wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2021 – 03:07 pm BST

PDB ID	:	7A5A
Title	:	Crimean-Congo Hemorrhagic Fever Virus Envelope Glycoprotein Gc W1191H/W1197A/W1199A Mutant in Postfusion Conformation (Monoclinic Crystal Form)
Authors	:	Hellert, J.; Guardado-Calvo, P.; Rey, F.A.
Deposited on	:	2020-08-20
Resolution	:	2.99 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

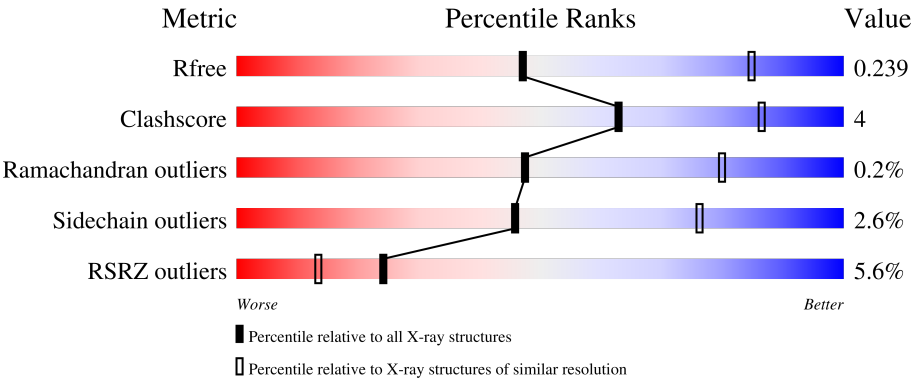
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	540	2% 81% 12% 6%
1	B	540	2% 80% 14% 6%
1	C	540	2% 82% 10% 8%
1	D	540	9% 80% 13% 8%
1	E	540	9% 77% 15% 8%

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Mol	Chain	Length	Quality of chain
1	F	540	7% 79% 13% 8%

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
2	NAG	A	1602	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23452 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3918	2454	669	760	35			
1	B	505	Total	C	N	O	S	0	0	0
			3918	2454	669	760	35			
1	C	498	Total	C	N	O	S	0	0	0
			3866	2423	660	748	35			
1	D	499	Total	C	N	O	S	0	0	0
			3873	2427	661	750	35			
1	E	499	Total	C	N	O	S	0	0	0
			3873	2427	661	750	35			
1	F	499	Total	C	N	O	S	0	0	0
			3873	2427	661	750	35			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1033	TRP	-	expression tag	UNP Q8JSZ3
A	1034	SER	-	expression tag	UNP Q8JSZ3
A	1035	HIS	-	expression tag	UNP Q8JSZ3
A	1036	PRO	-	expression tag	UNP Q8JSZ3
A	1037	GLN	-	expression tag	UNP Q8JSZ3
A	1038	PHE	-	expression tag	UNP Q8JSZ3
A	1039	GLU	-	expression tag	UNP Q8JSZ3
A	1040	LYS	-	expression tag	UNP Q8JSZ3
A	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
A	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
A	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
B	1033	TRP	-	expression tag	UNP Q8JSZ3
B	1034	SER	-	expression tag	UNP Q8JSZ3
B	1035	HIS	-	expression tag	UNP Q8JSZ3
B	1036	PRO	-	expression tag	UNP Q8JSZ3
B	1037	GLN	-	expression tag	UNP Q8JSZ3
B	1038	PHE	-	expression tag	UNP Q8JSZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1039	GLU	-	expression tag	UNP Q8JSZ3
B	1040	LYS	-	expression tag	UNP Q8JSZ3
B	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
B	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
B	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
C	1033	TRP	-	expression tag	UNP Q8JSZ3
C	1034	SER	-	expression tag	UNP Q8JSZ3
C	1035	HIS	-	expression tag	UNP Q8JSZ3
C	1036	PRO	-	expression tag	UNP Q8JSZ3
C	1037	GLN	-	expression tag	UNP Q8JSZ3
C	1038	PHE	-	expression tag	UNP Q8JSZ3
C	1039	GLU	-	expression tag	UNP Q8JSZ3
C	1040	LYS	-	expression tag	UNP Q8JSZ3
C	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
C	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
C	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
D	1033	TRP	-	expression tag	UNP Q8JSZ3
D	1034	SER	-	expression tag	UNP Q8JSZ3
D	1035	HIS	-	expression tag	UNP Q8JSZ3
D	1036	PRO	-	expression tag	UNP Q8JSZ3
D	1037	GLN	-	expression tag	UNP Q8JSZ3
D	1038	PHE	-	expression tag	UNP Q8JSZ3
D	1039	GLU	-	expression tag	UNP Q8JSZ3
D	1040	LYS	-	expression tag	UNP Q8JSZ3
D	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
D	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
D	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
E	1033	TRP	-	expression tag	UNP Q8JSZ3
E	1034	SER	-	expression tag	UNP Q8JSZ3
E	1035	HIS	-	expression tag	UNP Q8JSZ3
E	1036	PRO	-	expression tag	UNP Q8JSZ3
E	1037	GLN	-	expression tag	UNP Q8JSZ3
E	1038	PHE	-	expression tag	UNP Q8JSZ3
E	1039	GLU	-	expression tag	UNP Q8JSZ3
E	1040	LYS	-	expression tag	UNP Q8JSZ3
E	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
E	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
E	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
F	1033	TRP	-	expression tag	UNP Q8JSZ3
F	1034	SER	-	expression tag	UNP Q8JSZ3
F	1035	HIS	-	expression tag	UNP Q8JSZ3
F	1036	PRO	-	expression tag	UNP Q8JSZ3

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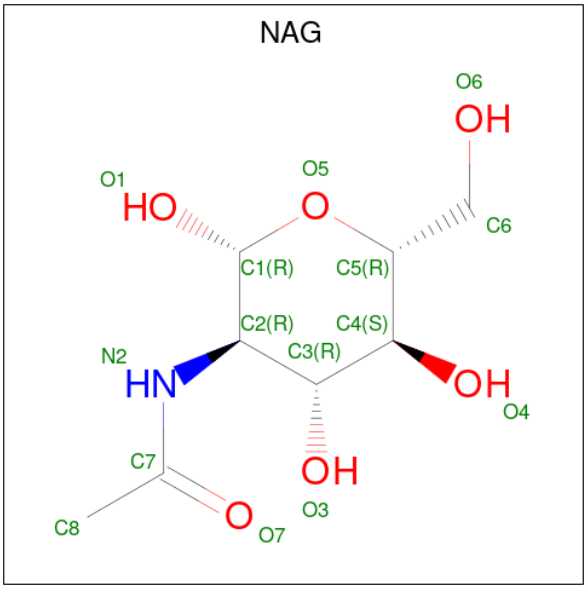
Chain	Residue	Modelled	Actual	Comment	Reference
F	1037	GLN	-	expression tag	UNP Q8JSZ3
F	1038	PHE	-	expression tag	UNP Q8JSZ3
F	1039	GLU	-	expression tag	UNP Q8JSZ3
F	1040	LYS	-	expression tag	UNP Q8JSZ3
F	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
F	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
F	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C N O 14 8 1 5	0	0
2	F	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

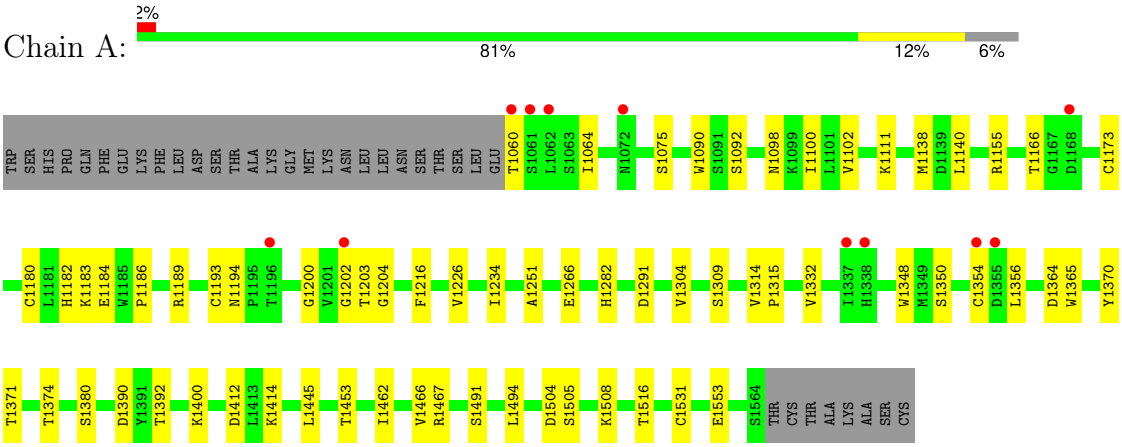
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	C	1	Total Cl 1 1	0	0
3	D	2	Total Cl 2 2	0	0

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.

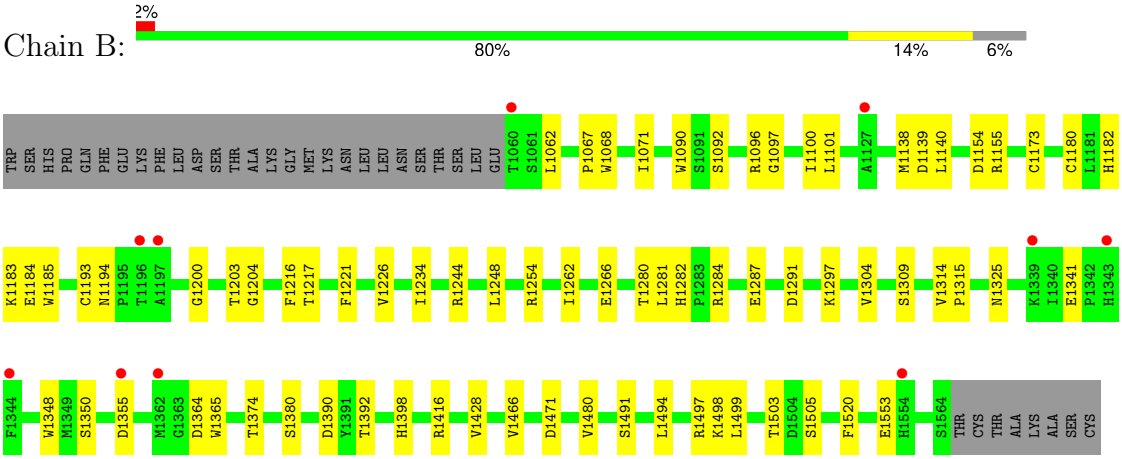
• Molecule 1: Envelopment polyprotein

Chain A:



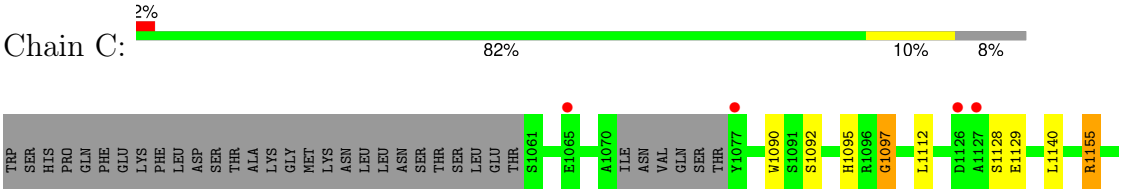
• Molecule 1: Envelopment polyprotein

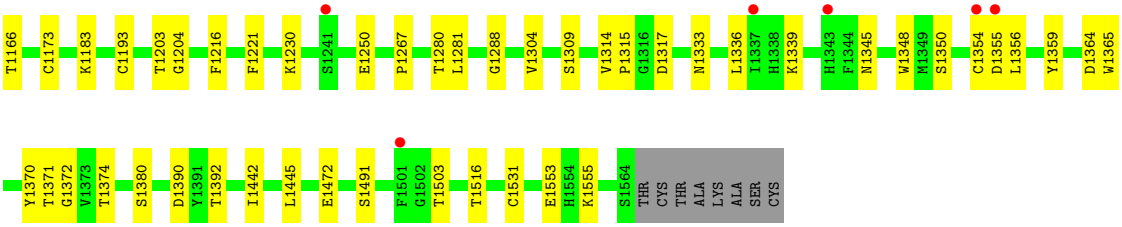
Chain B:



• Molecule 1: Envelopment polyprotein

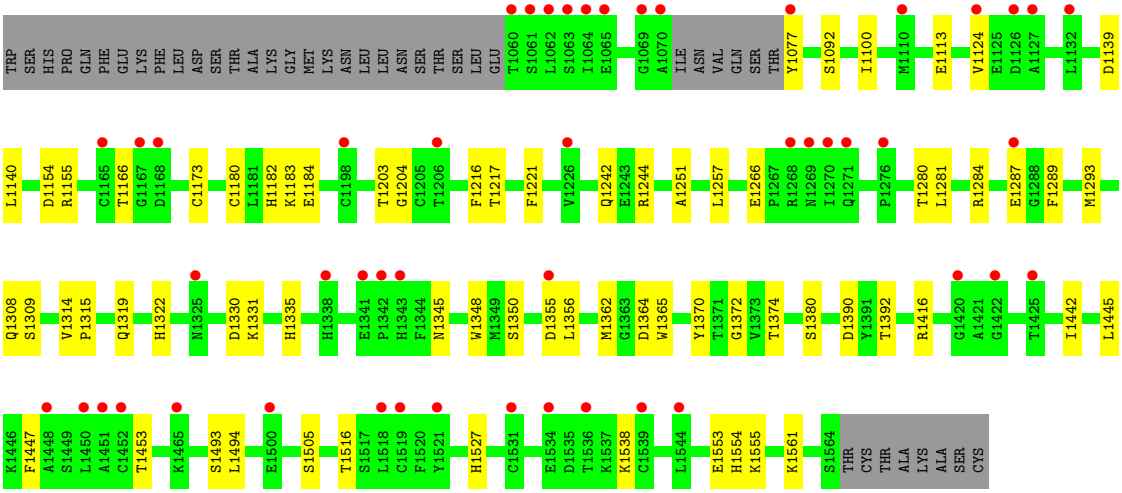
Chain C:





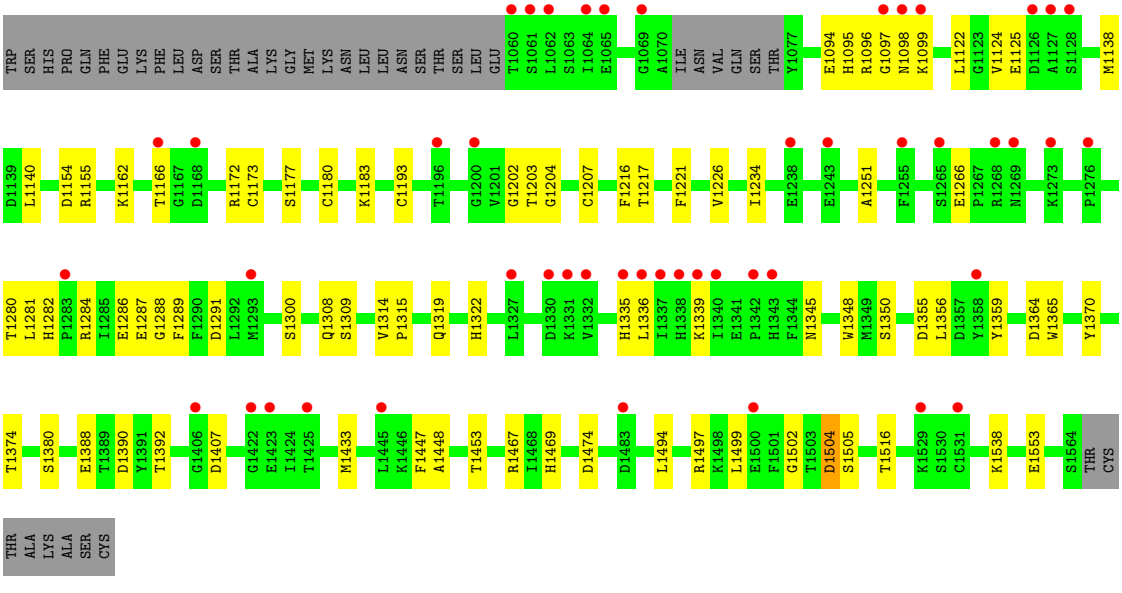
• Molecule 1: Envelopment polyprotein

Chain D:



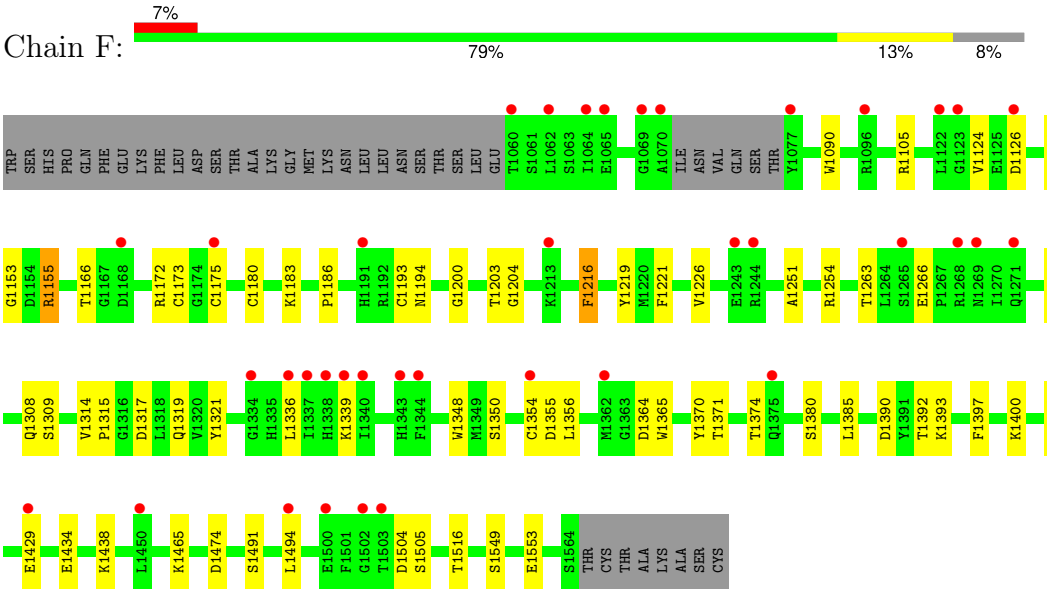
• Molecule 1: Envelopment polyprotein

Chain E:



• Molecule 1: Envelopment polyprotein

Chain F:


7%
79%
13%
8%
TRP SER HIS PRO GLN PHE GLU LYS PHE LEU ASP SER THR ALA LYS GLY MET LYS ASN LEU LEU LEU ASN SER THR SER LEU GLU T1060 S1061 L1062 S1063 I1064 E1065 G1069 A1070 ILE ASN VAL GLN SER THR Y1077 W1090 R1096 R1105 L1122 G1123 V1124 E1125 D1126 L1132 L1140
G1153 D1154 R1155 T1166 G1167 D1168 R1172 C1173 G1174 C1175 C1180 K1183 P1186 H1191 R1192 C1193 N1194 G1200 T1203 G1204 K1213 F1216 Y1219 M1220 F1221 V1226 E1243 R1244 A1251 R1254 T1263 L1264 S1265 E1266 P1267 R1268 N1269 I1270 Q1271 T1280 L1281 V1304
Q1308 S1309 V1314 P1315 G1316 D1317 L1318 Q1319 V1320 Y1321 G1334 H1335 L1336 I1337 H1338 K1339 I1340 H1343 F1344 W1348 M1349 S1350 C1354 D1355 L1356 M1362 G1363 D1364 W1365 Y1370 T1371 T1374 Q1375 S1380 L1385 D1390 Y1391 T1392 K1393 F1397 K1400 D1412 A1421 G1422
E1429 E1434 K1438 L1450 K1465 D1474 S1491 L1494 E1500 F1501 G1502 T1503 D1504 S1505 T1516 S1549 E1553 S1564 THR CYS THR ALA LYS ALA SER CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.97Å 108.26Å 223.53Å 90.00° 93.22° 90.00°	Depositor
Resolution (Å)	49.05 – 2.99 49.05 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.05-2.99) 91.1 (49.05-2.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.72 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.204 , 0.239 0.204 , 0.239	Depositor DCC
R_{free} test set	2001 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23452	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, NAG

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	0.30	0/4005	0.48	0/5432
1	B	0.30	0/4005	0.48	0/5432
1	C	0.29	0/3952	0.48	0/5357
1	D	0.26	0/3959	0.47	0/5367
1	E	0.26	0/3959	0.47	0/5367
1	F	0.26	0/3959	0.46	0/5367
All	All	0.28	0/23839	0.47	0/32322

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

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	3918	0	3810	32	0
1	B	3918	0	3810	38	0
1	C	3866	0	3756	29	0
1	D	3873	0	3764	40	0
1	E	3873	0	3764	43	0
1	F	3873	0	3764	38	0
2	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	26	1	0
2	C	28	0	26	0	0
2	D	14	0	13	1	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
All	All	23452	0	22785	199	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 4.

The worst 5 of 199 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:E:1355:ASP:OD2	1:F:1183:LYS:NZ	1.83	1.11
1:B:1355:ASP:OD2	1:C:1183:LYS:NZ	1.92	1.02
1:A:1467:ARG:NH1	1:A:1504:ASP:OD1	2.13	0.81
1:D:1287:GLU:O	1:D:1335:HIS:NE2	2.14	0.80
1:A:1314:VAL:HG21	1:B:1309:SER:HB2	1.64	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	503/540 (93%)	490 (97%)	13 (3%)	0	100 100
1	B	503/540 (93%)	490 (97%)	12 (2%)	1 (0%)	47 80
1	C	494/540 (92%)	481 (97%)	12 (2%)	1 (0%)	47 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	495/540 (92%)	481 (97%)	13 (3%)	1 (0%)	47 80
1	E	495/540 (92%)	479 (97%)	14 (3%)	2 (0%)	34 70
1	F	495/540 (92%)	482 (97%)	13 (3%)	0	100 100
All	All	2985/3240 (92%)	2903 (97%)	77 (3%)	5 (0%)	47 80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1097	GLY
1	E	1097	GLY
1	B	1097	GLY
1	D	1554	HIS
1	E	1504	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	448/479 (94%)	432 (96%)	16 (4%)	35 68
1	B	448/479 (94%)	437 (98%)	11 (2%)	47 77
1	C	441/479 (92%)	431 (98%)	10 (2%)	50 79
1	D	442/479 (92%)	433 (98%)	9 (2%)	55 81
1	E	442/479 (92%)	431 (98%)	11 (2%)	47 77
1	F	442/479 (92%)	430 (97%)	12 (3%)	44 75
All	All	2663/2874 (93%)	2594 (97%)	69 (3%)	46 76

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1126	ASP
1	F	1155	ARG
1	F	1226	VAL

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Mol	Chain	Res	Type
1	B	1304	VAL
1	B	1226	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1469	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)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
2	NAG	B	1601	1	14,14,15	0.19	0	17,19,21	0.36	0
2	NAG	B	1602	1	14,14,15	0.37	0	17,19,21	1.25	2 (11%)
2	NAG	D	1601	1	14,14,15	0.51	0	17,19,21	0.74	1 (5%)
2	NAG	F	1601	1	14,14,15	0.22	0	17,19,21	0.37	0
2	NAG	E	1601	1	14,14,15	0.17	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	1602	1	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	A	1601	1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	A	1602	1	14,14,15	0.22	0	17,19,21	0.48	0
2	NAG	C	1601	1	14,14,15	0.44	0	17,19,21	0.64	1 (5%)

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
2	NAG	B	1601	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1602	1	-	5/6/23/26	0/1/1/1
2	NAG	D	1601	1	-	1/6/23/26	0/1/1/1
2	NAG	F	1601	1	-	2/6/23/26	0/1/1/1
2	NAG	E	1601	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1602	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1601	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1602	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1602	NAG	C2-N2-C7	4.34	129.08	122.90
2	D	1601	NAG	C1-O5-C5	2.50	115.59	112.19
2	C	1601	NAG	C1-O5-C5	2.23	115.22	112.19
2	B	1602	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1602	NAG	O5-C5-C6-O6
2	B	1602	NAG	C4-C5-C6-O6
2	A	1601	NAG	C8-C7-N2-C2
2	A	1601	NAG	O7-C7-N2-C2
2	B	1602	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1602	NAG	1	0
2	D	1601	NAG	1	0

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

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^{th} 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	505/540 (93%)	0.13	11 (2%)	62	42	42, 69, 124, 171	0
1	B	505/540 (93%)	0.05	10 (1%)	65	45	40, 66, 123, 182	0
1	C	498/540 (92%)	0.11	10 (2%)	65	45	43, 71, 131, 191	0
1	D	499/540 (92%)	0.58	49 (9%)	7	4	68, 106, 158, 235	0
1	E	499/540 (92%)	0.51	48 (9%)	8	4	79, 114, 170, 230	0
1	F	499/540 (92%)	0.45	40 (8%)	12	6	70, 101, 157, 191	0
All	All	3005/3240 (92%)	0.30	168 (5%)	24	13	40, 90, 151, 235	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1097	GLY	7.7
1	D	1060	THR	7.6
1	D	1069	GLY	6.5
1	D	1127	ALA	5.6
1	E	1337	ILE	5.5

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 monosaccharides 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, 95^{th} 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	NAG	A	1601	14/15	0.62	0.36	134,144,150,151	0
2	NAG	D	1601	14/15	0.69	0.28	166,191,219,224	0
2	NAG	F	1601	14/15	0.72	0.32	145,165,170,170	0
2	NAG	A	1602	14/15	0.73	0.49	128,138,145,145	0
2	NAG	B	1601	14/15	0.74	0.34	137,145,152,153	0
2	NAG	C	1601	14/15	0.75	0.38	133,143,156,157	0
2	NAG	C	1602	14/15	0.78	0.32	139,157,162,163	0
3	CL	A	1604	1/1	0.79	0.12	87,87,87,87	0
2	NAG	B	1602	14/15	0.82	0.37	124,135,140,140	0
2	NAG	E	1601	14/15	0.83	0.26	163,174,178,183	0
3	CL	D	1603	1/1	0.91	0.63	94,94,94,94	0
3	CL	A	1603	1/1	0.94	0.65	94,94,94,94	0
3	CL	D	1602	1/1	0.97	0.59	82,82,82,82	0
3	CL	C	1603	1/1	0.99	0.29	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.