Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:54 AM GMT

PDB ID	:	3GE4
Title	:	Crystal structure of ferritin:DNA-binding protein DPS from Brucella Melitensis
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2009-02-25
Resolution	:	1.70 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:

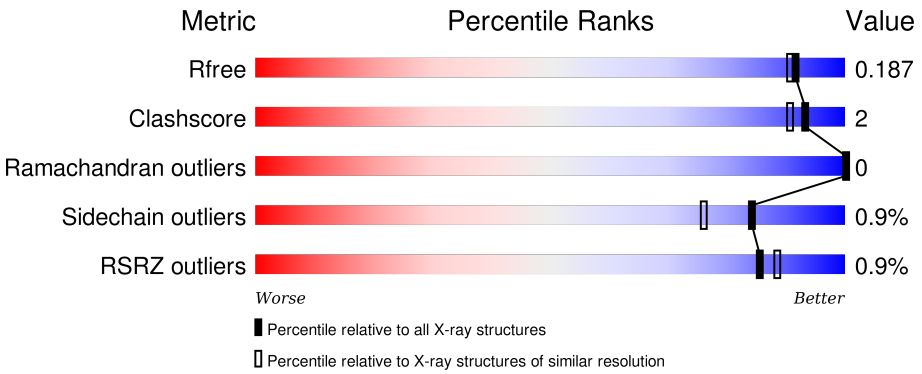
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	173	% 90% • 7%
1	B	173	% 87% 6% 7%
1	C	173	% 91% • 7%
1	D	173	86% 6% • 7%
1	E	173	87% • • 7%

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Mol	Chain	Length	Quality of chain
1	F	173	%, 91%, 7%
1	G	173	%, 88%, 7%
1	H	173	%, 90%, 7%
1	I	173	2%, 88%, 5%, 7%
1	J	173	87%, 6%, 7%
1	K	173	91%, 7%
1	L	173	2%, 91%, 7%

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
2	CA	G	167	-	-	-	X
2	CA	H	167	-	-	-	X
2	CA	K	167	-	-	-	X
2	CA	L	167	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17437 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 DNA PROTECTION DURING STARVATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	161	1271	795	218	255	3	0	5	0
			Total	C	N	O	S			
1	B	161	1272	795	214	260	3	0	8	0
			Total	C	N	O	S			
1	C	161	1258	787	213	255	3	0	5	0
			Total	C	N	O	S			
1	D	161	1282	803	219	257	3	0	7	0
			Total	C	N	O	S			
1	E	161	1265	791	216	255	3	0	5	0
			Total	C	N	O	S			
1	F	161	1268	794	215	256	3	0	6	0
			Total	C	N	O	S			
1	G	161	1254	785	213	253	3	0	4	0
			Total	C	N	O	S			
1	H	161	1270	796	215	256	3	0	7	0
			Total	C	N	O	S			
1	I	161	1259	788	212	256	3	0	5	0
			Total	C	N	O	S			
1	J	161	1272	797	213	259	3	0	8	0
			Total	C	N	O	S			
1	K	161	1272	796	217	256	3	0	6	0
			Total	C	N	O	S			
1	L	161	1281	802	216	260	3	0	9	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
A	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
A	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
A	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
A	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
A	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
A	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
B	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
B	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
B	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
B	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
B	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
B	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
B	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
B	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
C	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
C	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
C	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
C	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
C	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
C	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
C	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
C	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
D	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
D	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
D	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
D	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
D	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
D	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
D	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
D	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
E	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
E	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
E	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
E	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
E	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
E	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
E	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
E	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
F	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
F	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
F	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
F	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
F	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
F	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
F	0	HIS	-	EXPRESSION TAG	UNP Q8YE98

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
G	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
G	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
G	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
G	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
G	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
G	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
G	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
G	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
H	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
H	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
H	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
H	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
H	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
H	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
H	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
H	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
I	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
I	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
I	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
I	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
I	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
I	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
I	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
I	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
J	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
J	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
J	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
J	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
J	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
J	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
J	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
J	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
K	-6	MET	-	EXPRESSION TAG	UNP Q8YE98
K	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
K	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
K	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
K	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
K	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
K	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
K	1	HIS	-	EXPRESSION TAG	UNP Q8YE98
L	-6	MET	-	EXPRESSION TAG	UNP Q8YE98

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	ALA	-	EXPRESSION TAG	UNP Q8YE98
L	-4	HIS	-	EXPRESSION TAG	UNP Q8YE98
L	-3	HIS	-	EXPRESSION TAG	UNP Q8YE98
L	-2	HIS	-	EXPRESSION TAG	UNP Q8YE98
L	-1	HIS	-	EXPRESSION TAG	UNP Q8YE98
L	0	HIS	-	EXPRESSION TAG	UNP Q8YE98
L	1	HIS	-	EXPRESSION TAG	UNP Q8YE98

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	L	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	170	Total O 170 170	0	0
3	B	153	Total O 153 153	0	0

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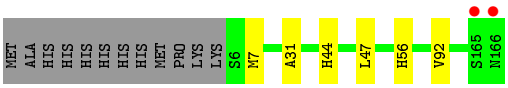
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	168	168	168	0	0
			Total	O		
3	D	191	191	191	0	0
			Total	O		
3	E	199	199	199	0	0
			Total	O		
3	F	193	193	193	0	0
			Total	O		
3	G	186	186	186	0	0
			Total	O		
3	H	198	198	198	0	0
			Total	O		
3	I	171	171	171	0	0
			Total	O		
3	J	207	207	207	0	0
			Total	O		
3	K	198	198	198	0	0
			Total	O		
3	L	167	167	167	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.

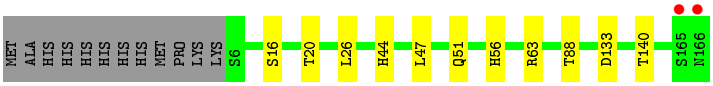
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain A:



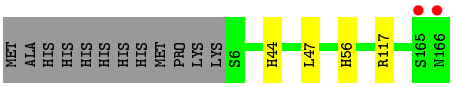
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain B:



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain C:



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

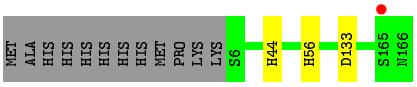
Chain D:

- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain E:

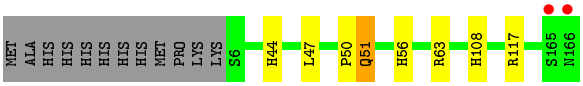
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain F:



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain G:

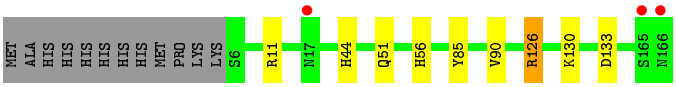


• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain H:

• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain I:



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

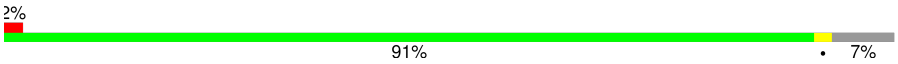
Chain J:

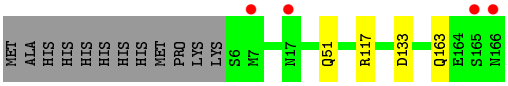
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain K:

• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.24Å 98.33Å 105.45Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	19.86 – 1.70 19.86 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.86-1.70) 99.8 (19.86-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.143 , 0.179 0.153 , 0.187	Depositor DCC
R_{free} test set	10665 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.1	EDS
Estimated twinning fraction	0.014 for k,h,-l 0.015 for -k,-h,-l 0.027 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 212708 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17437	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.71	1/1308 (0.1%)	0.75	0/1780
1	B	0.67	0/1312	0.71	1/1790 (0.1%)
1	C	0.71	1/1295 (0.1%)	0.72	0/1765
1	D	0.75	0/1325	0.78	0/1803
1	E	0.74	0/1302	0.78	2/1774 (0.1%)
1	F	0.72	0/1308	0.77	0/1782
1	G	0.73	1/1288 (0.1%)	0.77	1/1756 (0.1%)
1	H	0.73	1/1313 (0.1%)	0.75	1/1789 (0.1%)
1	I	0.71	0/1299	0.73	1/1773 (0.1%)
1	J	0.71	1/1318 (0.1%)	0.72	0/1797
1	K	0.72	0/1312	0.76	0/1786
1	L	0.68	0/1330	0.74	1/1812 (0.1%)
All	All	0.72	5/15710 (0.0%)	0.75	7/21407 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	117	ARG	CG-CD	-5.61	1.38	1.51
1	J	117	ARG	CG-CD	-5.30	1.38	1.51
1	H	117	ARG	CG-CD	-5.28	1.38	1.51
1	C	117	ARG	CG-CD	-5.18	1.39	1.51
1	A	31	ALA	CA-CB	5.14	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	117	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	I	11	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	G	63	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	B	63	ARG	NE-CZ-NH2	5.27	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	14	LEU	CA-CB-CG	5.19	127.23	115.30
1	H	126	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	L	117	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1271	0	1242	5	0
1	B	1272	0	1226	5	0
1	C	1258	0	1217	1	0
1	D	1282	0	1265	12	0
1	E	1265	0	1230	7	0
1	F	1268	0	1236	2	0
1	G	1254	0	1215	4	0
1	H	1270	0	1244	3	0
1	I	1259	0	1215	7	0
1	J	1272	0	1237	5	0
1	K	1272	0	1246	2	0
1	L	1281	0	1253	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	170	0	0	3	0
3	B	153	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	168	0	0	1	0
3	D	191	0	0	7	0
3	E	199	0	0	4	1
3	F	193	0	0	1	0
3	G	186	0	0	5	0
3	H	198	0	0	2	0
3	I	171	0	0	3	0
3	J	207	0	0	3	0
3	K	198	0	0	1	0
3	L	167	0	0	4	0
All	All	17437	0	14826	56	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (56) 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:A:7:MET:HE3	3:A:415:HOH:O	1.58	1.03
1:A:7:MET:CE	3:A:415:HOH:O	2.13	0.94
1:H:51:GLN:OE1	3:H:2198:HOH:O	1.91	0.89
1:G:51:GLN:OE1	3:G:2196:HOH:O	1.91	0.87
1:K:133[A]:ASP:OD2	3:K:188:HOH:O	1.96	0.82
1:E:51:GLN:OE1	3:E:2192:HOH:O	1.99	0.81
1:J:65[B]:GLU:OE1	3:J:744:HOH:O	2.03	0.77
1:E:133[B]:ASP:OD2	3:E:1876:HOH:O	2.04	0.76
1:L:133[B]:ASP:OD1	3:L:1465:HOH:O	2.06	0.74
1:E:133[B]:ASP:OD1	3:E:178:HOH:O	2.05	0.74
1:E:11:ARG:HD2	3:E:2079:HOH:O	1.90	0.72
1:L:51:GLN:OE1	3:L:640:HOH:O	2.09	0.71
1:J:133[B]:ASP:OD2	3:J:958:HOH:O	2.11	0.69
1:I:51:GLN:NE2	3:I:2193:HOH:O	1.94	0.69
1:L:133[B]:ASP:OD2	3:L:1301:HOH:O	2.12	0.67
1:G:108:HIS:ND1	3:G:2201:HOH:O	2.28	0.66
1:D:133[A]:ASP:OD2	3:D:1276:HOH:O	2.16	0.62
1:I:133[B]:ASP:OD1	3:I:1986:HOH:O	2.16	0.61
1:D:51:GLN:H	1:D:51:GLN:HE21	1.49	0.60
1:I:130:LYS:NZ	3:I:1392:HOH:O	2.28	0.59
3:G:179:HOH:O	1:I:126:ARG:HD3	2.02	0.59
1:D:133[A]:ASP:OD1	3:D:2077:HOH:O	2.16	0.58
3:B:470:HOH:O	1:D:126:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:MET:CE	3:D:1271:HOH:O	2.51	0.58
1:H:133:ASP:OD2	3:H:1885:HOH:O	2.16	0.57
1:G:50:PRO:HD2	3:G:2196:HOH:O	2.06	0.55
1:A:44:HIS:CE1	1:A:56:HIS:CE1	2.96	0.53
1:F:44:HIS:CE1	1:F:56:HIS:CE1	2.97	0.52
1:D:127:LYS:NZ	3:D:2070:HOH:O	2.33	0.51
1:B:16[A]:SER:O	1:B:20[A]:THR:HG23	2.09	0.51
1:D:7:MET:HE3	3:D:1271:HOH:O	2.08	0.50
1:A:7:MET:HE1	3:A:415:HOH:O	1.96	0.50
1:A:92:VAL:HB	1:B:88[B]:THR:HG22	1.94	0.50
1:G:44:HIS:CE1	1:G:56:HIS:CE1	3.00	0.49
1:B:44:HIS:CE1	1:B:56:HIS:CE1	3.01	0.49
1:F:133[A]:ASP:OD2	3:F:2194:HOH:O	2.19	0.49
1:L:163:GLN:O	3:L:1810:HOH:O	2.20	0.48
1:B:133[B]:ASP:OD1	3:B:773:HOH:O	2.19	0.47
3:C:170:HOH:O	1:E:126:ARG:HD3	2.14	0.47
1:H:44:HIS:CE1	1:H:56:HIS:CE1	3.03	0.47
1:D:7:MET:HE1	3:D:1271:HOH:O	2.13	0.46
1:D:75:GLU:OE1	3:D:1949:HOH:O	2.21	0.45
3:G:2125:HOH:O	1:I:130:LYS:HE3	2.16	0.45
1:K:44:HIS:CE1	1:K:56:HIS:CE1	3.04	0.45
1:I:44:HIS:CE1	1:I:56:HIS:CE1	3.04	0.45
1:D:39:ILE:HD13	1:D:117:ARG:HD3	1.99	0.45
1:E:44:HIS:CE1	1:E:56:HIS:CE1	3.05	0.44
1:D:21[B]:THR:HG22	1:D:22:MET:CE	2.48	0.44
1:E:39:ILE:HG23	1:E:100:TYR:CD1	2.53	0.43
1:C:44:HIS:CE1	1:C:56:HIS:CE1	3.07	0.42
1:I:85:TYR:HB3	1:I:90:VAL:HG11	2.00	0.42
1:D:85:TYR:HB3	1:D:90:VAL:HG11	2.02	0.41
1:J:39:ILE:HG23	1:J:100:TYR:CD1	2.56	0.41
1:B:26:LEU:HD21	1:B:140:THR:HG23	2.03	0.41
1:J:11:ARG:NH2	3:J:1319:HOH:O	2.53	0.40
1:J:44:HIS:CE1	1:J:56:HIS:CE1	3.09	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:588:HOH:O	3:E:2080:HOH:O[2_655]	2.16	0.04

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	164/173 (95%)	162 (99%)	2 (1%)	0	100	100
1	B	167/173 (96%)	164 (98%)	3 (2%)	0	100	100
1	C	164/173 (95%)	162 (99%)	2 (1%)	0	100	100
1	D	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
1	E	164/173 (95%)	161 (98%)	3 (2%)	0	100	100
1	F	165/173 (95%)	163 (99%)	2 (1%)	0	100	100
1	G	163/173 (94%)	160 (98%)	3 (2%)	0	100	100
1	H	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
1	I	165/173 (95%)	162 (98%)	3 (2%)	0	100	100
1	J	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
1	K	165/173 (95%)	162 (98%)	3 (2%)	0	100	100
1	L	168/173 (97%)	167 (99%)	1 (1%)	0	100	100
All	All	1984/2076 (96%)	1957 (99%)	27 (1%)	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	137/144 (95%)	136 (99%)	1 (1%)	88	82
1	B	137/144 (95%)	135 (98%)	2 (2%)	72	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	135/144 (94%)	134 (99%)	1 (1%)	88	82
1	D	140/144 (97%)	139 (99%)	1 (1%)	88	82
1	E	136/144 (94%)	133 (98%)	3 (2%)	60	39
1	F	137/144 (95%)	137 (100%)	0	100	100
1	G	134/144 (93%)	132 (98%)	2 (2%)	72	56
1	H	138/144 (96%)	137 (99%)	1 (1%)	88	82
1	I	135/144 (94%)	134 (99%)	1 (1%)	88	82
1	J	138/144 (96%)	136 (99%)	2 (1%)	74	59
1	K	138/144 (96%)	138 (100%)	0	100	100
1	L	140/144 (97%)	140 (100%)	0	100	100
All	All	1645/1728 (95%)	1631 (99%)	14 (1%)	84	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	B	47	LEU
1	B	51	GLN
1	C	47	LEU
1	D	51	GLN
1	E	14	LEU
1	E	51	GLN
1	E	126	ARG
1	G	47	LEU
1	G	51	GLN
1	H	51	GLN
1	I	126	ARG
1	J	47	LEU
1	J	51	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	ASN
1	D	51	GLN
1	E	51	GLN
1	G	51	GLN

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Mol	Chain	Res	Type
1	H	51	GLN
1	L	51	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	A	161/173 (93%)	-0.32	2 (1%)	81	85	11, 16, 25, 31	0
1	B	161/173 (93%)	-0.24	2 (1%)	81	85	12, 16, 26, 32	0
1	C	161/173 (93%)	-0.38	2 (1%)	81	85	9, 14, 22, 36	0
1	D	161/173 (93%)	-0.41	0	100	100	10, 14, 23, 31	0
1	E	161/173 (93%)	-0.50	0	100	100	8, 12, 21, 27	0
1	F	161/173 (93%)	-0.56	1 (0%)	90	92	7, 12, 20, 28	0
1	G	161/173 (93%)	-0.56	2 (1%)	81	85	7, 10, 20, 30	0
1	H	161/173 (93%)	-0.52	2 (1%)	81	85	7, 10, 20, 27	0
1	I	161/173 (93%)	-0.50	3 (1%)	70	74	8, 13, 22, 29	0
1	J	161/173 (93%)	-0.55	0	100	100	8, 12, 19, 23	0
1	K	161/173 (93%)	-0.56	0	100	100	9, 13, 20, 26	0
1	L	161/173 (93%)	-0.41	4 (2%)	61	65	9, 14, 24, 29	0
All	All	1932/2076 (93%)	-0.46	18 (0%)	85	88	7, 13, 23, 36	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	SER	3.4
1	G	165	SER	3.1
1	F	165	SER	2.9
1	G	166	ASN	2.9
1	A	165	SER	2.8
1	H	165[A]	SER	2.8
1	C	166	ASN	2.7
1	L	17	ASN	2.7
1	I	165	SER	2.7
1	I	17	ASN	2.6
1	B	165[A]	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	166	ASN	2.4
1	L	165[A]	SER	2.3
1	L	7	MET	2.2
1	A	166	ASN	2.1
1	H	166	ASN	2.1
1	L	166	ASN	2.0
1	B	166	ASN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	CA	K	167	1/1	0.99	0.11	5.64	20,20,20,20	0
2	CA	G	167	1/1	0.99	0.11	2.88	22,22,22,22	0
2	CA	H	167	1/1	0.99	0.09	2.76	18,18,18,18	0
2	CA	L	167	1/1	0.99	0.11	2.43	24,24,24,24	0
2	CA	J	167	1/1	0.99	0.10	1.97	22,22,22,22	0
2	CA	C	167	1/1	0.99	0.10	1.87	23,23,23,23	0
2	CA	I	167	1/1	0.99	0.10	1.84	26,26,26,26	0
2	CA	E	167	1/1	0.99	0.09	1.37	23,23,23,23	0
2	CA	B	167	1/1	0.99	0.10	1.11	24,24,24,24	0
2	CA	A	167	1/1	0.98	0.09	0.96	25,25,25,25	0
2	CA	D	167	1/1	0.99	0.09	0.77	25,25,25,25	0
2	CA	F	167	1/1	0.99	0.08	0.63	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.