



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 23, 2021 – 03:15 PM EST

PDB ID : 1TQ8
Title : Crystal Structure of protein Rv1636 from Mycobacterium tuberculosis H37Rv
Authors : Rajashankar, K.R.; Kniewel, R.; Solorzano, V.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-06-16
Resolution : 2.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

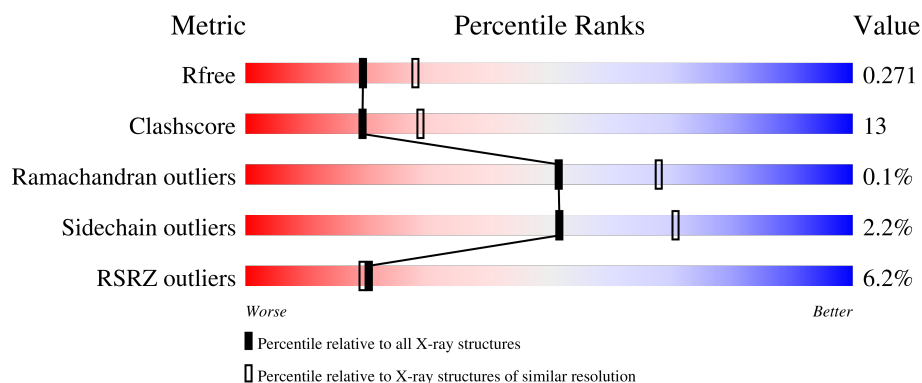
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. 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	163	<div> <div>61%</div> <div>15%</div> <div>•</div> <div>22%</div> </div>
1	B	163	<div> <div>6%</div> <div>58%</div> <div>20%</div> <div>22%</div> </div>
1	C	163	<div> <div>4%</div> <div>58%</div> <div>18%</div> <div>•</div> <div>22%</div> </div>
1	D	163	<div> <div>59%</div> <div>18%</div> <div>•</div> <div>22%</div> </div>
1	E	163	<div> <div>8%</div> <div>51%</div> <div>26%</div> <div>•</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	163	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (9%), green (52%), yellow (25%), and grey (22%). The segments are labeled with their respective percentages: 9%, 52%, 25%, and 22%. A small black dot is located on the yellow segment.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5753 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 hypothetical protein Rv1636.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	Se	0	0	0
			924	576	166	181	1			
1	B	127	Total	C	N	O	Se	0	0	0
			924	576	166	181	1			
1	C	127	Total	C	N	O	Se	0	0	0
			924	576	166	181	1			
1	D	127	Total	C	N	O	Se	0	0	0
			924	576	166	181	1			
1	E	126	Total	C	N	O	Se	0	0	0
			917	572	165	179	1			
1	F	127	Total	C	N	O	Se	0	0	0
			924	576	166	181	1			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP O06153
A	2	GLY	-	cloning artifact	UNP O06153
A	3	HIS	-	cloning artifact	UNP O06153
A	4	HIS	-	cloning artifact	UNP O06153
A	5	HIS	-	cloning artifact	UNP O06153
A	6	HIS	-	cloning artifact	UNP O06153
A	7	HIS	-	cloning artifact	UNP O06153
A	8	HIS	-	cloning artifact	UNP O06153
A	9	GLY	-	cloning artifact	UNP O06153
A	10	GLY	-	cloning artifact	UNP O06153
A	11	HIS	-	cloning artifact	UNP O06153
A	12	MET	-	cloning artifact	UNP O06153
A	13	SER	-	cloning artifact	UNP O06153
A	14	LEU	-	cloning artifact	UNP O06153
A	31	MSE	MET	modified residue	UNP O06153
A	160	GLU	-	cloning artifact	UNP O06153
A	161	GLY	-	cloning artifact	UNP O06153

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Chain	Residue	Modelled	Actual	Comment	Reference
A	162	GLY	-	cloning artifact	UNP O06153
A	163	SER	-	cloning artifact	UNP O06153
B	1	MSE	-	cloning artifact	UNP O06153
B	2	GLY	-	cloning artifact	UNP O06153
B	3	HIS	-	cloning artifact	UNP O06153
B	4	HIS	-	cloning artifact	UNP O06153
B	5	HIS	-	cloning artifact	UNP O06153
B	6	HIS	-	cloning artifact	UNP O06153
B	7	HIS	-	cloning artifact	UNP O06153
B	8	HIS	-	cloning artifact	UNP O06153
B	9	GLY	-	cloning artifact	UNP O06153
B	10	GLY	-	cloning artifact	UNP O06153
B	11	HIS	-	cloning artifact	UNP O06153
B	12	MET	-	cloning artifact	UNP O06153
B	13	SER	-	cloning artifact	UNP O06153
B	14	LEU	-	cloning artifact	UNP O06153
B	31	MSE	MET	modified residue	UNP O06153
B	160	GLU	-	cloning artifact	UNP O06153
B	161	GLY	-	cloning artifact	UNP O06153
B	162	GLY	-	cloning artifact	UNP O06153
B	163	SER	-	cloning artifact	UNP O06153
C	1	MSE	-	cloning artifact	UNP O06153
C	2	GLY	-	cloning artifact	UNP O06153
C	3	HIS	-	cloning artifact	UNP O06153
C	4	HIS	-	cloning artifact	UNP O06153
C	5	HIS	-	cloning artifact	UNP O06153
C	6	HIS	-	cloning artifact	UNP O06153
C	7	HIS	-	cloning artifact	UNP O06153
C	8	HIS	-	cloning artifact	UNP O06153
C	9	GLY	-	cloning artifact	UNP O06153
C	10	GLY	-	cloning artifact	UNP O06153
C	11	HIS	-	cloning artifact	UNP O06153
C	12	MET	-	cloning artifact	UNP O06153
C	13	SER	-	cloning artifact	UNP O06153
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C	31	MSE	MET	modified residue	UNP O06153
C	160	GLU	-	cloning artifact	UNP O06153
C	161	GLY	-	cloning artifact	UNP O06153
C	162	GLY	-	cloning artifact	UNP O06153
C	163	SER	-	cloning artifact	UNP O06153
D	1	MSE	-	cloning artifact	UNP O06153
D	2	GLY	-	cloning artifact	UNP O06153

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3	HIS	-	cloning artifact	UNP O06153
D	4	HIS	-	cloning artifact	UNP O06153
D	5	HIS	-	cloning artifact	UNP O06153
D	6	HIS	-	cloning artifact	UNP O06153
D	7	HIS	-	cloning artifact	UNP O06153
D	8	HIS	-	cloning artifact	UNP O06153
D	9	GLY	-	cloning artifact	UNP O06153
D	10	GLY	-	cloning artifact	UNP O06153
D	11	HIS	-	cloning artifact	UNP O06153
D	12	MET	-	cloning artifact	UNP O06153
D	13	SER	-	cloning artifact	UNP O06153
D	14	LEU	-	cloning artifact	UNP O06153
D	31	MSE	MET	modified residue	UNP O06153
D	160	GLU	-	cloning artifact	UNP O06153
D	161	GLY	-	cloning artifact	UNP O06153
D	162	GLY	-	cloning artifact	UNP O06153
D	163	SER	-	cloning artifact	UNP O06153
E	1	MSE	-	cloning artifact	UNP O06153
E	2	GLY	-	cloning artifact	UNP O06153
E	3	HIS	-	cloning artifact	UNP O06153
E	4	HIS	-	cloning artifact	UNP O06153
E	5	HIS	-	cloning artifact	UNP O06153
E	6	HIS	-	cloning artifact	UNP O06153
E	7	HIS	-	cloning artifact	UNP O06153
E	8	HIS	-	cloning artifact	UNP O06153
E	9	GLY	-	cloning artifact	UNP O06153
E	10	GLY	-	cloning artifact	UNP O06153
E	11	HIS	-	cloning artifact	UNP O06153
E	12	MET	-	cloning artifact	UNP O06153
E	13	SER	-	cloning artifact	UNP O06153
E	14	LEU	-	cloning artifact	UNP O06153
E	31	MSE	MET	modified residue	UNP O06153
E	160	GLU	-	cloning artifact	UNP O06153
E	161	GLY	-	cloning artifact	UNP O06153
E	162	GLY	-	cloning artifact	UNP O06153
E	163	SER	-	cloning artifact	UNP O06153
F	1	MSE	-	cloning artifact	UNP O06153
F	2	GLY	-	cloning artifact	UNP O06153
F	3	HIS	-	cloning artifact	UNP O06153
F	4	HIS	-	cloning artifact	UNP O06153
F	5	HIS	-	cloning artifact	UNP O06153
F	6	HIS	-	cloning artifact	UNP O06153

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Chain	Residue	Modelled	Actual	Comment	Reference
F	7	HIS	-	cloning artifact	UNP O06153
F	8	HIS	-	cloning artifact	UNP O06153
F	9	GLY	-	cloning artifact	UNP O06153
F	10	GLY	-	cloning artifact	UNP O06153
F	11	HIS	-	cloning artifact	UNP O06153
F	12	MET	-	cloning artifact	UNP O06153
F	13	SER	-	cloning artifact	UNP O06153
F	14	LEU	-	cloning artifact	UNP O06153
F	31	MSE	MET	modified residue	UNP O06153
F	160	GLU	-	cloning artifact	UNP O06153
F	161	GLY	-	cloning artifact	UNP O06153
F	162	GLY	-	cloning artifact	UNP O06153
F	163	SER	-	cloning artifact	UNP O06153

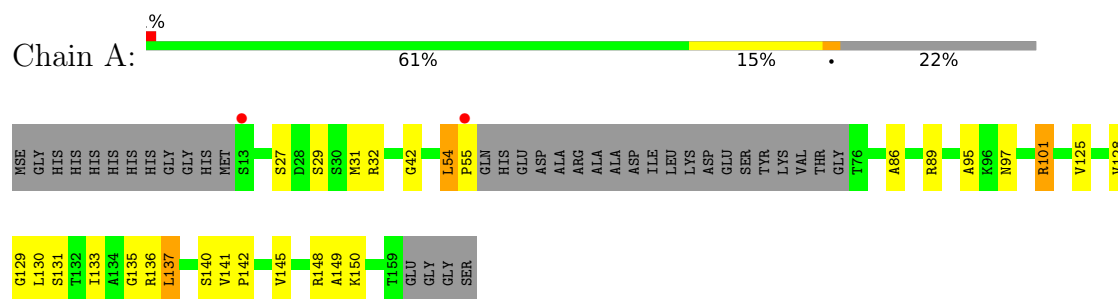
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	44	Total O 44 44	0	0
2	B	29	Total O 29 29	0	0
2	C	56	Total O 56 56	0	0
2	D	46	Total O 46 46	0	0
2	E	16	Total O 16 16	0	0
2	F	25	Total O 25 25	0	0

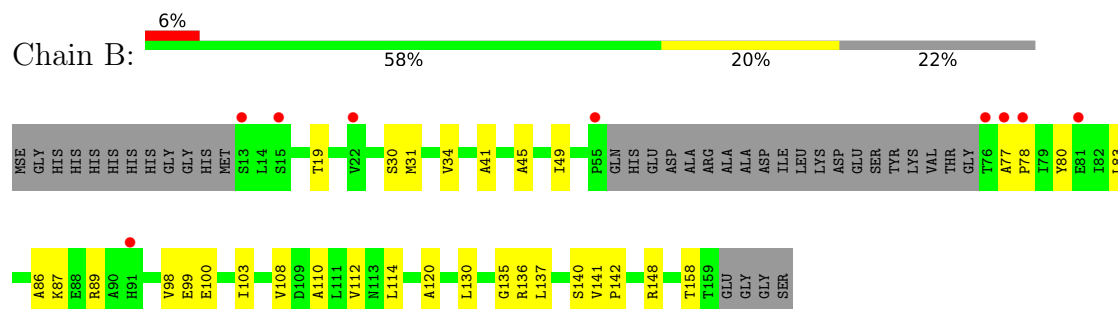
3 Residue-property plots [i](#)

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.

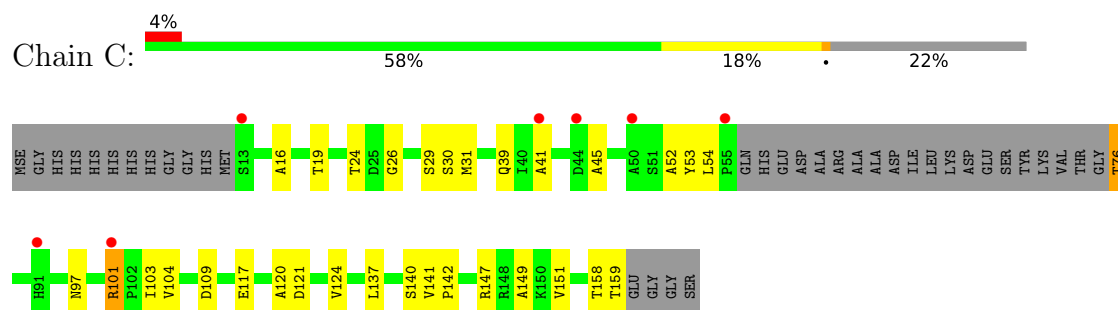
- Molecule 1: hypothetical protein Rv1636



- Molecule 1: hypothetical protein Rv1636

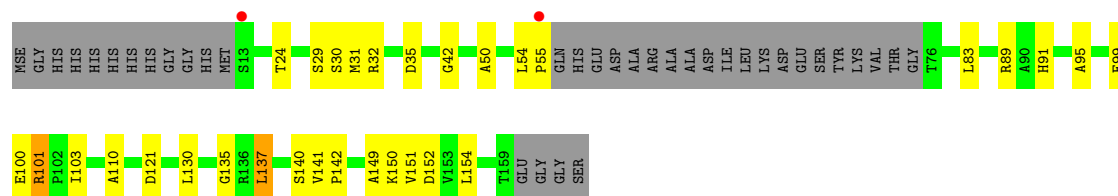


- Molecule 1: hypothetical protein Rv1636

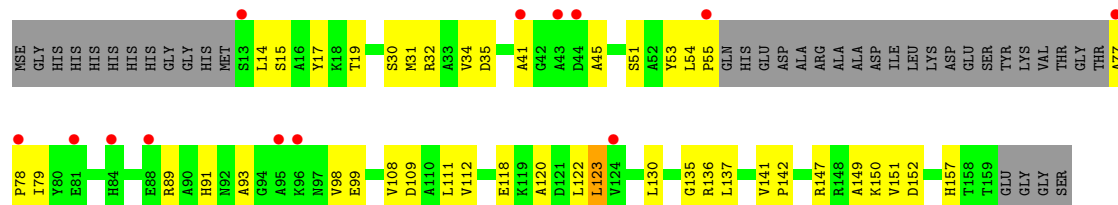


- Molecule 1: hypothetical protein Rv1636

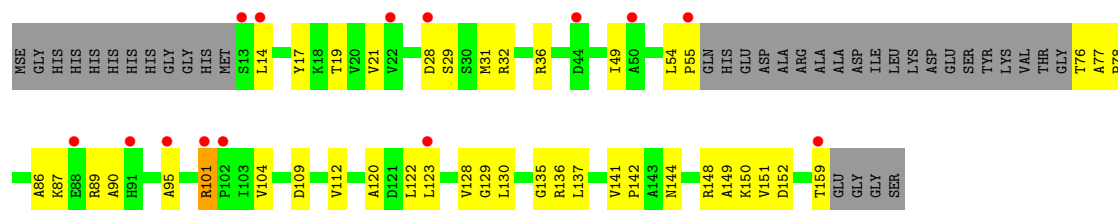




• Molecule 1: hypothetical protein Rv1636



• Molecule 1: hypothetical protein Rv1636



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.83Å 121.04Å 119.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.40 29.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.94-2.40) 97.4 (29.94-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.262 0.230 , 0.271	Depositor DCC
R_{free} test set	3894 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5753	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2430e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/932	0.59	0/1266
1	B	0.32	0/932	0.54	0/1266
1	C	0.35	0/932	0.58	0/1266
1	D	0.36	0/932	0.57	0/1266
1	E	0.29	0/925	0.50	0/1256
1	F	0.30	0/932	0.51	0/1266
All	All	0.33	0/5585	0.55	0/7586

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 [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	924	0	952	22	0
1	B	924	0	952	23	0
1	C	924	0	952	30	0
1	D	924	0	952	24	0
1	E	917	0	945	30	0
1	F	924	0	952	42	0
2	A	44	0	0	3	0
2	B	29	0	0	2	0
2	C	56	0	0	5	0
2	D	46	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	16	0	0	2	1
2	F	25	0	0	3	1
All	All	5753	0	5705	145	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 13.

The worst 5 of 145 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:54:LEU:HB2	1:A:55:PRO:HD3	1.52	0.91
1:C:76:THR:HG22	1:F:109:ASP:HB3	1.60	0.82
1:D:54:LEU:HB2	1:D:55:PRO:HD3	1.60	0.81
1:B:148:ARG:HD2	2:B:176:HOH:O	1.84	0.76
1:D:31:MSE:HG3	2:D:182:HOH:O	1.87	0.75

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)
2:E:165:HOH:O	2:F:179:HOH:O[2_545]	2.03	0.17

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	123/163 (76%)	119 (97%)	3 (2%)	1 (1%)	19	29
1	B	123/163 (76%)	118 (96%)	5 (4%)	0	100	100
1	C	123/163 (76%)	119 (97%)	4 (3%)	0	100	100
1	D	123/163 (76%)	118 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	122/163 (75%)	117 (96%)	5 (4%)	0	100	100
1	F	123/163 (76%)	118 (96%)	5 (4%)	0	100	100
All	All	737/978 (75%)	709 (96%)	27 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	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	97/122 (80%)	94 (97%)	3 (3%)	40	60
1	B	97/122 (80%)	97 (100%)	0	100	100
1	C	97/122 (80%)	92 (95%)	5 (5%)	23	38
1	D	97/122 (80%)	95 (98%)	2 (2%)	53	72
1	E	96/122 (79%)	94 (98%)	2 (2%)	53	72
1	F	97/122 (80%)	96 (99%)	1 (1%)	76	88
All	All	581/732 (79%)	568 (98%)	13 (2%)	52	71

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	76	THR
1	C	101	ARG
1	E	123	LEU
1	C	54	LEU
1	D	137	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	113	ASN
1	F	91	HIS
1	D	92	ASN
1	C	92	ASN
1	D	91	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 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 [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	126/163 (77%)	-0.00	2 (1%) 72 70	26, 39, 60, 80	0
1	B	126/163 (77%)	0.52	9 (7%) 16 14	26, 57, 77, 87	0
1	C	126/163 (77%)	0.14	7 (5%) 24 23	25, 42, 65, 76	0
1	D	126/163 (77%)	-0.06	2 (1%) 72 70	26, 38, 57, 78	0
1	E	125/163 (76%)	0.65	13 (10%) 6 6	36, 66, 83, 88	0
1	F	126/163 (77%)	0.53	14 (11%) 5 4	37, 55, 76, 84	0
All	All	755/978 (77%)	0.30	47 (6%) 20 19	25, 49, 78, 88	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	THR	6.9
1	B	77	ALA	5.7
1	E	55	PRO	5.1
1	E	78	PRO	4.9
1	E	77	ALA	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.