Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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:

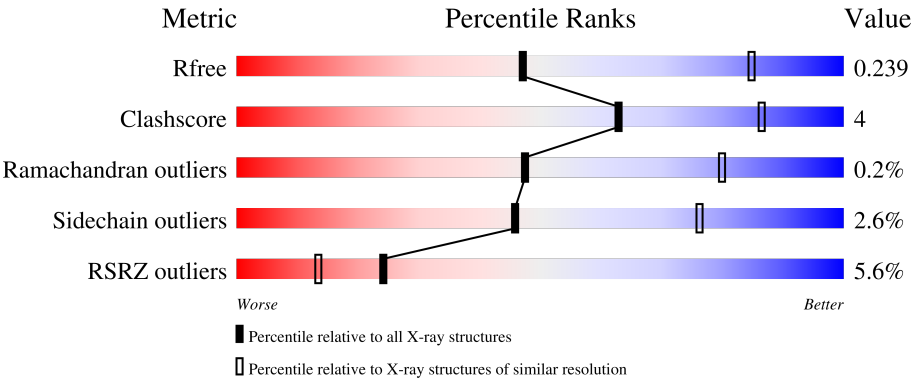
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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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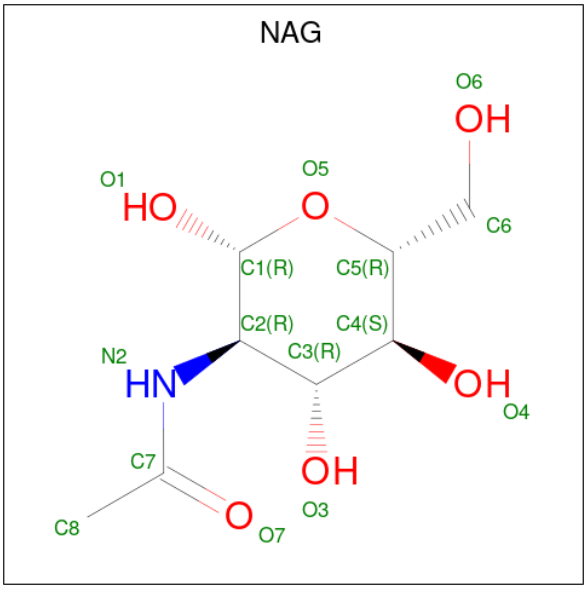
Chain	Residue	Modelled	Actual	Comment	Reference
F	1037	GLN	-	expression tag	UNP Q8JSZ3
F	1038	PHE	-	expression tag	UNP Q8JSZ3
F	1039	GLU	-	expression tag	UNP Q8JSZ3
F	1040	LYS	-	expression tag	UNP Q8JSZ3
F	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
F	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
F	1199	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).

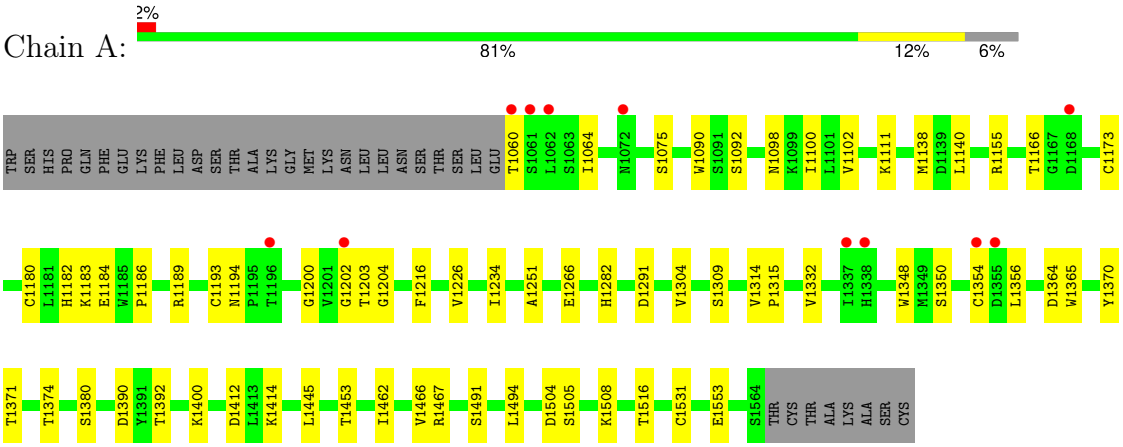
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	C	1	Total Cl 1 1	0	0
3	D	2	Total Cl 2 2	0	0

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.

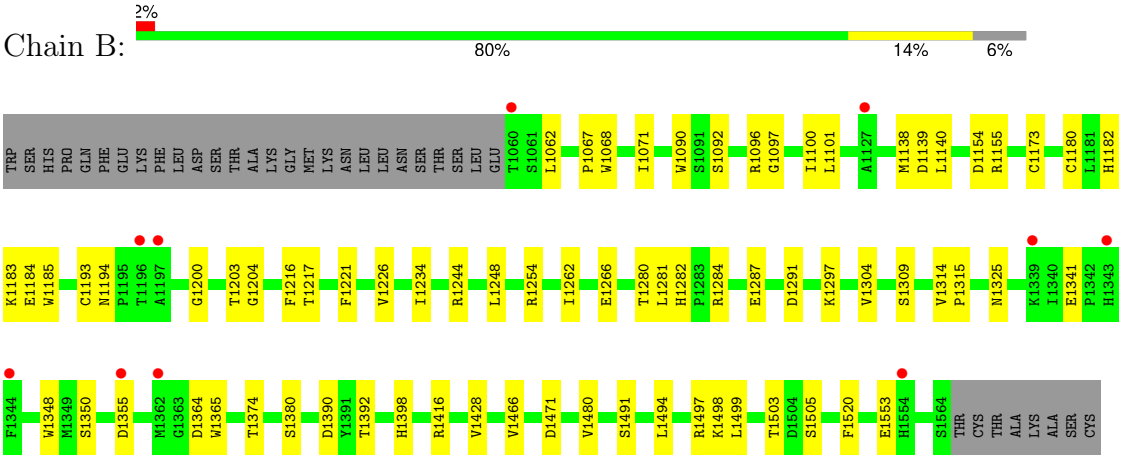
• Molecule 1: Envelopment polyprotein

Chain A:



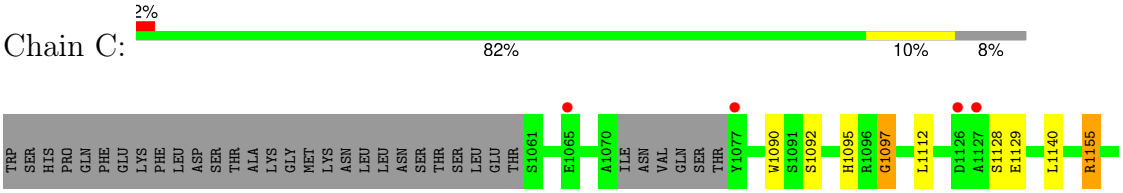
• Molecule 1: Envelopment polyprotein

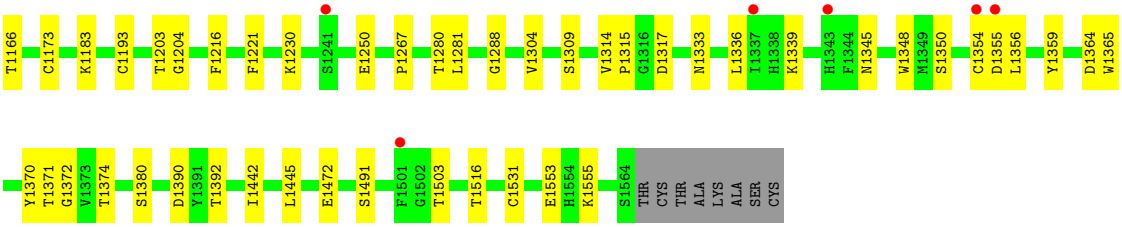
Chain B:



• Molecule 1: Envelopment polyprotein

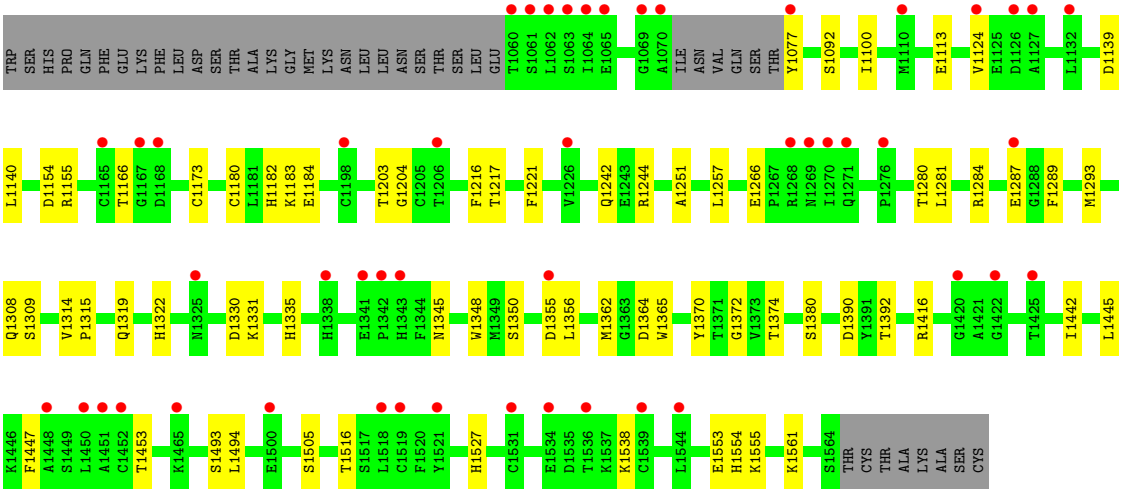
Chain C:





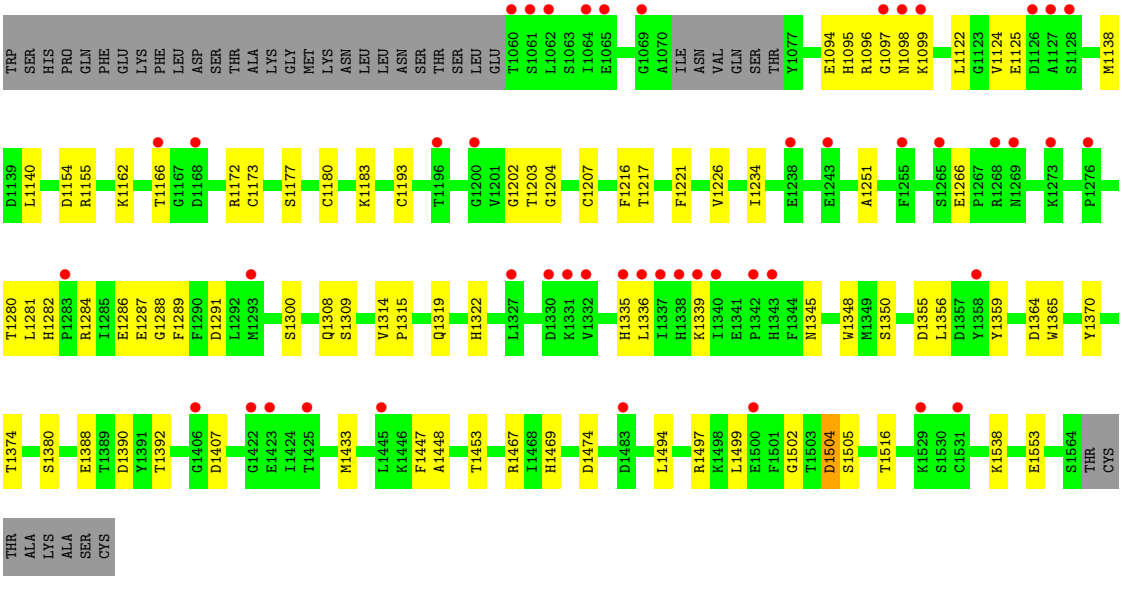
• Molecule 1: Envelopment polyprotein

Chain D:



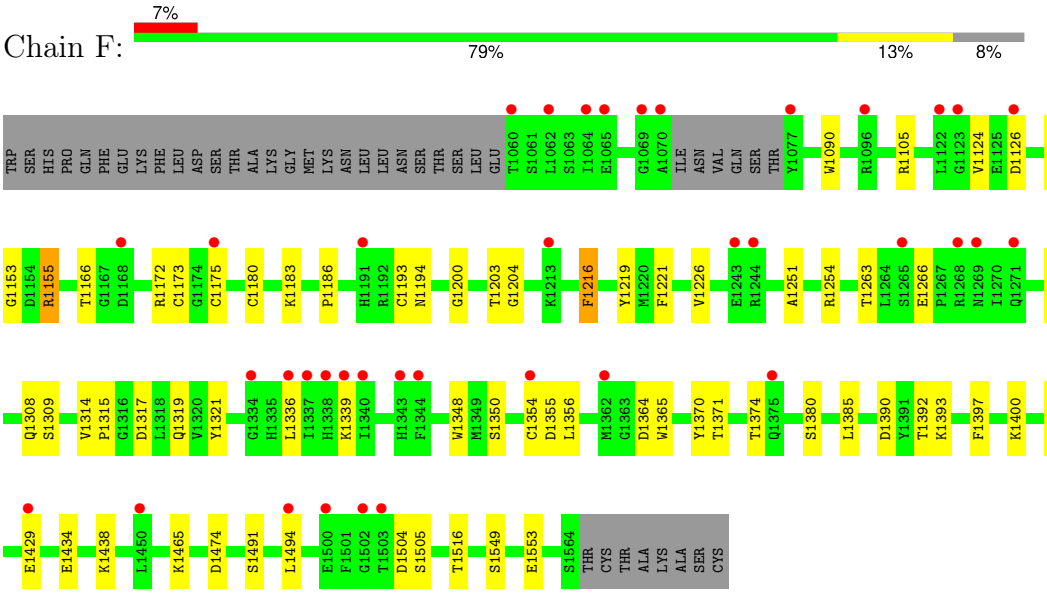
• Molecule 1: Envelopment polyprotein

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.

All (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
1:A:1183:LYS:NZ	1:C:1355:ASP:OD2	2.15	0.78
1:B:1314:VAL:HG21	1:C:1309:SER:HB2	1.68	0.74
1:F:1105:ARG:NH1	1:F:1429:GLU:HG3	2.04	0.72
1:F:1374:THR:HG23	1:F:1553:GLU:HG2	1.70	0.72
1:B:1284:ARG:HH21	1:B:1287:GLU:HG3	1.54	0.72
1:A:1092:SER:HB2	1:C:1090:TRP:HB2	1.73	0.70
1:A:1309:SER:HB2	1:C:1314:VAL:HG21	1.73	0.70
1:A:1390:ASP:OD1	1:A:1392:THR:OG1	2.11	0.68
1:E:1287:GLU:O	1:E:1335:HIS:NE2	2.24	0.68
1:D:1309:SER:HB2	1:F:1314:VAL:HG21	1.75	0.67
1:B:1390:ASP:OD1	1:B:1392:THR:OG1	2.12	0.67
1:B:1315:PRO:HD3	1:B:1380:SER:HB3	1.77	0.66
1:E:1094:GLU:OE2	1:E:1096:ARG:NH2	2.28	0.66
1:F:1390:ASP:OD1	1:F:1392:THR:OG1	2.14	0.66
1:C:1374:THR:HG23	1:C:1553:GLU:HG2	1.78	0.66
1:D:1374:THR:HG23	1:D:1553:GLU:HG2	1.78	0.65
1:E:1374:THR:HG23	1:E:1553:GLU:HG2	1.76	0.65
1:B:1096:ARG:HH11	1:B:1101:LEU:HD11	1.62	0.65
1:C:1390:ASP:OD1	1:C:1392:THR:OG1	2.15	0.65
1:D:1183:LYS:NZ	1:F:1355:ASP:OD2	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1284:ARG:HH21	1:E:1287:GLU:HG3	1.62	0.64
1:E:1314:VAL:HG21	1:F:1309:SER:HB2	1.79	0.64
1:D:1314:VAL:HG21	1:E:1309:SER:HB2	1.79	0.64
1:D:1390:ASP:OD1	1:D:1392:THR:OG1	2.16	0.64
1:D:1494:LEU:HD22	1:D:1505:SER:HB3	1.80	0.64
1:E:1286:GLU:HG2	1:E:1289:PHE:HB2	1.79	0.63
1:D:1289:PHE:HE2	1:D:1331:LYS:HD3	1.63	0.63
1:C:1315:PRO:HD3	1:C:1380:SER:HB3	1.79	0.63
1:A:1090:TRP:HB2	1:B:1092:SER:HB2	1.81	0.62
1:E:1494:LEU:HD22	1:E:1505:SER:HB3	1.80	0.62
1:A:1508:LYS:NZ	1:A:1508:LYS:HB3	2.15	0.62
1:F:1356:LEU:HD22	1:F:1370:TYR:HD2	1.66	0.61
1:F:1494:LEU:HD22	1:F:1505:SER:HB3	1.83	0.60
1:E:1474:ASP:N	1:E:1474:ASP:OD1	2.35	0.60
1:A:1356:LEU:HD22	1:A:1370:TYR:HD1	1.66	0.60
1:B:1374:THR:HG23	1:B:1553:GLU:HG2	1.83	0.60
1:B:1497:ARG:NH1	1:B:1499:LEU:O	2.35	0.59
1:A:1060:THR:HB	1:A:1075:SER:HB3	1.85	0.59
1:F:1474:ASP:OD1	1:F:1474:ASP:N	2.37	0.58
1:F:1354:CYS:HA	1:F:1371:THR:O	2.03	0.58
1:A:1315:PRO:HD3	1:A:1380:SER:HB3	1.85	0.58
1:E:1390:ASP:OD1	1:E:1392:THR:OG1	2.21	0.58
1:F:1221:PHE:HA	1:F:1280:THR:O	2.03	0.58
1:E:1154:ASP:OD2	1:E:1217:THR:HB	2.04	0.57
1:D:1315:PRO:HD3	1:D:1380:SER:HB3	1.86	0.57
1:C:1356:LEU:HD22	1:C:1370:TYR:HD1	1.69	0.56
1:E:1447:PHE:HB3	1:E:1538:LYS:HD2	1.86	0.56
1:E:1448:ALA:HB3	1:E:1467:ARG:HB3	1.87	0.56
1:D:1284:ARG:NH1	1:D:1287:GLU:HB2	2.20	0.56
1:E:1322:HIS:HB3	1:E:1407:ASP:OD2	2.06	0.56
1:F:1465:LYS:HD3	1:F:1504:ASP:OD2	2.06	0.56
1:D:1356:LEU:HD22	1:D:1370:TYR:HD2	1.71	0.55
1:D:1221:PHE:HB3	1:D:1281:LEU:HD23	1.88	0.55
1:B:1062:LEU:HD21	1:B:1244:ARG:HH11	1.71	0.55
2:B:1602:NAG:H3	2:B:1602:NAG:H83	1.89	0.55
1:B:1262:ILE:HD13	1:B:1428:VAL:HG22	1.88	0.54
1:F:1251:ALA:HB2	1:F:1266:GLU:HB3	1.89	0.54
1:F:1308:GLN:H	1:F:1319:GLN:HE22	1.56	0.54
1:B:1138:MET:HE1	1:B:1234:ILE:HG21	1.89	0.54
1:E:1251:ALA:HB2	1:E:1266:GLU:HB3	1.89	0.54
1:E:1315:PRO:HD3	1:E:1380:SER:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1098:ASN:HD21	1:E:1099:LYS:HE2	1.72	0.54
1:C:1445:LEU:HB2	1:C:1531:CYS:SG	2.48	0.53
1:C:1336:LEU:HD13	1:C:1339:LYS:HD2	1.91	0.53
1:F:1194:ASN:ND2	1:F:1200:GLY:O	2.42	0.53
1:C:1288:GLY:O	1:C:1333:ASN:HA	2.09	0.53
1:D:1251:ALA:HB2	1:D:1266:GLU:HB3	1.90	0.53
1:D:1561:LYS:O	2:D:1601:NAG:H83	2.09	0.53
1:B:1194:ASN:ND2	1:B:1200:GLY:O	2.41	0.53
1:C:1221:PHE:HB3	1:C:1281:LEU:HD23	1.91	0.53
1:D:1154:ASP:OD2	1:D:1217:THR:HB	2.08	0.52
1:E:1469:HIS:CE1	1:E:1499:LEU:HD23	2.44	0.52
1:B:1154:ASP:OD2	1:B:1217:THR:HB	2.10	0.52
1:A:1194:ASN:ND2	1:A:1200:GLY:O	2.43	0.52
1:E:1138:MET:HE1	1:E:1234:ILE:HG21	1.93	0.51
1:D:1183:LYS:HD3	1:D:1356:LEU:HB2	1.92	0.51
1:F:1364:ASP:OD1	1:F:1365:TRP:N	2.42	0.51
1:B:1096:ARG:HH11	1:B:1101:LEU:CD1	2.22	0.51
1:F:1392:THR:HA	1:F:1397:PHE:HE2	1.76	0.51
1:B:1182:HIS:ND1	1:B:1184:GLU:OE2	2.44	0.50
1:D:1221:PHE:HA	1:D:1280:THR:O	2.11	0.50
1:F:1348:TRP:CH2	1:F:1350:SER:HB2	2.47	0.50
1:E:1359:TYR:CG	1:F:1186:PRO:HD2	2.47	0.50
1:F:1390:ASP:OD2	1:F:1393:LYS:HE3	2.12	0.49
1:F:1221:PHE:HB3	1:F:1281:LEU:HD23	1.93	0.49
1:E:1122:LEU:HB3	1:E:1433:MET:HE2	1.94	0.49
1:F:1124:VAL:HA	1:F:1434:GLU:OE2	2.13	0.49
1:B:1139:ASP:OD1	1:B:1416:ARG:NH1	2.44	0.49
1:C:1155:ARG:NH2	1:C:1317:ASP:OD2	2.45	0.49
1:C:1345:ASN:OD1	1:C:1345:ASN:N	2.46	0.49
1:C:1348:TRP:CH2	1:C:1350:SER:HB2	2.47	0.48
1:B:1221:PHE:HB3	1:B:1281:LEU:HD23	1.94	0.48
1:F:1172:ARG:HB3	1:F:1175:CYS:HB2	1.96	0.48
1:E:1356:LEU:HD22	1:E:1370:TYR:HD2	1.78	0.48
1:C:1128:SER:OG	1:C:1129:GLU:N	2.47	0.48
1:D:1203:THR:OG1	1:D:1204:GLY:N	2.47	0.48
1:B:1068:TRP:HB2	1:B:1398:HIS:HB3	1.96	0.47
1:C:1203:THR:OG1	1:C:1204:GLY:N	2.46	0.47
1:F:1132:LEU:HD11	1:F:1438:LYS:HD2	1.96	0.47
1:F:1315:PRO:HD3	1:F:1380:SER:HB3	1.96	0.47
1:B:1203:THR:OG1	1:B:1204:GLY:N	2.47	0.47
1:E:1221:PHE:HA	1:E:1280:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1319:GLN:OE1	1:F:1321:TYR:OH	2.22	0.47
1:D:1322:HIS:NE2	1:F:1549:SER:OG	2.41	0.47
1:B:1068:TRP:NE1	1:B:1071:ILE:HD11	2.29	0.47
1:A:1348:TRP:CH2	1:A:1350:SER:HB2	2.50	0.47
1:A:1412:ASP:OD2	1:A:1414:LYS:HE2	2.14	0.47
1:B:1090:TRP:HB2	1:C:1092:SER:HB2	1.96	0.47
1:D:1442:ILE:HD12	1:D:1527:HIS:HB2	1.97	0.47
1:E:1203:THR:OG1	1:E:1204:GLY:N	2.47	0.47
1:B:1466:VAL:HG11	1:B:1494:LEU:HD13	1.96	0.46
1:E:1497:ARG:HD2	1:E:1502:GLY:HA2	1.97	0.46
1:F:1254:ARG:HG2	1:F:1263:THR:HG23	1.97	0.46
1:F:1203:THR:OG1	1:F:1204:GLY:N	2.48	0.46
1:A:1400:LYS:HA	1:A:1412:ASP:O	2.16	0.46
1:D:1372:GLY:C	1:D:1555:LYS:HD2	2.36	0.46
1:B:1348:TRP:CH2	1:B:1350:SER:HB2	2.50	0.46
1:F:1153:GLY:HA3	1:F:1216:PHE:HB3	1.98	0.46
1:D:1447:PHE:HB3	1:D:1538:LYS:HD2	1.98	0.45
1:C:1221:PHE:HA	1:C:1280:THR:O	2.17	0.45
1:D:1356:LEU:HD22	1:D:1370:TYR:CD2	2.52	0.45
1:B:1067:PRO:HD3	1:B:1248:LEU:HD11	1.98	0.45
1:E:1348:TRP:CH2	1:E:1350:SER:HB2	2.51	0.45
1:A:1186:PRO:HD2	1:C:1359:TYR:CG	2.51	0.45
1:A:1356:LEU:HD22	1:A:1370:TYR:CD1	2.51	0.45
1:C:1354:CYS:HA	1:C:1371:THR:O	2.17	0.45
1:A:1251:ALA:HB2	1:A:1266:GLU:HB3	1.99	0.45
1:E:1288:GLY:HA3	1:E:1335:HIS:CD2	2.52	0.45
1:A:1364:ASP:OD1	1:A:1365:TRP:N	2.44	0.45
1:F:1155:ARG:NH2	1:F:1317:ASP:OD2	2.44	0.45
1:A:1494:LEU:HD22	1:A:1505:SER:HB3	1.98	0.45
1:B:1471:ASP:O	1:B:1498:LYS:HE2	2.16	0.45
1:F:1356:LEU:HD22	1:F:1370:TYR:CD2	2.48	0.45
1:B:1183:LYS:HD3	1:B:1185:TRP:CZ2	2.52	0.44
1:D:1362:MET:HE3	1:E:1202:GLY:HA3	1.99	0.44
1:A:1466:VAL:HG11	1:A:1494:LEU:HD13	1.98	0.44
1:D:1092:SER:HB3	1:F:1090:TRP:HB2	1.98	0.44
1:E:1364:ASP:OD1	1:E:1365:TRP:N	2.47	0.44
1:E:1124:VAL:HG12	1:E:1125:GLU:HG2	1.99	0.44
1:E:1300:SER:OG	1:E:1388:GLU:OE2	2.24	0.44
1:A:1182:HIS:ND1	1:A:1184:GLU:OE2	2.49	0.44
1:B:1364:ASP:OD1	1:B:1365:TRP:N	2.48	0.44
1:D:1345:ASN:OD1	1:D:1345:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:THR:OG1	1:A:1204:GLY:N	2.49	0.44
1:A:1445:LEU:HB2	1:A:1531:CYS:SG	2.58	0.44
1:D:1284:ARG:HH11	1:D:1287:GLU:HB2	1.82	0.44
1:E:1172:ARG:NH2	1:E:1177:SER:O	2.42	0.44
1:A:1189:ARG:O	1:A:1202:GLY:N	2.42	0.44
1:B:1281:LEU:HB2	1:B:1297:LYS:HB2	2.00	0.43
1:E:1356:LEU:HD22	1:E:1370:TYR:CD2	2.54	0.43
1:C:1230:LYS:NZ	1:C:1250:GLU:OE2	2.33	0.43
1:D:1364:ASP:OD1	1:D:1365:TRP:N	2.50	0.43
1:B:1096:ARG:HD3	1:B:1101:LEU:HD12	2.00	0.43
1:E:1336:LEU:HD13	1:E:1339:LYS:HD2	2.00	0.43
1:D:1113:GLU:OE2	1:D:1493:SER:HB3	2.18	0.43
1:D:1139:ASP:OD1	1:D:1416:ARG:NH2	2.52	0.43
1:D:1348:TRP:CH2	1:D:1350:SER:HB2	2.54	0.43
1:D:1124:VAL:HG13	1:E:1095:HIS:O	2.19	0.43
1:F:1336:LEU:HD13	1:F:1339:LYS:HD2	2.01	0.43
1:E:1308:GLN:H	1:E:1319:GLN:HE22	1.66	0.43
1:F:1219:TYR:CE1	1:F:1385:LEU:HD11	2.54	0.43
1:D:1308:GLN:H	1:D:1319:GLN:HE22	1.65	0.42
1:E:1345:ASN:OD1	1:E:1345:ASN:N	2.52	0.42
1:D:1077:TYR:HD2	1:D:1244:ARG:NH1	2.17	0.42
1:C:1356:LEU:HD22	1:C:1370:TYR:CD1	2.51	0.42
1:B:1254:ARG:HA	1:B:1262:ILE:O	2.19	0.42
1:A:1374:THR:HG23	1:A:1553:GLU:HG2	2.00	0.42
1:A:1354:CYS:HA	1:A:1371:THR:O	2.19	0.42
1:B:1221:PHE:HA	1:B:1280:THR:O	2.20	0.42
1:E:1162:LYS:HB2	1:E:1207:CYS:HB3	2.02	0.42
1:E:1448:ALA:N	1:E:1467:ARG:O	2.46	0.42
1:B:1325:ASN:ND2	1:B:1341:GLU:HG2	2.35	0.42
1:C:1372:GLY:C	1:C:1555:LYS:HD2	2.41	0.42
1:D:1092:SER:CB	1:F:1090:TRP:HB2	2.50	0.41
1:C:1112:LEU:HD11	1:C:1267:PRO:HB3	2.03	0.41
1:F:1400:LYS:HA	1:F:1412:ASP:O	2.20	0.41
1:A:1138:MET:HE2	1:A:1234:ILE:HG21	2.03	0.41
1:B:1494:LEU:HD22	1:B:1505:SER:HB3	2.02	0.41
1:D:1445:LEU:HD23	1:D:1445:LEU:HA	1.94	0.41
1:B:1480:VAL:HG13	1:B:1520:PHE:HB3	2.01	0.41
1:C:1095:HIS:NE2	1:C:1097:GLY:O	2.52	0.41
1:C:1442:ILE:HA	1:C:1472:GLU:O	2.20	0.41
1:C:1364:ASP:OD1	1:C:1365:TRP:N	2.44	0.41
1:A:1111:LYS:NZ	1:B:1266:GLU:OE1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1282:HIS:HB3	1:A:1291:ASP:O	2.21	0.41
1:D:1293:MET:HG2	1:D:1330:ASP:HB3	2.03	0.41
1:E:1221:PHE:HB3	1:E:1281:LEU:HD23	2.02	0.41
1:E:1282:HIS:HB3	1:E:1291:ASP:O	2.20	0.41
1:A:1064:ILE:HD12	1:A:1138:MET:HE1	2.03	0.40
1:D:1182:HIS:ND1	1:D:1184:GLU:OE2	2.48	0.40
1:D:1355:ASP:OD2	1:E:1183:LYS:NZ	2.34	0.40
1:D:1242:GLN:HB3	1:D:1257:LEU:HD21	2.03	0.40
1:A:1462:ILE:O	1:A:1508:LYS:HA	2.22	0.40
1:B:1282:HIS:HB3	1:B:1291:ASP:O	2.22	0.40

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
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

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Mol	Chain	Res	Type
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

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1098	ASN
1	A	1100	ILE
1	A	1102	VAL
1	A	1140	LEU
1	A	1155	ARG
1	A	1166	THR
1	A	1173	CYS
1	A	1180	CYS
1	A	1193	CYS
1	A	1216	PHE
1	A	1226	VAL
1	A	1304	VAL
1	A	1332	VAL
1	A	1453	THR
1	A	1491	SER

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Mol	Chain	Res	Type
1	A	1516	THR
1	B	1100	ILE
1	B	1140	LEU
1	B	1155	ARG
1	B	1173	CYS
1	B	1180	CYS
1	B	1193	CYS
1	B	1216	PHE
1	B	1226	VAL
1	B	1304	VAL
1	B	1491	SER
1	B	1503	THR
1	C	1140	LEU
1	C	1155	ARG
1	C	1166	THR
1	C	1173	CYS
1	C	1193	CYS
1	C	1216	PHE
1	C	1304	VAL
1	C	1491	SER
1	C	1503	THR
1	C	1516	THR
1	D	1100	ILE
1	D	1140	LEU
1	D	1155	ARG
1	D	1166	THR
1	D	1173	CYS
1	D	1180	CYS
1	D	1216	PHE
1	D	1453	THR
1	D	1516	THR
1	E	1140	LEU
1	E	1155	ARG
1	E	1166	THR
1	E	1173	CYS
1	E	1180	CYS
1	E	1193	CYS
1	E	1216	PHE
1	E	1226	VAL
1	E	1453	THR
1	E	1504	ASP
1	E	1516	THR

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Mol	Chain	Res	Type
1	F	1126	ASP
1	F	1140	LEU
1	F	1155	ARG
1	F	1166	THR
1	F	1173	CYS
1	F	1180	CYS
1	F	1193	CYS
1	F	1216	PHE
1	F	1226	VAL
1	F	1304	VAL
1	F	1491	SER
1	F	1516	THR

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
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.

All (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
2	B	1602	NAG	O7-C7-N2-C2
2	C	1602	NAG	C8-C7-N2-C2
2	C	1602	NAG	O7-C7-N2-C2
2	E	1601	NAG	C8-C7-N2-C2
2	E	1601	NAG	O7-C7-N2-C2
2	F	1601	NAG	C8-C7-N2-C2
2	F	1601	NAG	O7-C7-N2-C2
2	C	1602	NAG	O5-C5-C6-O6
2	B	1601	NAG	C4-C5-C6-O6
2	C	1602	NAG	C4-C5-C6-O6
2	B	1601	NAG	O5-C5-C6-O6
2	A	1601	NAG	C4-C5-C6-O6
2	D	1601	NAG	C3-C2-N2-C7
2	A	1602	NAG	C3-C2-N2-C7
2	B	1602	NAG	C3-C2-N2-C7
2	A	1602	NAG	C1-C2-N2-C7

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

All (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
1	D	1064	ILE	5.4
1	D	1534	GLU	5.3
1	E	1338	HIS	5.1
1	F	1069	GLY	4.8
1	F	1064	ILE	4.8
1	E	1339	LYS	4.4
1	D	1063	SER	4.4
1	D	1341	GLU	4.4
1	D	1061	SER	4.4
1	F	1339	LYS	4.1
1	F	1334	GLY	4.1
1	E	1265	SER	4.1
1	D	1070	ALA	4.0
1	E	1336	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	1062	LEU	4.0
1	F	1271	GLN	3.9
1	F	1338	HIS	3.9
1	A	1060	THR	3.8
1	D	1451	ALA	3.8
1	D	1518	LEU	3.7
1	E	1060	THR	3.7
1	F	1060	THR	3.7
1	E	1061	SER	3.6
1	E	1069	GLY	3.6
1	F	1337	ILE	3.5
1	E	1062	LEU	3.5
1	D	1536	THR	3.4
1	D	1269	ASN	3.4
1	F	1340	ILE	3.4
1	F	1422	GLY	3.4
1	E	1127	ALA	3.4
1	E	1269	ASN	3.3
1	D	1126	ASP	3.3
1	F	1243	GLU	3.3
1	D	1422	GLY	3.3
1	E	1243	GLU	3.3
1	E	1335	HIS	3.3
1	A	1355	ASP	3.3
1	E	1098	ASN	3.2
1	D	1448	ALA	3.2
1	B	1343	HIS	3.2
1	A	1061	SER	3.1
1	C	1126	ASP	3.1
1	F	1494	LEU	3.1
1	C	1127	ALA	3.0
1	F	1503	THR	3.0
1	F	1336	LEU	3.0
1	E	1422	GLY	3.0
1	E	1065	GLU	3.0
1	A	1168	ASP	3.0
1	D	1270	ILE	3.0
1	E	1445	LEU	2.9
1	B	1197	ALA	2.9
1	E	1500	GLU	2.9
1	A	1354	CYS	2.9
1	E	1128	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1196	THR	2.9
1	E	1343	HIS	2.9
1	F	1244	ARG	2.9
1	D	1342	PRO	2.8
1	E	1064	ILE	2.8
1	D	1062	LEU	2.8
1	F	1265	SER	2.8
1	E	1166	THR	2.8
1	D	1065	GLU	2.7
1	E	1406	GLY	2.7
1	D	1077	TYR	2.7
1	D	1521	TYR	2.6
1	C	1501	PHE	2.6
1	F	1344	PHE	2.6
1	E	1126	ASP	2.6
1	B	1362	MET	2.6
1	B	1554	HIS	2.6
1	F	1362	MET	2.5
1	B	1344	PHE	2.5
1	D	1325	ASN	2.5
1	E	1331	LYS	2.5
1	C	1355	ASP	2.5
1	E	1276	PRO	2.5
1	D	1420	GLY	2.5
1	F	1168	ASP	2.5
1	A	1202	GLY	2.5
1	D	1450	LEU	2.5
1	B	1339	LYS	2.4
1	E	1283	PRO	2.4
1	D	1343	HIS	2.4
1	F	1065	GLU	2.4
1	D	1165	CYS	2.4
1	F	1191	HIS	2.4
1	C	1354	CYS	2.4
1	E	1342	PRO	2.4
1	C	1337	ILE	2.4
1	D	1425	THR	2.4
1	F	1269	ASN	2.4
1	A	1337	ILE	2.4
1	F	1213	LYS	2.4
1	D	1539	CYS	2.4
1	F	1123	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	1168	ASP	2.3
1	E	1340	ILE	2.3
1	E	1238	GLU	2.3
1	D	1276	PRO	2.3
1	E	1327	LEU	2.3
1	F	1502	GLY	2.3
1	E	1358	TYR	2.3
1	B	1127	ALA	2.3
1	A	1062	LEU	2.3
1	E	1529	LYS	2.3
1	D	1338	HIS	2.3
1	F	1429	GLU	2.3
1	D	1271	GLN	2.3
1	A	1338	HIS	2.3
1	E	1255	PHE	2.3
1	F	1500	GLU	2.3
1	F	1175	CYS	2.3
1	B	1060	THR	2.3
1	F	1126	ASP	2.3
1	F	1070	ALA	2.3
1	F	1450	LEU	2.3
1	A	1072	ASN	2.2
1	E	1268	ARG	2.2
1	E	1332	VAL	2.2
1	F	1096	ARG	2.2
1	D	1519	CYS	2.2
1	F	1268	ARG	2.2
1	E	1200	GLY	2.2
1	E	1483	ASP	2.2
1	D	1544	LEU	2.2
1	E	1293	MET	2.2
1	D	1452	CYS	2.2
1	D	1531	CYS	2.2
1	D	1206	THR	2.2
1	F	1343	HIS	2.2
1	F	1375	GLN	2.2
1	D	1132	LEU	2.2
1	E	1273	LYS	2.2
1	D	1287	GLU	2.2
1	D	1500	GLU	2.2
1	E	1531	CYS	2.1
1	D	1268	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	1110	MET	2.1
1	D	1355	ASP	2.1
1	E	1196	THR	2.1
1	F	1354	CYS	2.1
1	C	1241	SER	2.1
1	C	1343	HIS	2.1
1	E	1330	ASP	2.1
1	D	1167	GLY	2.1
1	E	1425	THR	2.1
1	C	1065	GLU	2.1
1	D	1226	VAL	2.1
1	C	1077	TYR	2.1
1	F	1077	TYR	2.1
1	F	1421	ALA	2.1
1	E	1099	LYS	2.1
1	A	1196	THR	2.0
1	E	1423	GLU	2.0
1	E	1168	ASP	2.0
1	D	1124	VAL	2.0
1	D	1465	LYS	2.0
1	D	1198	CYS	2.0
1	F	1122	LEU	2.0
1	B	1355	ASP	2.0

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)

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<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.