C	N	O	S	0	0	0
			536	328	98	108	2			
1	E	78	Total	C	N	O	S	0	0	0
			541	330	101	108	2			
1	F	78	Total	C	N	O	S	0	0	0
			536	328	98	108	2			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1000	ALA	-	CLONING ARTIFACT	UNP Q48152
A	1001	SER	-	CLONING ARTIFACT	UNP Q48152
A	1002	TRP	-	CLONING ARTIFACT	UNP Q48152
A	1003	SER	-	CLONING ARTIFACT	UNP Q48152
A	1004	HIS	-	CLONING ARTIFACT	UNP Q48152
A	1005	PRO	-	CLONING ARTIFACT	UNP Q48152
A	1006	GLN	-	CLONING ARTIFACT	UNP Q48152
A	1007	PHE	-	CLONING ARTIFACT	UNP Q48152
A	1008	GLU	-	CLONING ARTIFACT	UNP Q48152
A	1009	LYS	-	CLONING ARTIFACT	UNP Q48152
A	1010	SER	-	CLONING ARTIFACT	UNP Q48152
A	1011	GLY	-	CLONING ARTIFACT	UNP Q48152
A	1012	GLY	-	CLONING ARTIFACT	UNP Q48152
A	1013	GLY	-	CLONING ARTIFACT	UNP Q48152
A	1014	GLY	-	CLONING ARTIFACT	UNP Q48152
A	1015	GLY	-	CLONING ARTIFACT	UNP Q48152
A	1016	LEU	-	CLONING ARTIFACT	UNP Q48152

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1017	VAL	-	CLONING ARTIFACT	UNP Q48152
A	1018	PRO	-	CLONING ARTIFACT	UNP Q48152
A	1019	ARG	-	CLONING ARTIFACT	UNP Q48152
A	1020	GLY	-	CLONING ARTIFACT	UNP Q48152
A	1021	SER	-	CLONING ARTIFACT	UNP Q48152
B	1000	ALA	-	CLONING ARTIFACT	UNP Q48152
B	1001	SER	-	CLONING ARTIFACT	UNP Q48152
B	1002	TRP	-	CLONING ARTIFACT	UNP Q48152
B	1003	SER	-	CLONING ARTIFACT	UNP Q48152
B	1004	HIS	-	CLONING ARTIFACT	UNP Q48152
B	1005	PRO	-	CLONING ARTIFACT	UNP Q48152
B	1006	GLN	-	CLONING ARTIFACT	UNP Q48152
B	1007	PHE	-	CLONING ARTIFACT	UNP Q48152
B	1008	GLU	-	CLONING ARTIFACT	UNP Q48152
B	1009	LYS	-	CLONING ARTIFACT	UNP Q48152
B	1010	SER	-	CLONING ARTIFACT	UNP Q48152
B	1011	GLY	-	CLONING ARTIFACT	UNP Q48152
B	1012	GLY	-	CLONING ARTIFACT	UNP Q48152
B	1013	GLY	-	CLONING ARTIFACT	UNP Q48152
B	1014	GLY	-	CLONING ARTIFACT	UNP Q48152
B	1015	GLY	-	CLONING ARTIFACT	UNP Q48152
B	1016	LEU	-	CLONING ARTIFACT	UNP Q48152
B	1017	VAL	-	CLONING ARTIFACT	UNP Q48152
B	1018	PRO	-	CLONING ARTIFACT	UNP Q48152
B	1019	ARG	-	CLONING ARTIFACT	UNP Q48152
B	1020	GLY	-	CLONING ARTIFACT	UNP Q48152
B	1021	SER	-	CLONING ARTIFACT	UNP Q48152
C	1000	ALA	-	CLONING ARTIFACT	UNP Q48152
C	1001	SER	-	CLONING ARTIFACT	UNP Q48152
C	1002	TRP	-	CLONING ARTIFACT	UNP Q48152
C	1003	SER	-	CLONING ARTIFACT	UNP Q48152
C	1004	HIS	-	CLONING ARTIFACT	UNP Q48152
C	1005	PRO	-	CLONING ARTIFACT	UNP Q48152
C	1006	GLN	-	CLONING ARTIFACT	UNP Q48152
C	1007	PHE	-	CLONING ARTIFACT	UNP Q48152
C	1008	GLU	-	CLONING ARTIFACT	UNP Q48152
C	1009	LYS	-	CLONING ARTIFACT	UNP Q48152
C	1010	SER	-	CLONING ARTIFACT	UNP Q48152
C	1011	GLY	-	CLONING ARTIFACT	UNP Q48152
C	1012	GLY	-	CLONING ARTIFACT	UNP Q48152
C	1013	GLY	-	CLONING ARTIFACT	UNP Q48152
C	1014	GLY	-	CLONING ARTIFACT	UNP Q48152

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1015	GLY	-	CLONING ARTIFACT	UNP Q48152
C	1016	LEU	-	CLONING ARTIFACT	UNP Q48152
C	1017	VAL	-	CLONING ARTIFACT	UNP Q48152
C	1018	PRO	-	CLONING ARTIFACT	UNP Q48152
C	1019	ARG	-	CLONING ARTIFACT	UNP Q48152
C	1020	GLY	-	CLONING ARTIFACT	UNP Q48152
C	1021	SER	-	CLONING ARTIFACT	UNP Q48152
D	1000	ALA	-	CLONING ARTIFACT	UNP Q48152
D	1001	SER	-	CLONING ARTIFACT	UNP Q48152
D	1002	TRP	-	CLONING ARTIFACT	UNP Q48152
D	1003	SER	-	CLONING ARTIFACT	UNP Q48152
D	1004	HIS	-	CLONING ARTIFACT	UNP Q48152
D	1005	PRO	-	CLONING ARTIFACT	UNP Q48152
D	1006	GLN	-	CLONING ARTIFACT	UNP Q48152
D	1007	PHE	-	CLONING ARTIFACT	UNP Q48152
D	1008	GLU	-	CLONING ARTIFACT	UNP Q48152
D	1009	LYS	-	CLONING ARTIFACT	UNP Q48152
D	1010	SER	-	CLONING ARTIFACT	UNP Q48152
D	1011	GLY	-	CLONING ARTIFACT	UNP Q48152
D	1012	GLY	-	CLONING ARTIFACT	UNP Q48152
D	1013	GLY	-	CLONING ARTIFACT	UNP Q48152
D	1014	GLY	-	CLONING ARTIFACT	UNP Q48152
D	1015	GLY	-	CLONING ARTIFACT	UNP Q48152
D	1016	LEU	-	CLONING ARTIFACT	UNP Q48152
D	1017	VAL	-	CLONING ARTIFACT	UNP Q48152
D	1018	PRO	-	CLONING ARTIFACT	UNP Q48152
D	1019	ARG	-	CLONING ARTIFACT	UNP Q48152
D	1020	GLY	-	CLONING ARTIFACT	UNP Q48152
D	1021	SER	-	CLONING ARTIFACT	UNP Q48152
E	1000	ALA	-	CLONING ARTIFACT	UNP Q48152
E	1001	SER	-	CLONING ARTIFACT	UNP Q48152
E	1002	TRP	-	CLONING ARTIFACT	UNP Q48152
E	1003	SER	-	CLONING ARTIFACT	UNP Q48152
E	1004	HIS	-	CLONING ARTIFACT	UNP Q48152
E	1005	PRO	-	CLONING ARTIFACT	UNP Q48152
E	1006	GLN	-	CLONING ARTIFACT	UNP Q48152
E	1007	PHE	-	CLONING ARTIFACT	UNP Q48152
E	1008	GLU	-	CLONING ARTIFACT	UNP Q48152
E	1009	LYS	-	CLONING ARTIFACT	UNP Q48152
E	1010	SER	-	CLONING ARTIFACT	UNP Q48152
E	1011	GLY	-	CLONING ARTIFACT	UNP Q48152
E	1012	GLY	-	CLONING ARTIFACT	UNP Q48152

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1013	GLY	-	CLONING ARTIFACT	UNP Q48152
E	1014	GLY	-	CLONING ARTIFACT	UNP Q48152
E	1015	GLY	-	CLONING ARTIFACT	UNP Q48152
E	1016	LEU	-	CLONING ARTIFACT	UNP Q48152
E	1017	VAL	-	CLONING ARTIFACT	UNP Q48152
E	1018	PRO	-	CLONING ARTIFACT	UNP Q48152
E	1019	ARG	-	CLONING ARTIFACT	UNP Q48152
E	1020	GLY	-	CLONING ARTIFACT	UNP Q48152
E	1021	SER	-	CLONING ARTIFACT	UNP Q48152
F	1000	ALA	-	CLONING ARTIFACT	UNP Q48152
F	1001	SER	-	CLONING ARTIFACT	UNP Q48152
F	1002	TRP	-	CLONING ARTIFACT	UNP Q48152
F	1003	SER	-	CLONING ARTIFACT	UNP Q48152
F	1004	HIS	-	CLONING ARTIFACT	UNP Q48152
F	1005	PRO	-	CLONING ARTIFACT	UNP Q48152
F	1006	GLN	-	CLONING ARTIFACT	UNP Q48152
F	1007	PHE	-	CLONING ARTIFACT	UNP Q48152
F	1008	GLU	-	CLONING ARTIFACT	UNP Q48152
F	1009	LYS	-	CLONING ARTIFACT	UNP Q48152
F	1010	SER	-	CLONING ARTIFACT	UNP Q48152
F	1011	GLY	-	CLONING ARTIFACT	UNP Q48152
F	1012	GLY	-	CLONING ARTIFACT	UNP Q48152
F	1013	GLY	-	CLONING ARTIFACT	UNP Q48152
F	1014	GLY	-	CLONING ARTIFACT	UNP Q48152
F	1015	GLY	-	CLONING ARTIFACT	UNP Q48152
F	1016	LEU	-	CLONING ARTIFACT	UNP Q48152
F	1017	VAL	-	CLONING ARTIFACT	UNP Q48152
F	1018	PRO	-	CLONING ARTIFACT	UNP Q48152
F	1019	ARG	-	CLONING ARTIFACT	UNP Q48152
F	1020	GLY	-	CLONING ARTIFACT	UNP Q48152
F	1021	SER	-	CLONING ARTIFACT	UNP Q48152

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	31	Total O 31 31	0	0
2	B	47	Total O 47 47	0	0
2	C	31	Total O 31 31	0	0
2	D	33	Total O 33 33	0	0

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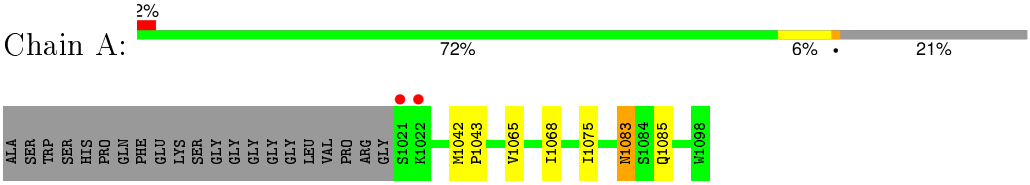
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	40	Total O 40 40	0	0
2	F	39	Total O 39 39	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

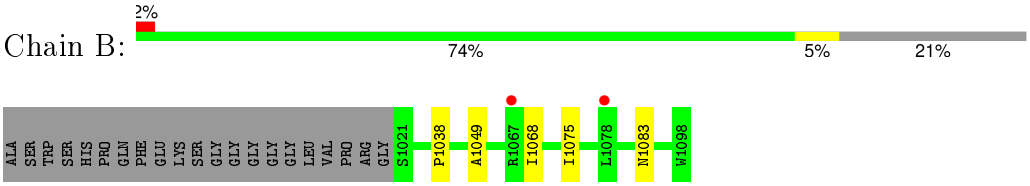
- Molecule 1: Adhesin

Chain A:



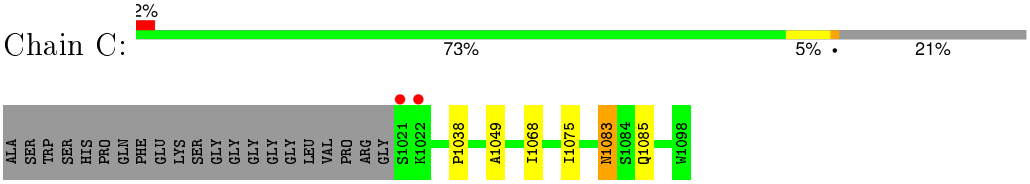
- Molecule 1: Adhesin

Chain B:



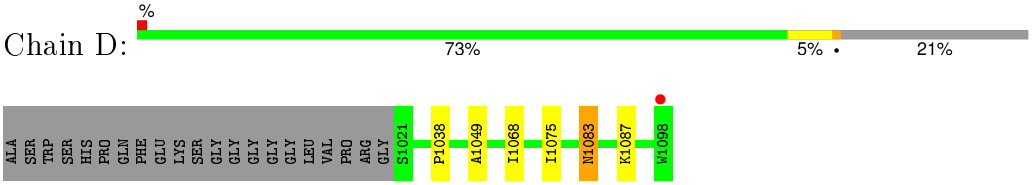
- Molecule 1: Adhesin

Chain C:



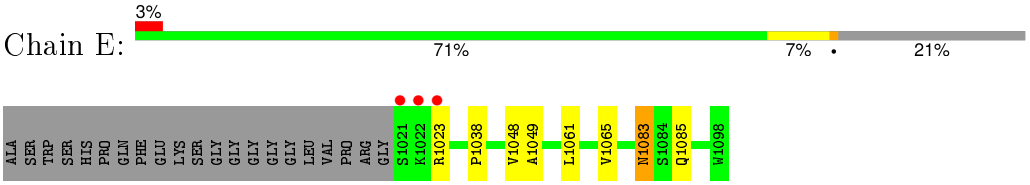
- Molecule 1: Adhesin

Chain D:



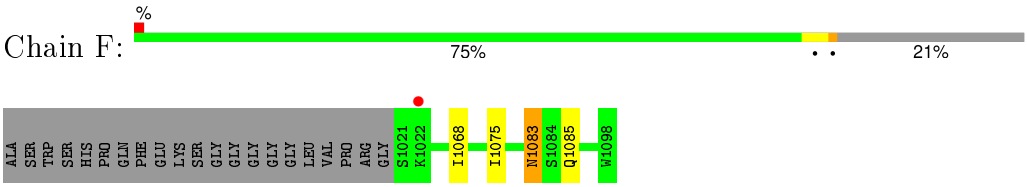
- Molecule 1: Adhesin

Chain E:



- Molecule 1: Adhesin

Chain F:


%
75%
21%
ALA
SER
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS
SER
GLY
GLY
GLY
GLY
GLY
LEU
VAL
PRO
ARG
GLY
S1021
K1022
I1068
I1075
N1083
S1094
Q1095
W1098

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.26Å 82.26Å 82.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.00) 99.2 (19.98-1.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.215 0.223 , 0.243	Depositor DCC
R_{free} test set	1949 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.9	EDS
Estimated twinning fraction	0.022 for -h,l,k 0.026 for -l,-k,-h 0.019 for k,h,-l 0.013 for k,l,h 0.013 for l,h,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 52073 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3432	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.28	0/540	0.44	0/729
1	B	0.28	0/530	0.44	0/714
1	C	0.29	0/541	0.45	0/730
1	D	0.29	0/541	0.45	0/730
1	E	0.29	0/546	0.46	0/736
1	F	0.29	0/541	0.45	0/730
All	All	0.29	0/3239	0.45	0/4369

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	535	0	538	4	0
1	B	527	0	532	2	0
1	C	536	0	540	3	0
1	D	536	0	540	3	0
1	E	541	0	549	6	0
1	F	536	0	540	2	0
2	A	31	0	0	0	0
2	B	47	0	0	0	0
2	C	31	0	0	0	0
2	D	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	40	0	0	0	0
2	F	39	0	0	0	0
All	All	3432	0	3239	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 3.

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:E:1023:ARG:HH11	1:E:1023:ARG:HG2	1.55	0.71
1:B:1038:PRO:HD2	1:B:1049:ALA:HB1	1.90	0.52
1:E:1048:VAL:HG22	1:E:1065:VAL:HG12	1.95	0.49
1:E:1038:PRO:HD2	1:E:1049:ALA:HB1	1.95	0.47
1:B:1068:ILE:HG12	1:B:1075:ILE:HG12	1.98	0.46
1:F:1068:ILE:HG12	1:F:1075:ILE:HG12	1.98	0.46
1:F:1083:ASN:HD22	1:F:1085:GLN:H	1.64	0.45
1:C:1038:PRO:HD2	1:C:1049:ALA:HB1	1.97	0.45
1:C:1068:ILE:HG12	1:C:1075:ILE:HG12	1.97	0.45
1:D:1038:PRO:HD2	1:D:1049:ALA:HB1	1.99	0.44
1:D:1068:ILE:HG12	1:D:1075:ILE:HG12	2.00	0.44
1:A:1068:ILE:HG12	1:A:1075:ILE:HG12	1.98	0.44
1:C:1083:ASN:HD22	1:C:1085:GLN:H	1.66	0.43
1:D:1083:ASN:ND2	1:D:1087:LYS:H	2.16	0.43
1:E:1023:ARG:HG2	1:E:1023:ARG:NH1	2.27	0.42
1:A:1065:VAL:HG11	1:E:1061:LEU:HD13	2.01	0.42
1:E:1083:ASN:HD22	1:E:1085:GLN:H	1.68	0.41
1:A:1083:ASN:HD22	1:A:1085:GLN:H	1.68	0.41
1:A:1042:MET:HA	1:A:1043:PRO:HD3	1.91	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	76/99 (77%)	76 (100%)	0	0	100	100
1	B	76/99 (77%)	76 (100%)	0	0	100	100
1	C	76/99 (77%)	76 (100%)	0	0	100	100
1	D	76/99 (77%)	76 (100%)	0	0	100	100
1	E	76/99 (77%)	76 (100%)	0	0	100	100
1	F	76/99 (77%)	76 (100%)	0	0	100	100
All	All	456/594 (77%)	456 (100%)	0	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	A	53/68 (78%)	52 (98%)	1 (2%)	65	67
1	B	52/68 (76%)	51 (98%)	1 (2%)	65	67
1	C	53/68 (78%)	52 (98%)	1 (2%)	65	67
1	D	53/68 (78%)	52 (98%)	1 (2%)	65	67
1	E	54/68 (79%)	53 (98%)	1 (2%)	65	67
1	F	53/68 (78%)	52 (98%)	1 (2%)	65	67
All	All	318/408 (78%)	312 (98%)	6 (2%)	65	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1083	ASN
1	B	1083	ASN
1	C	1083	ASN
1	D	1083	ASN

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Mol	Chain	Res	Type
1	E	1083	ASN
1	F	1083	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1083	ASN
1	B	1083	ASN
1	B	1085	GLN
1	C	1083	ASN
1	D	1083	ASN
1	D	1085	GLN
1	E	1083	ASN
1	F	1083	ASN

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 carbohydrates 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	A	78/99 (78%)	0.19	2 (2%)	59	60	5, 8, 9, 10	0
1	B	78/99 (78%)	0.16	2 (2%)	59	60	6, 7, 10, 11	0
1	C	78/99 (78%)	0.02	2 (2%)	59	60	4, 7, 10, 11	0
1	D	78/99 (78%)	-0.01	1 (1%)	79	80	6, 7, 10, 10	0
1	E	78/99 (78%)	0.18	3 (3%)	44	45	6, 7, 10, 13	0
1	F	78/99 (78%)	0.14	1 (1%)	79	80	5, 8, 10, 12	0
All	All	468/594 (78%)	0.11	11 (2%)	62	63	4, 7, 10, 13	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	SER	3.6
1	E	1021	SER	3.4
1	D	1098	TRP	3.4
1	A	1022	LYS	3.3
1	C	1022	LYS	3.1
1	E	1023	ARG	2.5
1	C	1021	SER	2.4
1	B	1067	ARG	2.2
1	F	1022	LYS	2.1
1	E	1022	LYS	2.1
1	B	1078	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates 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.