



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2017 – 05:48 AM EDT

PDB ID : 2IOU  
Title : Major Tropism Determinant P1 (Mtd-P1) Variant Complexed with Bordetella  
brochiseptica Virulence Factor Pertactin extracellular domain (Prn-E).  
Authors : Miller, J.L.; Ghosh, P.  
Deposited on : unknown  
Resolution : 3.16 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

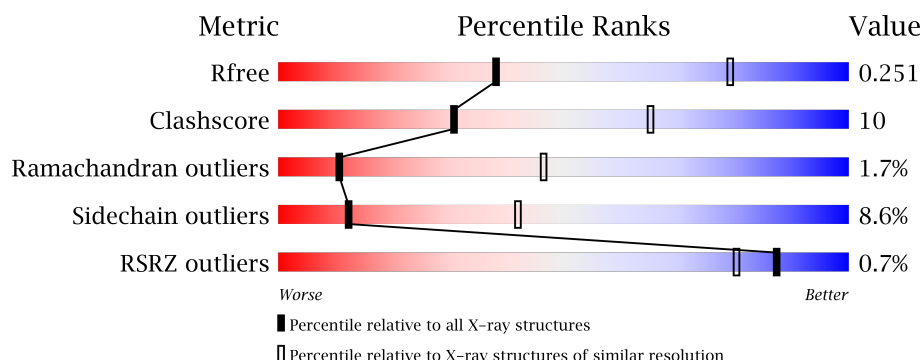
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 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))
$R_{free}$	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	<div> <div>80%</div> <div>19%</div> <div>..</div> </div>
1	B	376	<div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	C	376	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	D	376	<div> <div>85%</div> <div>15%</div> <div>.</div> </div>
1	E	376	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	376	
2	G	535	
2	H	535	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	3	-	-	-	X
3	MG	D	4	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23900 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 Major Tropism Determinant P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	B	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	C	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	D	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	E	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	F	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			

- Molecule 2 is a protein called Pertactin Extracellular Domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	508	Total	C	N	O	S	54	0	0
			3674	2265	686	717	6			
2	H	508	Total	C	N	O	S	54	0	0
			3674	2265	686	717	6			

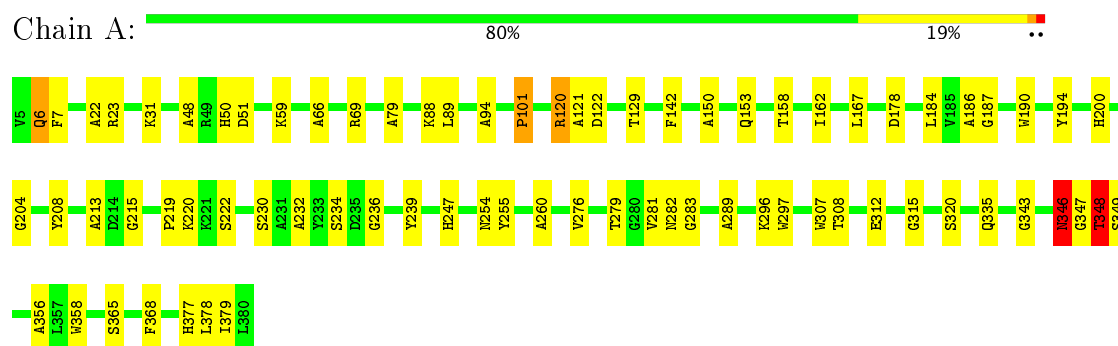
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	2	Total	Mg	0	0
			2	2		

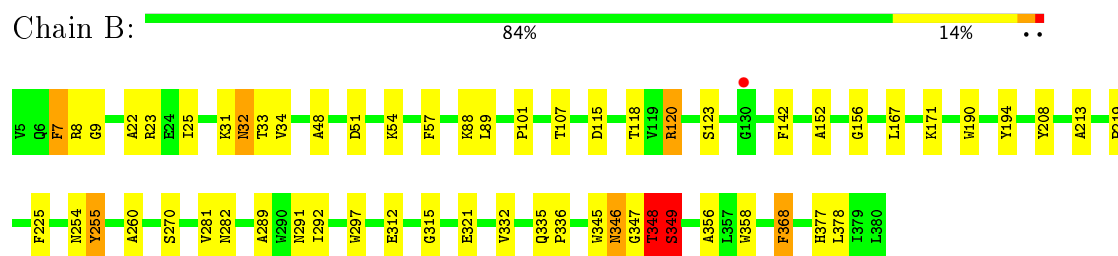
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

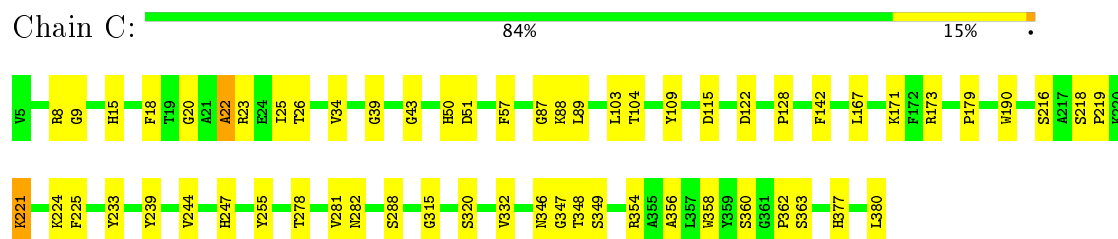
#### • Molecule 1: Major Tropism Determinant P1



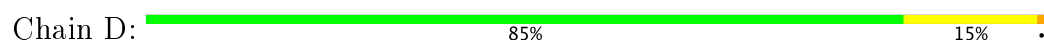
#### • Molecule 1: Major Tropism Determinant P1

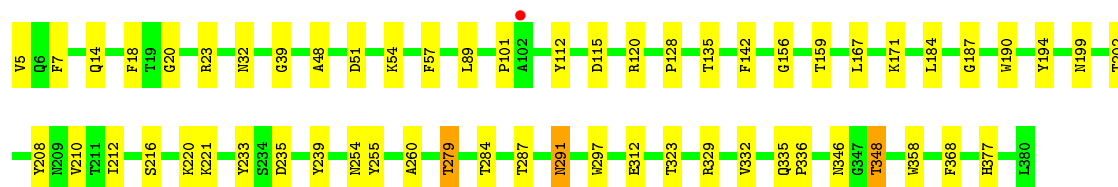


#### • Molecule 1: Major Tropism Determinant P1

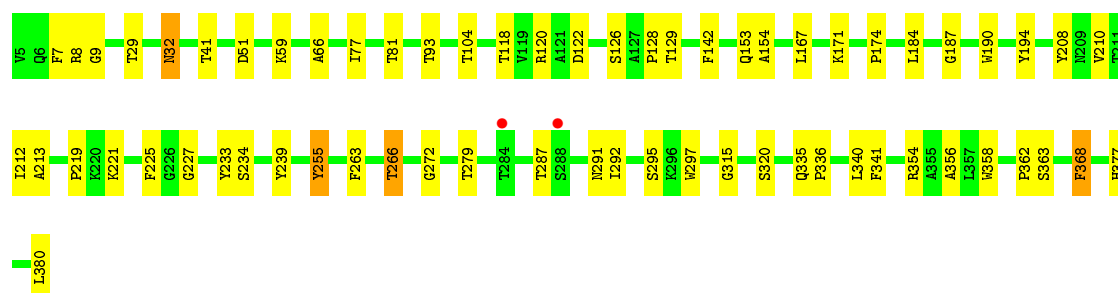
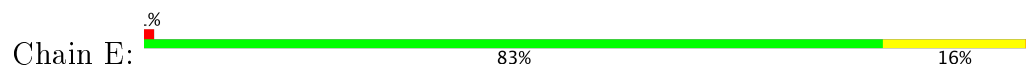


#### • Molecule 1: Major Tropism Determinant P1

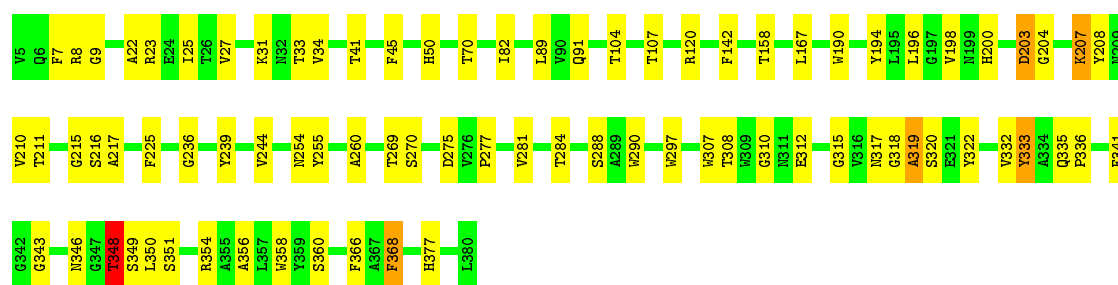
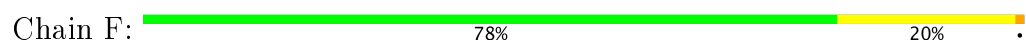




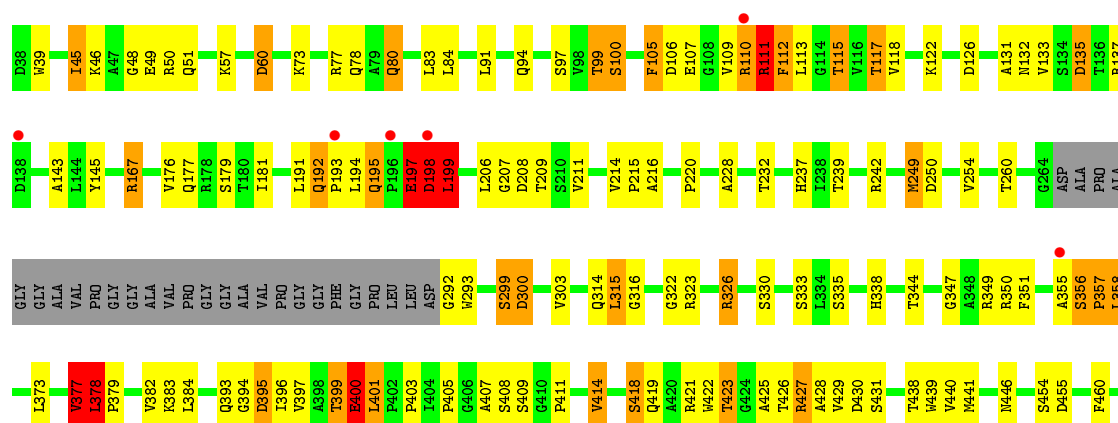
• Molecule 1: Major Tropism Determinant P1

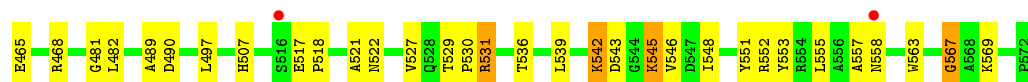


• Molecule 1: Major Tropism Determinant P1

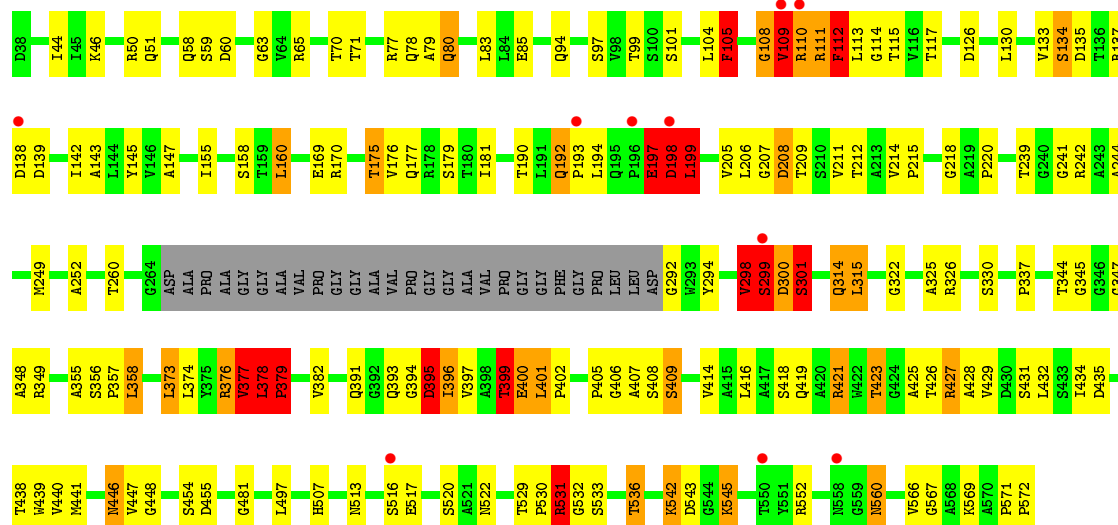


• Molecule 2: Pertactin Extracellular Domain





● Molecule 2: Pertactin Extracellular Domain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	413.46 Å 413.46 Å 98.86 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.63 – 3.16 49.60 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.63-3.16) 99.9 (49.60-3.16)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.19 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.224 , 0.249 0.227 , 0.251	Depositor DCC
$R_{free}$ test set	8334 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.45	2/2828 (0.1%)	0.59	1/3856 (0.0%)
1	B	1.67	4/2828 (0.1%)	0.79	7/3856 (0.2%)
1	C	0.44	0/2828	0.55	0/3856
1	D	0.44	0/2828	0.57	2/3856 (0.1%)
1	E	0.43	0/2828	0.54	0/3856
1	F	0.87	5/2828 (0.2%)	0.83	8/3856 (0.2%)
2	G	1.57	12/3731 (0.3%)	1.31	26/5073 (0.5%)
2	H	3.57	23/3731 (0.6%)	1.64	48/5073 (0.9%)
All	All	1.68	46/24430 (0.2%)	0.98	92/33282 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	F	1	0
2	G	0	9
2	H	0	7
All	All	1	18

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	408	SER	CB-OG	153.18	3.41	1.42
2	H	299	SER	CB-OG	96.94	2.68	1.42
1	B	349	SER	CB-OG	-67.15	0.55	1.42
2	G	377	VAL	CB-CG2	64.35	2.88	1.52
2	H	379	PRO	N-CD	63.04	2.36	1.47

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	300	ASP	CB-CG-OD1	-39.30	82.93	118.30
2	H	300	ASP	CB-CG-OD2	38.97	153.38	118.30
2	G	377	VAL	CG1-CB-CG2	-35.82	53.59	110.90
2	H	378	LEU	C-N-CD	-33.40	47.13	120.60
2	G	377	VAL	CA-CB-CG2	-29.63	66.46	110.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	349	SER	CA

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	346	ASN	Mainchain
1	B	349	SER	Mainchain
2	G	111	ARG	Mainchain,Peptide
2	G	197	GLU	Mainchain,Peptide
2	G	198	ASP	Sidechain

## 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	2758	0	2615	51	0
1	B	2758	0	2614	52	0
1	C	2758	0	2615	40	0
1	D	2758	0	2615	37	0
1	E	2758	0	2615	45	0
1	F	2758	0	2614	66	0
2	G	3674	0	3666	120	0
2	H	3674	0	3665	128	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
All	All	23900	0	23019	487	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 10.

The worst 5 of 487 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)
2:H:401:LEU:CB	2:H:401:LEU:CG	1.84	1.51
2:G:399:THR:CB	2:G:399:THR:CG2	1.99	1.39
1:F:348:THR:CB	1:F:348:THR:OG1	1.74	1.35
2:H:379:PRO:CB	2:H:379:PRO:CG	2.12	1.28
1:F:348:THR:CB	1:F:348:THR:CG2	2.12	1.27

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	374/376 (100%)	350 (94%)	22 (6%)	2 (0%)	32	73
1	B	374/376 (100%)	350 (94%)	21 (6%)	3 (1%)	22	64
1	C	374/376 (100%)	352 (94%)	20 (5%)	2 (0%)	32	73
1	D	374/376 (100%)	348 (93%)	24 (6%)	2 (0%)	32	73
1	E	374/376 (100%)	346 (92%)	28 (8%)	0	100	100
1	F	374/376 (100%)	348 (93%)	23 (6%)	3 (1%)	22	64
2	G	504/535 (94%)	439 (87%)	42 (8%)	23 (5%)	3	19
2	H	504/535 (94%)	444 (88%)	41 (8%)	19 (4%)	4	24
All	All	3252/3326 (98%)	2977 (92%)	221 (7%)	54 (2%)	11	46

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	112	PHE

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Mol	Chain	Res	Type
2	G	199	LEU
2	G	300	ASP
2	G	355	ALA
2	G	378	LEU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/271 (100%)	254 (94%)	17 (6%)	21	58
1	B	271/271 (100%)	261 (96%)	10 (4%)	39	75
1	C	271/271 (100%)	260 (96%)	11 (4%)	35	71
1	D	271/271 (100%)	256 (94%)	15 (6%)	25	62
1	E	271/271 (100%)	252 (93%)	19 (7%)	18	53
1	F	271/271 (100%)	254 (94%)	17 (6%)	21	58
2	G	375/388 (97%)	316 (84%)	59 (16%)	3	13
2	H	375/388 (97%)	318 (85%)	57 (15%)	3	15
All	All	2376/2402 (99%)	2171 (91%)	205 (9%)	12	42

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	50	ARG
2	G	237	HIS
2	H	423	THR
2	G	78	GLN
2	G	117	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	377	HIS

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Mol	Chain	Res	Type
1	F	209	ASN
2	H	363	GLN
1	E	248	HIS
1	F	247	HIS

### 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 4 ligands modelled in this entry, 4 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	4
2	G	3
1	F	2
1	B	1
1	A	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	348:THR	C	349:SER	N	1.19
1	B	349:SER	C	350:LEU	N	1.19
1	F	350:LEU	C	351:SER	N	1.19
1	H	399:THR	C	400:GLU	N	1.15
1	G	111:ARG	C	112:PHE	N	1.08

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	376/376 (100%)	-0.22	0 100 100	47, 61, 75, 83	0
1	B	376/376 (100%)	-0.13	1 (0%) 93 92	46, 65, 75, 80	0
1	C	376/376 (100%)	-0.22	0 100 100	44, 58, 71, 80	0
1	D	376/376 (100%)	-0.13	1 (0%) 93 92	52, 66, 75, 80	0
1	E	376/376 (100%)	-0.00	2 (0%) 90 85	58, 75, 89, 97	0
1	F	376/376 (100%)	-0.08	0 100 100	51, 69, 83, 91	0
2	G	502/535 (93%)	0.06	8 (1%) 72 58	57, 71, 92, 109	0
2	H	502/535 (93%)	0.17	10 (1%) 65 49	63, 81, 105, 120	0
All	All	3260/3326 (98%)	-0.05	22 (0%) 87 80	44, 68, 92, 120	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	558	ASN	3.8
2	H	193	PRO	3.7
2	H	550	THR	2.9
1	E	284	THR	2.7
2	G	198	ASP	2.7

### 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MG	A	3	1/1	0.91	0.55	15.23	51,51,51,51	0
3	MG	D	4	1/1	0.96	0.59	14.53	57,57,57,57	0
3	MG	B	1	1/1	0.97	0.23	1.00	50,50,50,50	0
3	MG	D	2	1/1	0.97	0.23	0.28	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.