



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2025 – 01:34 PM JST

PDB ID : 9JKC
Title : Crystal structure of Aspergillus fumigatus polmycovirus 1 ploymerase
(residues 85-763) in its apo state
Authors : Jia, H.; Cao, S.; Gong, P.
Deposited on : 2024-09-15
Resolution : 3.40 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 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

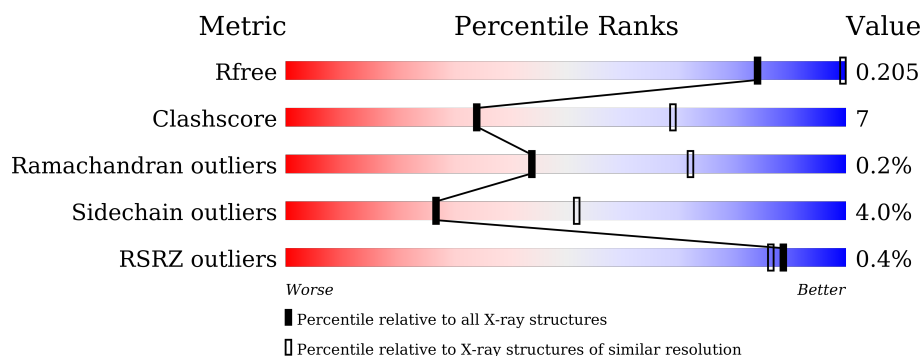
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	690	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 77% 18% • • </div> </div>
1	B	690	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 78% 16% • • </div> </div>
1	C	690	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 78% 16% • 5% </div> </div>
1	D	690	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 75% 19% • 5% </div> </div>
1	E	690	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 79% 16% • • </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25293 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 RNA dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5100	3214	920	945	21			
1	B	660	Total	C	N	O	S	0	1	0
			5100	3215	916	948	21			
1	C	656	Total	C	N	O	S	0	0	0
			5041	3186	908	926	21			
1	D	655	Total	C	N	O	S	0	0	0
			4988	3149	894	924	21			
1	E	660	Total	C	N	O	S	0	0	0
			5035	3175	908	931	21			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MET	-	initiating methionine	UNP A0A0H5BRR0
A	764	GLY	-	expression tag	UNP A0A0H5BRR0
A	765	SER	-	expression tag	UNP A0A0H5BRR0
A	766	SER	-	expression tag	UNP A0A0H5BRR0
A	767	SER	-	expression tag	UNP A0A0H5BRR0
A	768	HIS	-	expression tag	UNP A0A0H5BRR0
A	769	HIS	-	expression tag	UNP A0A0H5BRR0
A	770	HIS	-	expression tag	UNP A0A0H5BRR0
A	771	HIS	-	expression tag	UNP A0A0H5BRR0
A	772	HIS	-	expression tag	UNP A0A0H5BRR0
A	773	HIS	-	expression tag	UNP A0A0H5BRR0
B	84	MET	-	initiating methionine	UNP A0A0H5BRR0
B	764	GLY	-	expression tag	UNP A0A0H5BRR0
B	765	SER	-	expression tag	UNP A0A0H5BRR0
B	766	SER	-	expression tag	UNP A0A0H5BRR0
B	767	SER	-	expression tag	UNP A0A0H5BRR0
B	768	HIS	-	expression tag	UNP A0A0H5BRR0
B	769	HIS	-	expression tag	UNP A0A0H5BRR0
B	770	HIS	-	expression tag	UNP A0A0H5BRR0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	771	HIS	-	expression tag	UNP A0A0H5BRR0
B	772	HIS	-	expression tag	UNP A0A0H5BRR0
B	773	HIS	-	expression tag	UNP A0A0H5BRR0
C	84	MET	-	initiating methionine	UNP A0A0H5BRR0
C	764	GLY	-	expression tag	UNP A0A0H5BRR0
C	765	SER	-	expression tag	UNP A0A0H5BRR0
C	766	SER	-	expression tag	UNP A0A0H5BRR0
C	767	SER	-	expression tag	UNP A0A0H5BRR0
C	768	HIS	-	expression tag	UNP A0A0H5BRR0
C	769	HIS	-	expression tag	UNP A0A0H5BRR0
C	770	HIS	-	expression tag	UNP A0A0H5BRR0
C	771	HIS	-	expression tag	UNP A0A0H5BRR0
C	772	HIS	-	expression tag	UNP A0A0H5BRR0
C	773	HIS	-	expression tag	UNP A0A0H5BRR0
D	84	MET	-	initiating methionine	UNP A0A0H5BRR0
D	764	GLY	-	expression tag	UNP A0A0H5BRR0
D	765	SER	-	expression tag	UNP A0A0H5BRR0
D	766	SER	-	expression tag	UNP A0A0H5BRR0
D	767	SER	-	expression tag	UNP A0A0H5BRR0
D	768	HIS	-	expression tag	UNP A0A0H5BRR0
D	769	HIS	-	expression tag	UNP A0A0H5BRR0
D	770	HIS	-	expression tag	UNP A0A0H5BRR0
D	771	HIS	-	expression tag	UNP A0A0H5BRR0
D	772	HIS	-	expression tag	UNP A0A0H5BRR0
D	773	HIS	-	expression tag	UNP A0A0H5BRR0
E	84	MET	-	initiating methionine	UNP A0A0H5BRR0
E	764	GLY	-	expression tag	UNP A0A0H5BRR0
E	765	SER	-	expression tag	UNP A0A0H5BRR0
E	766	SER	-	expression tag	UNP A0A0H5BRR0
E	767	SER	-	expression tag	UNP A0A0H5BRR0
E	768	HIS	-	expression tag	UNP A0A0H5BRR0
E	769	HIS	-	expression tag	UNP A0A0H5BRR0
E	770	HIS	-	expression tag	UNP A0A0H5BRR0
E	771	HIS	-	expression tag	UNP A0A0H5BRR0
E	772	HIS	-	expression tag	UNP A0A0H5BRR0
E	773	HIS	-	expression tag	UNP A0A0H5BRR0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0

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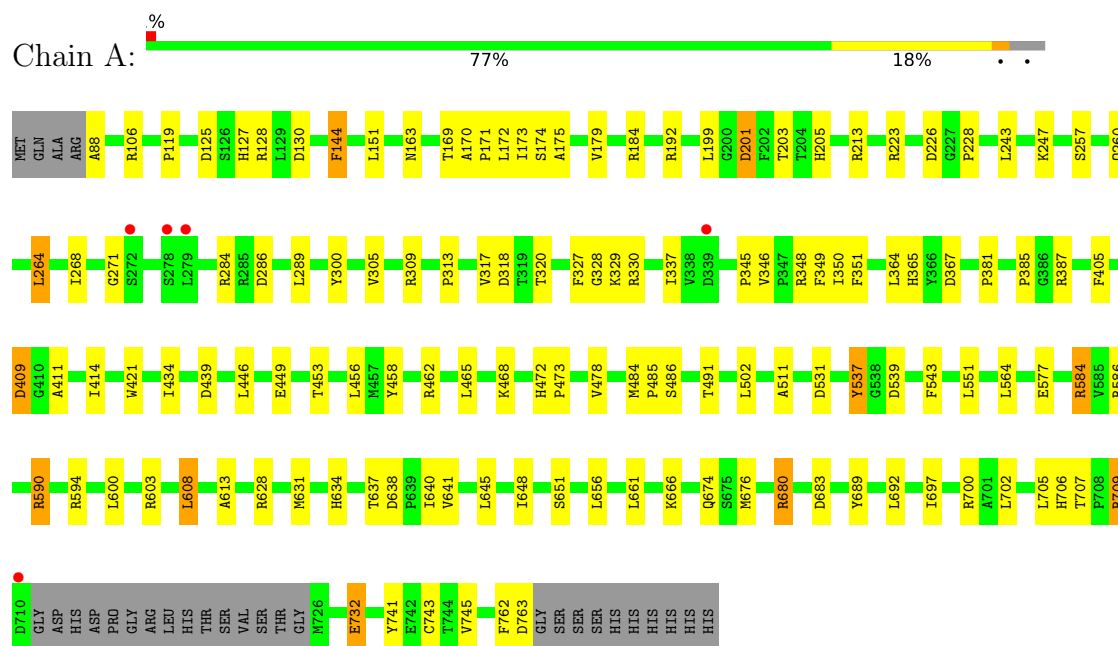
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	10	Total 10	O 10	0	0
2	C	6	Total 6	O 6	0	0
2	D	6	Total 6	O 6	0	0
2	E	1	Total 1	O 1	0	0

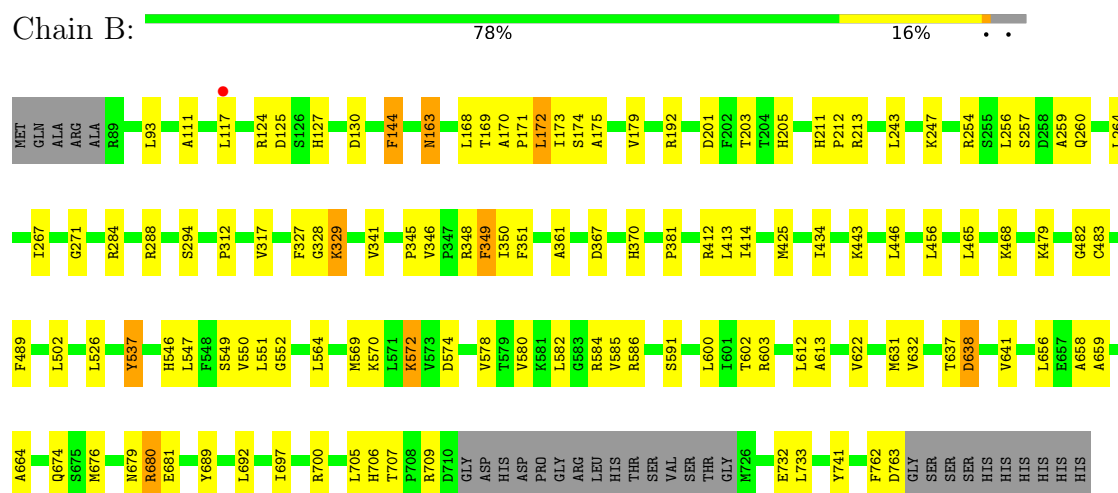
3 Residue-property plots

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: RNA dependent RNA polymerase

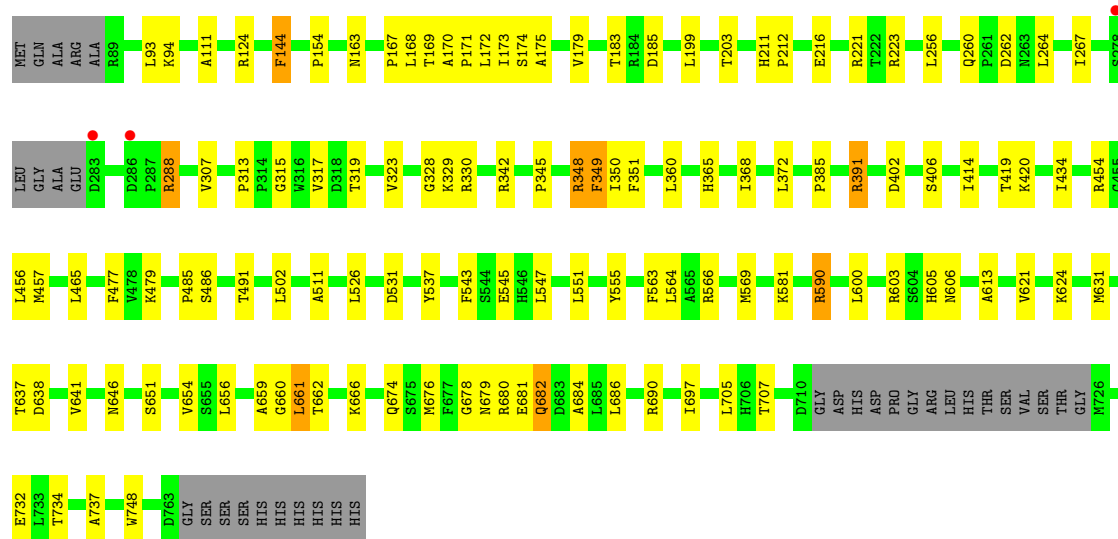


• Molecule 1: RNA dependent RNA polymerase




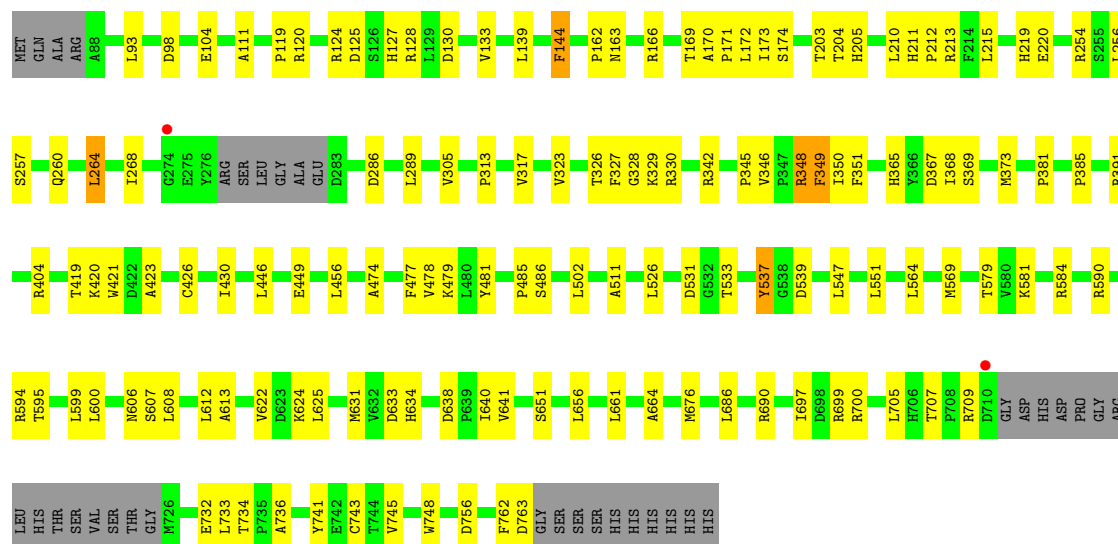
• Molecule 1: RNA dependent RNA polymerase

Chain C:  78% 16% 5%




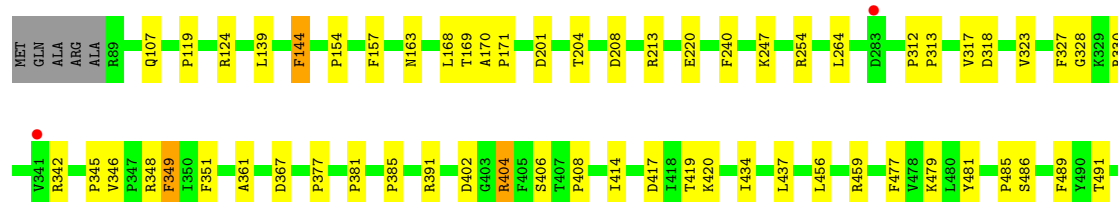
• Molecule 1: RNA dependent RNA polymerase

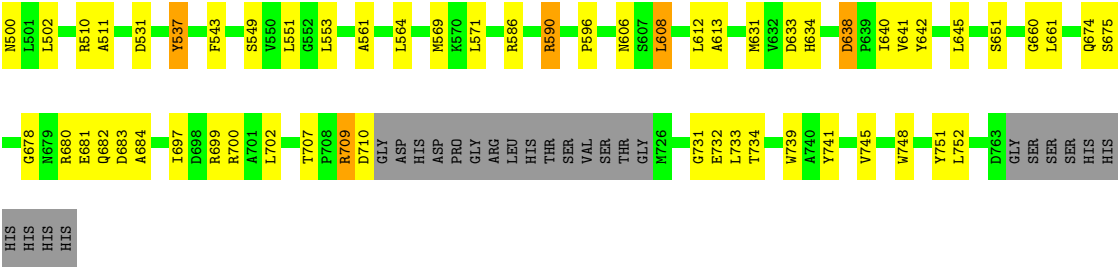
Chain D:  75% 19% 5%



• Molecule 1: RNA dependent RNA polymerase

Chain E:  79% 16% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	257.96Å 182.92Å 118.68Å 90.00° 103.79° 90.00°	Depositor
Resolution (Å)	29.88 – 3.40 29.88 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.88-3.40) 99.2 (29.88-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.158 , 0.206 0.158 , 0.205	Depositor DCC
R_{free} test set	3750 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25293	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.51	0/5216	0.70	0/7083
1	B	0.51	0/5216	0.70	0/7083
1	C	0.49	0/5156	0.69	0/7005
1	D	0.48	0/5102	0.69	0/6942
1	E	0.44	0/5151	0.65	0/7005
All	All	0.49	0/25841	0.69	0/35118

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	5100	0	4975	83	0
1	B	5100	0	4975	74	0
1	C	5041	0	4920	76	0
1	D	4988	0	4816	80	0
1	E	5035	0	4869	70	0
2	A	6	0	0	0	0
2	B	10	0	0	1	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	E	1	0	0	0	0
All	All	25293	0	24555	373	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 7.

The worst 5 of 373 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:169:THR:HG22	1:A:613:ALA:HA	1.53	0.88
1:B:169:THR:HG22	1:B:613:ALA:HA	1.58	0.84
1:D:169:THR:HG22	1:D:613:ALA:HA	1.60	0.84
1:E:169:THR:HG22	1:E:613:ALA:HA	1.63	0.80
1:C:169:THR:HG22	1:C:613:ALA:HA	1.65	0.79

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	657/690 (95%)	613 (93%)	43 (6%)	1 (0%)	44	72
1	B	657/690 (95%)	614 (94%)	39 (6%)	4 (1%)	22	50
1	C	650/690 (94%)	612 (94%)	36 (6%)	2 (0%)	37	66
1	D	649/690 (94%)	614 (95%)	34 (5%)	1 (0%)	44	72
1	E	656/690 (95%)	619 (94%)	37 (6%)	0	100	100
All	All	3269/3450 (95%)	3072 (94%)	189 (6%)	8 (0%)	44	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	531	ASP
1	B	341	VAL
1	D	531	ASP
1	B	582	LEU
1	A	531	ASP

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	528/575 (92%)	502 (95%)	26 (5%)	21	48
1	B	530/575 (92%)	513 (97%)	17 (3%)	34	59
1	C	520/575 (90%)	500 (96%)	20 (4%)	28	54
1	D	510/575 (89%)	491 (96%)	19 (4%)	29	54
1	E	515/575 (90%)	493 (96%)	22 (4%)	25	50
All	All	2603/2875 (90%)	2499 (96%)	104 (4%)	27	52

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	590	ARG
1	D	391	ARG
1	E	608	LEU
1	C	606	ASN
1	D	172	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	674	GLN
1	D	634	HIS
1	E	618	HIS
1	D	674	GLN
1	C	634	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 oligosaccharides 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	661/690 (95%)	-0.70	5 (0%) 82 75	22, 41, 72, 120	0
1	B	660/690 (95%)	-0.73	1 (0%) 92 92	18, 41, 75, 113	1 (0%)
1	C	656/690 (95%)	-0.64	3 (0%) 87 83	25, 44, 74, 113	0
1	D	655/690 (94%)	-0.69	2 (0%) 90 89	28, 44, 73, 111	0
1	E	660/690 (95%)	-0.52	2 (0%) 90 89	28, 54, 83, 122	0
All	All	3292/3450 (95%)	-0.66	13 (0%) 89 86	18, 45, 78, 122	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	278	SER	3.3
1	A	278	SER	3.2
1	C	283	ASP	3.2
1	E	283	ASP	3.0
1	D	710	ASP	2.6

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.