



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:36 AM UTC

PDB ID : 2WWT / pdb_00002wwt
Title : Intracellular subtilisin precursor from *B. clausii*
Authors : Vevodova, J.; Gamble, M.; Ariza, A.; Dodson, E.; Jones, D.D.; Wilson, K.S.
Deposited on : 2009-10-27
Resolution : 2.68 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

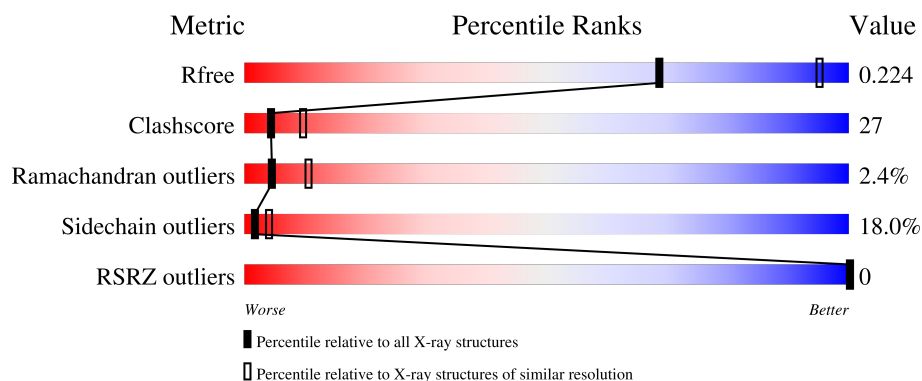
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	329	
1	B	329	
1	C	329	
1	D	329	
1	E	329	

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Mol	Chain	Length	Quality of chain
1	F	329	53% 33% 6% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13310 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 INTRACELLULAR SUBTILISIN PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2200	1387	373	433	7			
1	B	298	Total	C	N	O	S	0	0	0
			2194	1384	372	431	7			
1	C	300	Total	C	N	O	S	0	0	0
			2209	1392	374	436	7			
1	D	306	Total	C	N	O	S	0	0	0
			2258	1421	382	448	7			
1	E	299	Total	C	N	O	S	6	0	0
			2200	1387	373	433	7			
1	F	302	Total	C	N	O	S	0	0	0
			2224	1401	376	440	7			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	LEU	-	expression tag	UNP D0AB41
A	323	GLU	-	expression tag	UNP D0AB41
A	324	HIS	-	expression tag	UNP D0AB41
A	325	HIS	-	expression tag	UNP D0AB41
A	326	HIS	-	expression tag	UNP D0AB41
A	327	HIS	-	expression tag	UNP D0AB41
A	328	HIS	-	expression tag	UNP D0AB41
A	329	HIS	-	expression tag	UNP D0AB41
A	250	ALA	SER	engineered mutation	UNP D0AB41
B	322	LEU	-	expression tag	UNP D0AB41
B	323	GLU	-	expression tag	UNP D0AB41
B	324	HIS	-	expression tag	UNP D0AB41
B	325	HIS	-	expression tag	UNP D0AB41
B	326	HIS	-	expression tag	UNP D0AB41
B	327	HIS	-	expression tag	UNP D0AB41
B	328	HIS	-	expression tag	UNP D0AB41
B	329	HIS	-	expression tag	UNP D0AB41

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Chain	Residue	Modelled	Actual	Comment	Reference
B	250	ALA	SER	engineered mutation	UNP D0AB41
C	322	LEU	-	expression tag	UNP D0AB41
C	323	GLU	-	expression tag	UNP D0AB41
C	324	HIS	-	expression tag	UNP D0AB41
C	325	HIS	-	expression tag	UNP D0AB41
C	326	HIS	-	expression tag	UNP D0AB41
C	327	HIS	-	expression tag	UNP D0AB41
C	328	HIS	-	expression tag	UNP D0AB41
C	329	HIS	-	expression tag	UNP D0AB41
C	250	ALA	SER	engineered mutation	UNP D0AB41
D	322	LEU	-	expression tag	UNP D0AB41
D	323	GLU	-	expression tag	UNP D0AB41
D	324	HIS	-	expression tag	UNP D0AB41
D	325	HIS	-	expression tag	UNP D0AB41
D	326	HIS	-	expression tag	UNP D0AB41
D	327	HIS	-	expression tag	UNP D0AB41
D	328	HIS	-	expression tag	UNP D0AB41
D	329	HIS	-	expression tag	UNP D0AB41
D	250	ALA	SER	engineered mutation	UNP D0AB41
E	322	LEU	-	expression tag	UNP D0AB41
E	323	GLU	-	expression tag	UNP D0AB41
E	324	HIS	-	expression tag	UNP D0AB41
E	325	HIS	-	expression tag	UNP D0AB41
E	326	HIS	-	expression tag	UNP D0AB41
E	327	HIS	-	expression tag	UNP D0AB41
E	328	HIS	-	expression tag	UNP D0AB41
E	329	HIS	-	expression tag	UNP D0AB41
E	250	ALA	SER	engineered mutation	UNP D0AB41
F	322	LEU	-	expression tag	UNP D0AB41
F	323	GLU	-	expression tag	UNP D0AB41
F	324	HIS	-	expression tag	UNP D0AB41
F	325	HIS	-	expression tag	UNP D0AB41
F	326	HIS	-	expression tag	UNP D0AB41
F	327	HIS	-	expression tag	UNP D0AB41
F	328	HIS	-	expression tag	UNP D0AB41
F	329	HIS	-	expression tag	UNP D0AB41
F	250	ALA	SER	engineered mutation	UNP D0AB41

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0

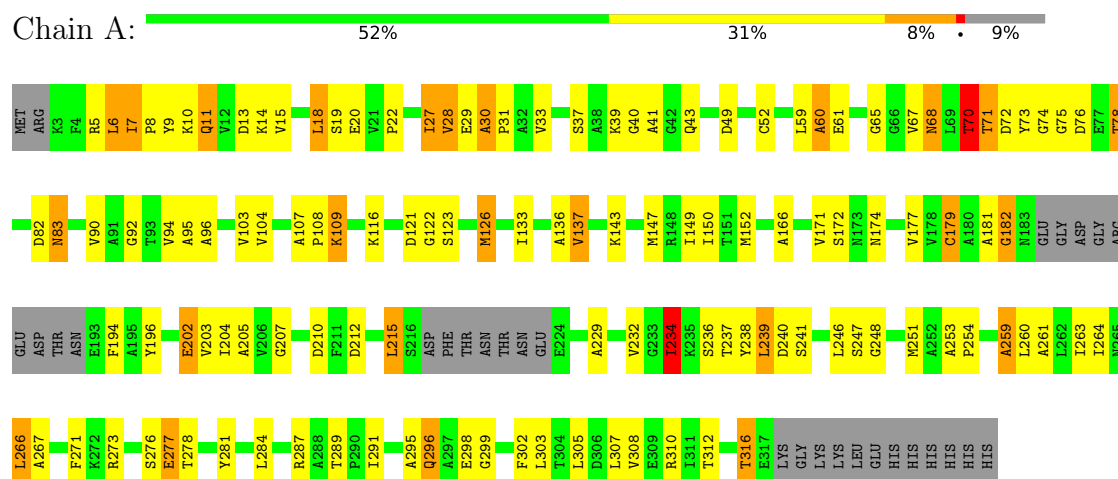
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	3	Total O 3 3	0	0
3	C	4	Total O 4 4	0	0
3	D	3	Total O 3 3	0	0
3	E	3	Total O 3 3	0	0
3	F	3	Total O 3 3	0	0

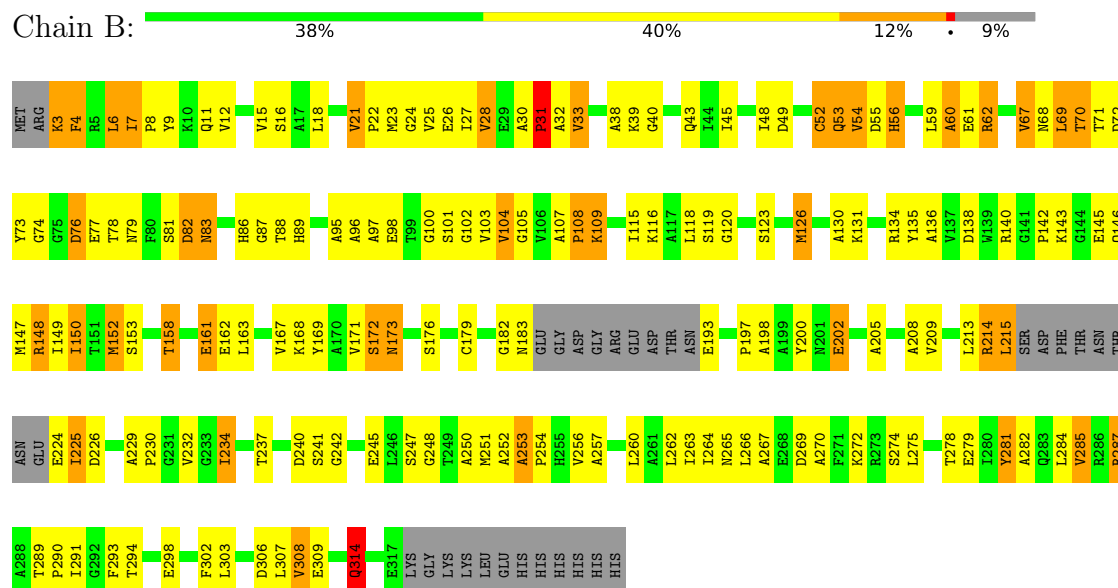
3 Residue-property plots

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: INTRACELLULAR SUBTILISIN PROTEASE

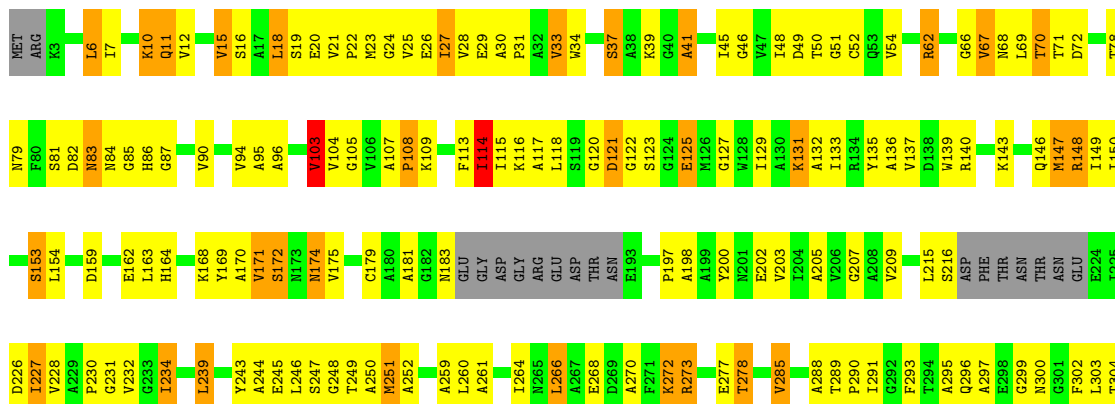
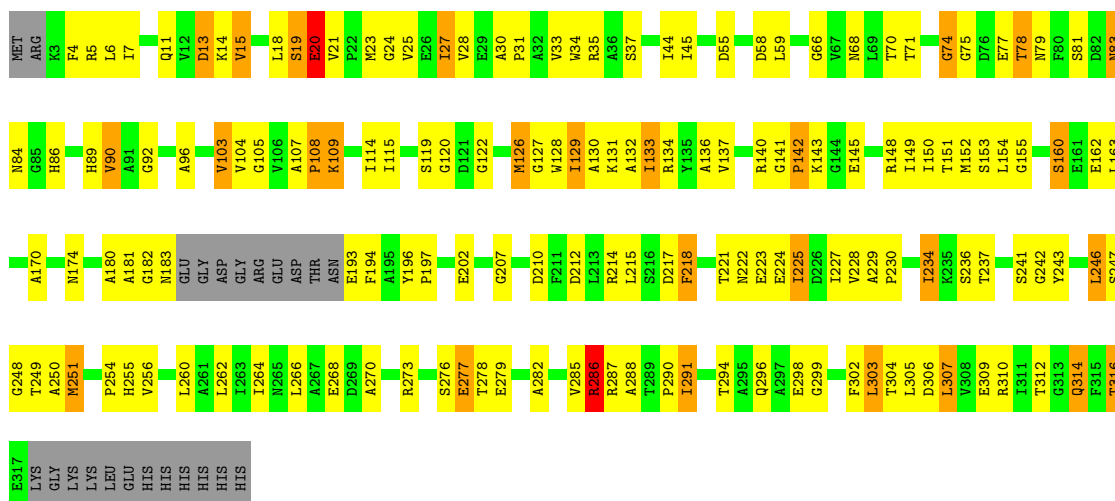


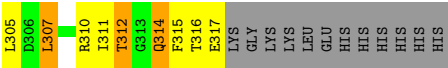
• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE



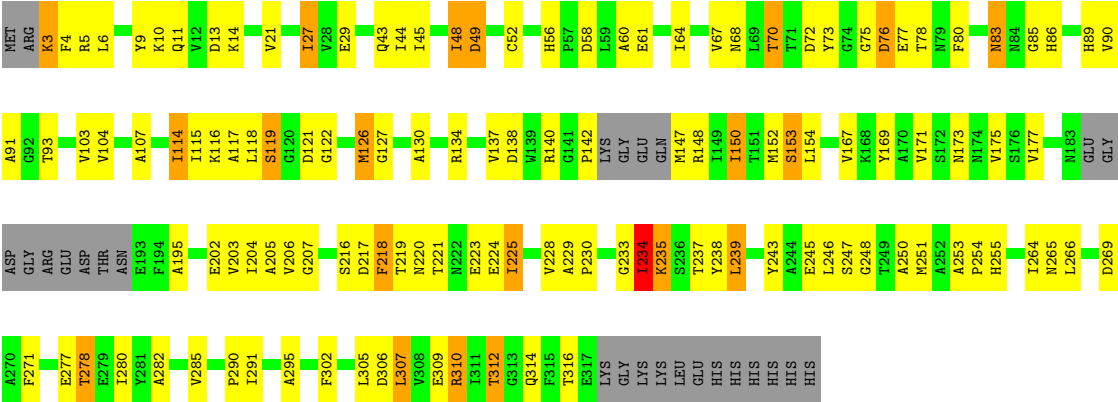
• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE







● Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	121.64Å 121.64Å 106.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	105.57 – 2.68 105.34 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.8 (105.57-2.68) 99.0 (105.34-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.166 , 0.252 (Not available) , 0.224	Depositor DCC
R_{free} test set	2916 reflections (5.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 17.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.094 for -h,-k,l 0.097 for h,-h-k,-l 0.245 for -k,-h,-l	Xtriage
Reported twinning fraction	0.720 for H, K, L 0.280 for -H, H+K, -L	Depositor
Outliers	0 of 48934 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13310	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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

5.1 Standard geometry

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

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	1.20	9/2237 (0.4%)	1.33	15/3039 (0.5%)
1	B	0.97	1/2231 (0.0%)	1.25	21/3031 (0.7%)
1	C	1.17	2/2246 (0.1%)	1.36	17/3051 (0.6%)
1	D	1.06	1/2297 (0.0%)	1.24	7/3123 (0.2%)
1	E	0.99	1/2237 (0.0%)	1.23	11/3039 (0.4%)
1	F	0.91	0/2261	1.19	9/3073 (0.3%)
All	All	1.05	14/13509 (0.1%)	1.27	80/18356 (0.4%)

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	A	0	2
1	C	0	1
All	All	0	3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	ALA	CA-CB	-8.11	1.40	1.53
1	C	63	ILE	CA-CB	7.76	1.62	1.53
1	A	205	ALA	CA-CB	-7.45	1.42	1.53
1	C	204	ILE	CA-CB	7.26	1.61	1.53
1	A	207	GLY	C-O	7.03	1.30	1.23

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	74	GLY	N-CA-C	10.31	124.61	113.58
1	C	156	GLY	CA-C-N	-9.13	110.53	120.94
1	C	156	GLY	C-N-CA	-9.13	110.53	120.94
1	D	314	GLN	N-CA-C	8.54	122.14	109.59
1	C	314	GLN	N-CA-C	7.82	122.45	109.46

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASP	Peptide
1	A	181	ALA	Peptide
1	C	313	GLY	Peptide

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	2200	0	2166	84	0
1	B	2194	0	2160	156	0
1	C	2209	0	2172	106	0
1	D	2258	0	2211	143	0
1	E	2200	0	2166	126	0
1	F	2224	0	2175	116	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
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	1	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
All	All	13310	0	13050	704	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 27.

The worst 5 of 704 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:234:ILE:HD11	1:A:251:MET:CB	1.55	1.36
1:A:234:ILE:CD1	1:A:251:MET:HB3	1.55	1.34
1:F:234:ILE:HD11	1:F:251:MET:HB3	1.20	1.14
1:B:136:ALA:HA	1:B:147:MET:HE2	1.22	1.09
1:C:285:VAL:HG21	1:D:282:ALA:HB1	1.31	1.08

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	293/329 (89%)	266 (91%)	23 (8%)	4 (1%)	9	21
1	B	292/329 (89%)	253 (87%)	30 (10%)	9 (3%)	3	7
1	C	294/329 (89%)	261 (89%)	25 (8%)	8 (3%)	4	9
1	D	302/329 (92%)	259 (86%)	35 (12%)	8 (3%)	4	9
1	E	293/329 (89%)	261 (89%)	22 (8%)	10 (3%)	3	6
1	F	296/329 (90%)	263 (89%)	30 (10%)	3 (1%)	12	28
All	All	1770/1974 (90%)	1563 (88%)	165 (9%)	42 (2%)	4	10

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	GLY
1	A	239	LEU
1	B	32	ALA
1	B	60	ALA
1	B	182	GLY

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	224/252 (89%)	190 (85%)	34 (15%)	3	6
1	B	223/252 (88%)	179 (80%)	44 (20%)	1	3
1	C	225/252 (89%)	180 (80%)	45 (20%)	1	3
1	D	231/252 (92%)	190 (82%)	41 (18%)	2	4
1	E	224/252 (89%)	178 (80%)	46 (20%)	1	3
1	F	228/252 (90%)	194 (85%)	34 (15%)	3	6
All	All	1355/1512 (90%)	1111 (82%)	244 (18%)	2	4

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	266	LEU
1	F	83	ASN
1	D	160	SER
1	F	76	ASP
1	F	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	89	HIS
1	F	164	HIS
1	F	255	HIS
1	C	296	GLN
1	C	201	ASN

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](#)

Of 5 ligands modelled in this entry, 5 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	299/329 (90%)	-1.24	0 100 100	19, 29, 44, 59	0
1	B	298/329 (90%)	-1.04	0 100 100	22, 42, 67, 89	0
1	C	300/329 (91%)	-1.24	0 100 100	19, 28, 44, 77	0
1	D	306/329 (93%)	-1.10	0 100 100	20, 37, 56, 69	0
1	E	299/329 (90%)	-1.06	0 100 100	25, 42, 63, 70	1 (0%)
1	F	302/329 (91%)	-1.03	0 100 100	28, 48, 74, 98	0
All	All	1804/1974 (91%)	-1.12	0 100 100	19, 37, 65, 98	1 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	NA	B	401	1/1	0.98	0.03	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	D	401	1/1	0.98	0.03	37,37,37,37	0
2	NA	E	401	1/1	0.98	0.05	33,33,33,33	0
2	NA	C	401	1/1	0.99	0.02	22,22,22,22	0
2	NA	F	401	1/1	1.00	0.03	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.