



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:08 am BST

PDB ID : 2X8J
Title : Intracellular subtilisin precursor from *B. clausii*
Authors : Vedodova, J.; Gamble, M.; Ariza, A.; Dodson, E.; Jones, D.D.; Wilson, K.S.
Deposited on : 2010-03-09
Resolution : 1.56 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 : 2.11
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) : 2.11

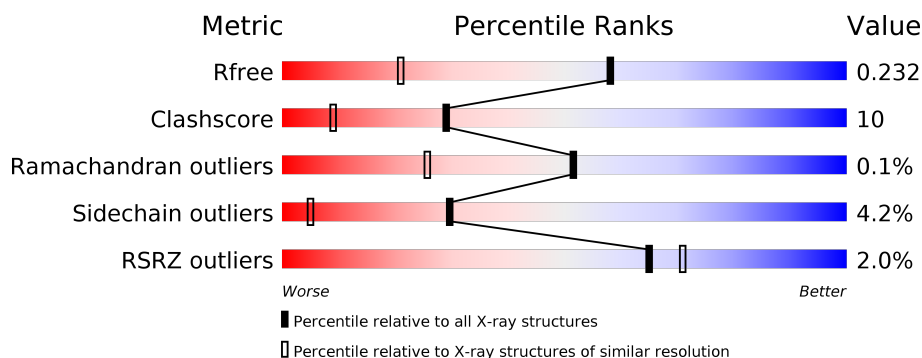
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 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	327	<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% 13% • 7% </div> </div>
1	C	327	<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;"> 81% 9% • 7% </div> </div>
1	D	327	<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% 12% •• 6% </div> </div>
1	E	327	<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;"> 76% 15% • 6% </div> </div>
1	F	327	<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% 14% •• 6% </div> </div>
2	B	327	<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;"> 76% 15% •• 6% </div> </div>

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
5	GOL	D	1319	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15480 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	303	Total	C	N	O	S	3	8	0
			2308	1447	398	455	8			
1	C	304	Total	C	N	O	S	3	7	0
			2316	1453	396	457	10			
1	D	308	Total	C	N	O	S	0	6	0
			2329	1461	396	461	11			
1	E	307	Total	C	N	O	S	3	5	0
			2312	1448	397	456	11			
1	F	307	Total	C	N	O	S	0	5	0
			2311	1449	396	458	8			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	HIS	-	expression tag	UNP D0AB41
A	323	HIS	-	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
C	322	HIS	-	expression tag	UNP D0AB41
C	323	HIS	-	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
D	322	HIS	-	expression tag	UNP D0AB41
D	323	HIS	-	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
E	322	HIS	-	expression tag	UNP D0AB41

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	323	HIS	-	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
F	322	HIS	-	expression tag	UNP D0AB41
F	323	HIS	-	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
A	250	ALA	SER	engineered mutation	UNP D0AB41
C	250	ALA	SER	engineered mutation	UNP D0AB41
D	250	ALA	SER	engineered mutation	UNP D0AB41
E	250	ALA	SER	engineered mutation	UNP D0AB41
F	250	ALA	SER	engineered mutation	UNP D0AB41

- Molecule 2 is a protein called INTRACELLULAR SUBTILISIN PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	7	0
			2325	1455	398	463	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	322	HIS	-	expression tag	UNP D0AB41
B	323	HIS	-	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	250	ALA	SER	engineered mutation	UNP D0AB41

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

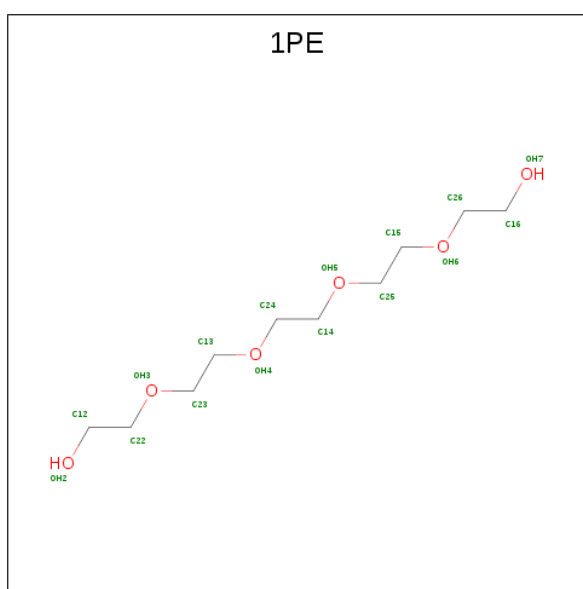
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

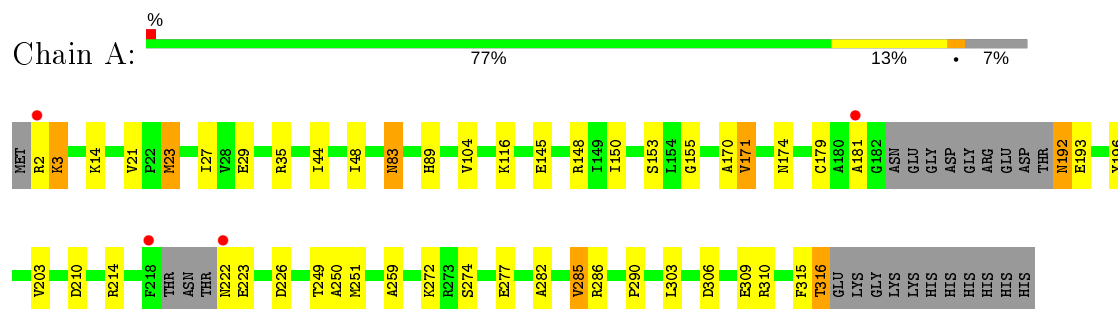
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	241	Total	O	0	0
			241	241		
6	B	208	Total	O	0	0
			208	208		
6	C	264	Total	O	0	0
			264	264		
6	D	213	Total	O	0	0
			213	213		
6	E	265	Total	O	0	0
			265	265		
6	F	310	Total	O	0	0
			310	310		

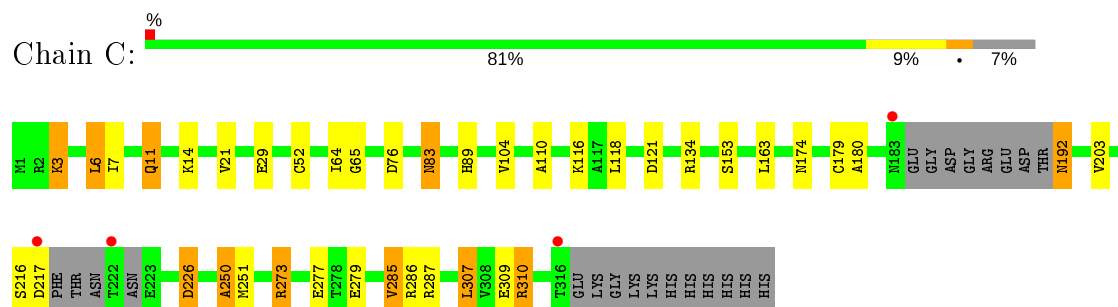
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

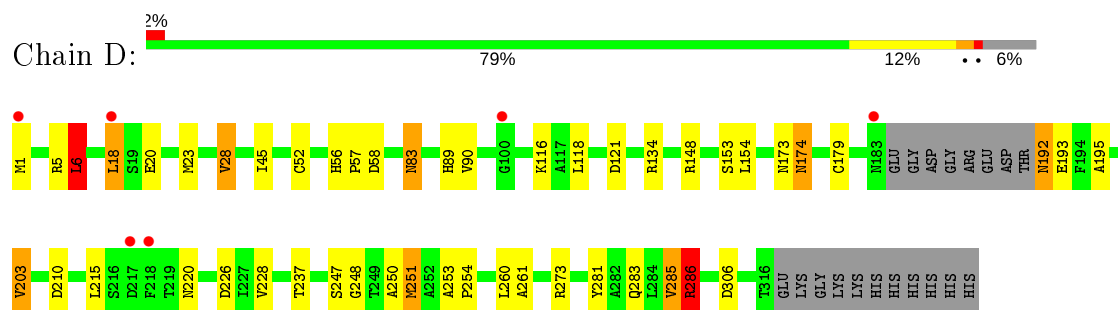
• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE



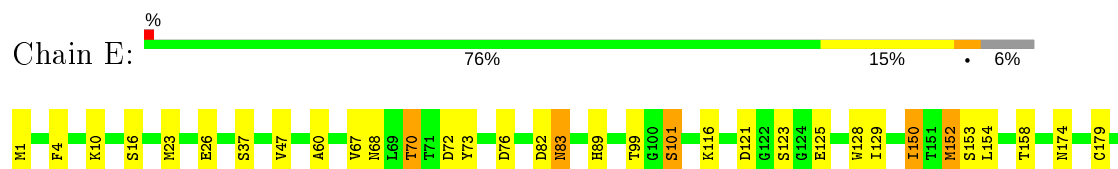
• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE

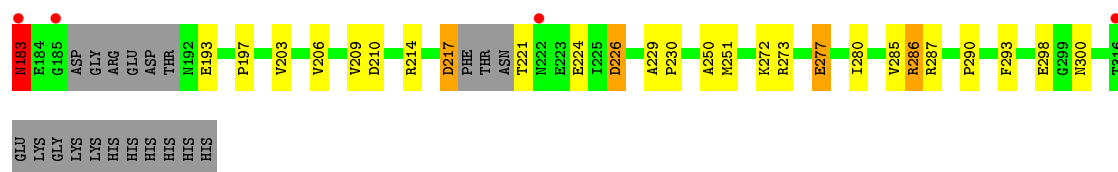


• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE

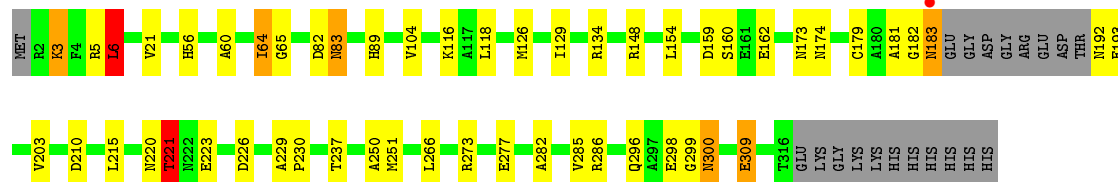


• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE

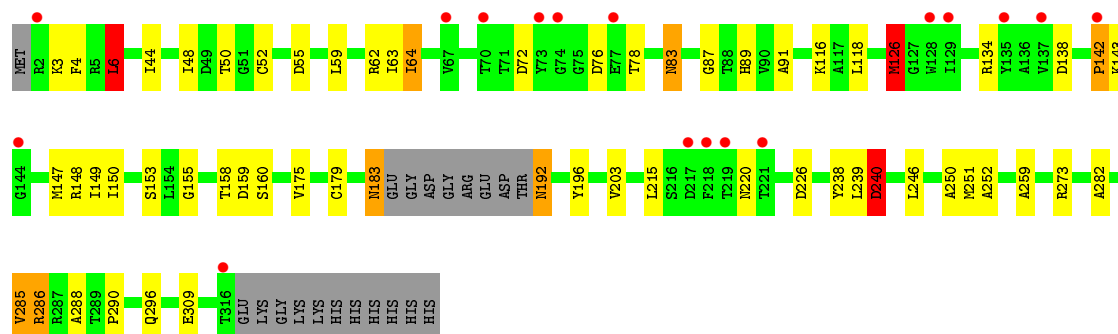
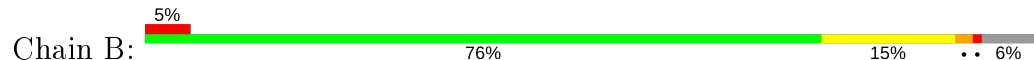




• Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE



• Molecule 2: INTRACELLULAR SUBTILISIN PROTEASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	125.66Å 125.66Å 106.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.98 – 1.56 75.98 – 1.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.98-1.56) 99.7 (75.98-1.56)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.230 0.192 , 0.232	Depositor DCC
R_{free} test set	16527 reflections (6.16%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.019 for h,-h-k,-l 0.013 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15480	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 1PE, CSX, 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	1.30	3/2332 (0.1%)	1.05	7/3162 (0.2%)
1	C	1.38	7/2339 (0.3%)	1.28	16/3172 (0.5%)
1	D	1.23	6/2354 (0.3%)	1.14	16/3194 (0.5%)
1	E	23.32	15/2335 (0.6%)	1.60	21/3165 (0.7%)
1	F	1.30	6/2336 (0.3%)	1.17	11/3173 (0.3%)
2	B	1.29	8/2342 (0.3%)	1.11	7/3178 (0.2%)
All	All	9.58	45/14038 (0.3%)	1.24	78/19044 (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	E	1	0

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	ASN	CB-CG	852.16	21.11	1.51
1	E	183	ASN	CA-CB	734.18	20.62	1.53
1	A	3	LYS	CG-CD	-25.61	0.65	1.52
1	C	3	LYS	CG-CD	-20.87	0.81	1.52
2	B	285	VAL	CB-CG2	-11.32	1.29	1.52

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	183	ASN	CA-CB-CG	-48.43	6.85	113.40
1	E	183	ASN	CB-CG-OD1	19.86	161.31	121.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	183	ASN	CB-CG-ND2	-17.42	74.89	116.70
1	C	310	ARG	NE-CZ-NH2	-12.37	114.12	120.30
1	C	310	ARG	NE-CZ-NH1	12.02	126.31	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	183	ASN	CA

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	2308	0	2254	38	0
1	C	2316	0	2274	40	0
1	D	2329	0	2280	46	0
1	E	2312	0	2268	58	0
1	F	2311	0	2260	61	0
2	B	2325	0	2266	51	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	13	3	0
4	B	10	0	13	3	0
4	C	10	0	13	3	0
4	D	10	0	13	3	0
4	E	10	0	13	2	0
4	F	10	0	13	4	0
5	C	6	0	8	0	0
5	D	6	0	8	6	0
6	A	241	0	0	3	0
6	B	208	0	0	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	264	0	0	7	0
6	D	213	0	0	3	0
6	E	265	0	0	10	0
6	F	310	0	0	8	0
All	All	15480	0	13696	267	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 267 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)
4:F:1318:IPE:C14	4:F:1318:IPE:OH5	1.65	1.42
1:E:273[A]:ARG:NH1	6:E:2234:HOH:O	1.58	1.28
1:E:129:ILE:HG12	6:E:2116:HOH:O	1.08	1.25
1:F:309:GLU:HG3	6:F:2296:HOH:O	1.43	1.18
1:A:309:GLU:HG3	6:A:2233:HOH:O	1.46	1.15

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	303/327 (93%)	294 (97%)	9 (3%)	0	100	100
1	C	304/327 (93%)	295 (97%)	9 (3%)	0	100	100
1	D	308/327 (94%)	300 (97%)	8 (3%)	0	100	100
1	E	304/327 (93%)	295 (97%)	9 (3%)	0	100	100
1	F	306/327 (94%)	293 (96%)	13 (4%)	0	100	100
2	B	307/327 (94%)	295 (96%)	11 (4%)	1 (0%)	41	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1832/1962 (93%)	1772 (97%)	59 (3%)	1 (0%)	51 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	142	PRO

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	234/249 (94%)	222 (95%)	12 (5%)	24 3
1	C	236/249 (95%)	229 (97%)	7 (3%)	41 12
1	D	238/249 (96%)	228 (96%)	10 (4%)	30 5
1	E	235/249 (94%)	224 (95%)	11 (5%)	26 4
1	F	236/249 (95%)	226 (96%)	10 (4%)	30 5
2	B	237/248 (96%)	224 (94%)	13 (6%)	21 3
All	All	1416/1493 (95%)	1353 (96%)	63 (4%)	30 4

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	83	ASN
1	D	83	ASN
1	F	160[B]	SER
1	C	192	ASN
1	C	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	192	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	89	HIS
1	F	201	ASN
1	C	201	ASN
1	D	220	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

13 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CSX	C	179[A]	1	3,5,7	1.69	1 (33%)	1,5,8	3.20	1 (100%)
1	CSX	E	179[B]	1	3,6,7	1.71	1 (33%)	1,6,8	0.95	0
1	CSX	F	179[B]	1	3,6,7	0.98	0	1,6,8	0.17	0
1	CSX	A	179[A]	1	3,6,7	1.10	0	1,6,8	0.85	0
2	CSX	B	52	2	3,6,7	1.11	0	1,6,8	0.42	0
2	CSX	B	179[B]	2	3,6,7	1.20	0	1,6,8	1.66	0
1	CSX	C	179[B]	1	3,6,7	0.85	0	1,6,8	1.52	0
1	CSX	A	179[B]	1	3,5,7	1.42	1 (33%)	1,5,8	2.27	1 (100%)
1	CSX	D	179[B]	1	3,6,7	0.63	0	1,6,8	0.83	0
1	CSX	E	179[A]	1	3,6,7	0.90	0	1,6,8	0.09	0
2	CSX	B	179[A]	2	3,5,7	1.44	0	1,5,8	1.31	0
1	CSX	F	179[A]	1	3,6,7	0.92	0	1,6,8	0.40	0
1	CSX	D	179[A]	1	3,6,7	1.32	0	1,6,8	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSX	C	179[A]	1	-	0/1/4/7	-
1	CSX	E	179[B]	1	-	0/1/5/7	-
1	CSX	F	179[B]	1	-	0/1/5/7	-
1	CSX	A	179[A]	1	-	0/1/5/7	-
2	CSX	B	52	2	-	1/1/5/7	-
2	CSX	B	179[B]	2	-	0/1/5/7	-
1	CSX	C	179[B]	1	-	0/1/5/7	-
1	CSX	A	179[B]	1	-	0/1/4/7	-
1	CSX	D	179[B]	1	-	0/1/5/7	-
1	CSX	E	179[A]	1	-	0/1/5/7	-
2	CSX	B	179[A]	2	-	0/1/4/7	-
1	CSX	F	179[A]	1	-	0/1/5/7	-
1	CSX	D	179[A]	1	-	0/1/5/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	179[B]	CSX	CB-CA	-2.76	1.46	1.53
1	C	179[A]	CSX	O-C	2.55	1.30	1.19
1	A	179[B]	CSX	CB-CA	-2.07	1.48	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179[A]	CSX	CA-CB-SG	3.20	120.35	113.36
1	A	179[B]	CSX	CA-CB-SG	-2.27	108.40	113.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	52	CSX	N-CA-CB-SG

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	179[A]	CSX	2	0
2	B	52	CSX	1	0
1	A	179[B]	CSX	2	0
1	E	179[A]	CSX	2	0
2	B	179[A]	CSX	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	179[A]	CSX	2	0
1	D	179[A]	CSX	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	1PE	E	1318	-	9,9,15	2.42	4 (44%)	8,8,14	0.59	0
4	1PE	C	1319	-	9,9,15	2.31	5 (55%)	8,8,14	0.57	0
4	1PE	B	1318	-	9,9,15	1.52	3 (33%)	8,8,14	1.36	2 (25%)
5	GOL	D	1319	-	5,5,5	0.24	0	5,5,5	0.48	0
4	1PE	D	1318	-	9,9,15	1.86	4 (44%)	8,8,14	1.09	0
4	1PE	F	1318	-	9,9,15	2.52	4 (44%)	8,8,14	0.67	0
5	GOL	C	1320	-	5,5,5	0.30	0	5,5,5	0.39	0
4	1PE	A	1318	-	9,9,15	1.37	2 (22%)	8,8,14	1.13	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	E	1318	-	-	3/7/7/13	-
4	1PE	C	1319	-	-	3/7/7/13	-
4	1PE	B	1318	-	-	3/7/7/13	-
5	GOL	D	1319	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	D	1318	-	-	3/7/7/13	-
4	1PE	F	1318	-	-	3/7/7/13	-
5	GOL	C	1320	-	-	2/4/4/4	-
4	1PE	A	1318	-	-	3/7/7/13	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1318	1PE	OH5-C14	4.45	1.65	1.42
4	E	1318	1PE	OH5-C14	4.02	1.62	1.42
4	E	1318	1PE	OH4-C24	3.93	1.59	1.42
4	F	1318	1PE	OH4-C24	3.55	1.57	1.42
4	C	1319	1PE	OH3-C23	3.47	1.57	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1318	1PE	OH3-C22-C12	2.54	121.22	110.07
4	A	1318	1PE	OH3-C22-C12	2.18	119.66	110.07
4	B	1318	1PE	OH3-C23-C13	2.09	119.80	110.39

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1318	1PE	C14-C24-OH4-C13
4	F	1318	1PE	C14-C24-OH4-C13
4	E	1318	1PE	C14-C24-OH4-C13
5	C	1320	GOL	C1-C2-C3-O3
4	B	1318	1PE	OH4-C13-C23-OH3

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1318	1PE	2	0
4	C	1319	1PE	3	0
4	B	1318	1PE	3	0
5	D	1319	GOL	6	0
4	D	1318	1PE	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1318	1PE	4	0
4	A	1318	1PE	3	0

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
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	179[A]:CSX	C	180:ALA	N	1.15
1	A	179[B]:CSX	C	180:ALA	N	1.14

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	302/327 (92%)	-0.20	4 (1%) 77 82	14, 26, 42, 60	1 (0%)
1	C	303/327 (92%)	-0.37	4 (1%) 77 82	12, 20, 38, 55	1 (0%)
1	D	307/327 (93%)	-0.12	6 (1%) 65 71	12, 26, 44, 54	0
1	E	306/327 (93%)	-0.19	4 (1%) 77 82	10, 20, 37, 60	1 (0%)
1	F	306/327 (93%)	-0.23	1 (0%) 94 95	10, 21, 37, 47	0
2	B	305/327 (93%)	0.22	17 (5%) 24 28	14, 27, 44, 62	0
All	All	1829/1962 (93%)	-0.15	36 (1%) 65 71	10, 23, 41, 62	3 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	185	GLY	8.3
1	C	316	THR	6.0
1	E	316	THR	5.6
2	B	74	GLY	4.5
2	B	144	GLY	3.9

6.2 Non-standard residues in protein, DNA, RNA chains [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	CSX	B	52	7/8	0.92	0.11	27,29,31,31	0
2	CSX	B	179[B]	7/8	0.95	0.10	20,22,23,26	7
2	CSX	B	179[A]	6/8	0.95	0.10	22,22,23,23	6
1	CSX	D	179[B]	7/8	0.96	0.08	15,16,20,24	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSX	E	179[A]	7/8	0.96	0.09	7,11,16,18	7
1	CSX	E	179[B]	7/8	0.96	0.09	11,12,16,17	7
1	CSX	D	179[A]	7/8	0.96	0.08	15,15,19,24	7
1	CSX	A	179[B]	6/8	0.97	0.07	19,20,21,25	6
1	CSX	A	179[A]	7/8	0.97	0.07	19,19,21,22	7
1	CSX	C	179[A]	6/8	0.97	0.07	11,12,13,18	6
1	CSX	F	179[B]	7/8	0.97	0.09	12,13,15,23	7
1	CSX	F	179[A]	7/8	0.97	0.09	10,14,21,23	7
1	CSX	C	179[B]	7/8	0.97	0.07	11,13,18,19	7

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. 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(\AA^2)	Q<0.9
5	GOL	C	1320	6/6	0.75	0.16	53,57,57,58	0
5	GOL	D	1319	6/6	0.81	0.20	27,34,40,42	0
3	NA	A	1317	1/1	0.92	0.08	30,30,30,30	0
3	NA	D	1317	1/1	0.92	0.10	30,30,30,30	0
4	1PE	B	1318	10/16	0.93	0.09	15,20,24,27	0
3	NA	B	1317	1/1	0.93	0.07	26,26,26,26	0
4	1PE	C	1319	10/16	0.94	0.07	10,15,20,20	0
4	1PE	E	1318	10/16	0.95	0.07	8,13,20,21	0
4	1PE	A	1318	10/16	0.95	0.07	11,19,23,23	0
3	NA	E	1317	1/1	0.96	0.06	19,19,19,19	0
4	1PE	F	1318	10/16	0.96	0.09	9,14,19,19	0
4	1PE	D	1318	10/16	0.96	0.06	7,16,20,22	0
3	NA	C	1317	1/1	0.96	0.06	23,23,23,23	0
3	NA	F	1317	1/1	0.97	0.06	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.