W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2017 – 02:39 PM EST

PDB ID : 5TJ4

Title : Gasdermin-B C-terminal domain containing the polymorphism residues Gly299:Pro306 fused to maltose binding protein

Authors : Chao, L.K.; Herzberg, O.

Deposited on : 2016-10-03

Resolution : 3.50 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:
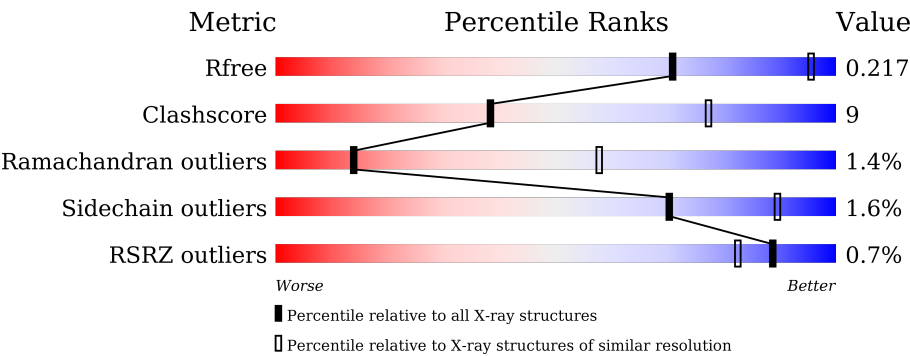
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	Percentile Ranks	Value
Rfree		0.217
Clashscore		9
Ramachandran outliers		1.4%
Sidechain outliers		1.6%
RSRZ outliers		0.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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. 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	561	84% 13% ••
1	B	561	84% 13% ••
1	C	561	80% 16% ••
1	D	561	81% 14% • •
1	E	561	85% 13% ••
1	F	561	83% 11% • •

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Mol	Chain	Length	Quality of chain
1	G	561	82% · · 13%
1	H	561	81% · · 13%
1	I	561	81% · 5% 13%
1	J	561	86% · · 11%

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	MAL	C	1501	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 39838 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 Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4066	2613	658	781	14			
1	B	554	Total	C	N	O	S	0	0	0
			4064	2603	664	784	13			
1	C	554	Total	C	N	O	S	0	0	0
			4070	2608	664	785	13			
1	D	541	Total	C	N	O	S	0	0	0
			3959	2542	643	762	12			
1	E	556	Total	C	N	O	S	0	0	0
			4077	2618	669	777	13			
1	F	541	Total	C	N	O	S	0	0	0
			3956	2546	633	765	12			
1	G	543	Total	C	N	O	S	0	0	0
			3885	2504	629	740	12			
1	H	537	Total	C	N	O	S	0	0	0
			3832	2459	623	739	11			
1	I	535	Total	C	N	O	S	0	0	0
			3795	2437	619	727	12			
1	J	548	Total	C	N	O	S	0	0	0
			3902	2500	638	754	10			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	ASP	see remark 999	UNP A0A178SBV6
A	83	ALA	LYS	see remark 999	UNP A0A178SBV6
A	172	ALA	GLU	see remark 999	UNP A0A178SBV6
A	173	ALA	ASN	see remark 999	UNP A0A178SBV6
A	239	ALA	LYS	see remark 999	UNP A0A178SBV6
A	362	ALA	LYS	see remark 999	UNP A0A178SBV6
A	363	ALA	ASP	see remark 999	UNP A0A178SBV6
A	367	ASN	-	linker	UNP A0A178SBV6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	-	linker	UNP A0A178SBV6
A	369	ALA	-	linker	UNP A0A178SBV6
A	370	ALA	-	linker	UNP A0A178SBV6
A	1220	MET	MET	linker	UNP Q8TAX9
B	82	ALA	ASP	see remark 999	UNP A0A178SBV6
B	83	ALA	LYS	see remark 999	UNP A0A178SBV6
B	172	ALA	GLU	see remark 999	UNP A0A178SBV6
B	173	ALA	ASN	see remark 999	UNP A0A178SBV6
B	239	ALA	LYS	see remark 999	UNP A0A178SBV6
B	362	ALA	LYS	see remark 999	UNP A0A178SBV6
B	363	ALA	ASP	see remark 999	UNP A0A178SBV6
B	367	ASN	-	linker	UNP A0A178SBV6
B	368	ALA	-	linker	UNP A0A178SBV6
B	369	ALA	-	linker	UNP A0A178SBV6
B	370	ALA	-	linker	UNP A0A178SBV6
B	1220	MET	MET	linker	UNP Q8TAX9
C	82	ALA	ASP	see remark 999	UNP A0A178SBV6
C	83	ALA	LYS	see remark 999	UNP A0A178SBV6
C	172	ALA	GLU	see remark 999	UNP A0A178SBV6
C	173	ALA	ASN	see remark 999	UNP A0A178SBV6
C	239	ALA	LYS	see remark 999	UNP A0A178SBV6
C	362	ALA	LYS	see remark 999	UNP A0A178SBV6
C	363	ALA	ASP	see remark 999	UNP A0A178SBV6
C	367	ASN	-	linker	UNP A0A178SBV6
C	368	ALA	-	linker	UNP A0A178SBV6
C	369	ALA	-	linker	UNP A0A178SBV6
C	370	ALA	-	linker	UNP A0A178SBV6
C	1220	MET	MET	linker	UNP Q8TAX9
D	82	ALA	ASP	see remark 999	UNP A0A178SBV6
D	83	ALA	LYS	see remark 999	UNP A0A178SBV6
D	172	ALA	GLU	see remark 999	UNP A0A178SBV6
D	173	ALA	ASN	see remark 999	UNP A0A178SBV6
D	239	ALA	LYS	see remark 999	UNP A0A178SBV6
D	362	ALA	LYS	see remark 999	UNP A0A178SBV6
D	363	ALA	ASP	see remark 999	UNP A0A178SBV6
D	367	ASN	-	linker	UNP A0A178SBV6
D	368	ALA	-	linker	UNP A0A178SBV6
D	369	ALA	-	linker	UNP A0A178SBV6
D	370	ALA	-	linker	UNP A0A178SBV6
D	1220	MET	MET	linker	UNP Q8TAX9
E	82	ALA	ASP	see remark 999	UNP A0A178SBV6
E	83	ALA	LYS	see remark 999	UNP A0A178SBV6

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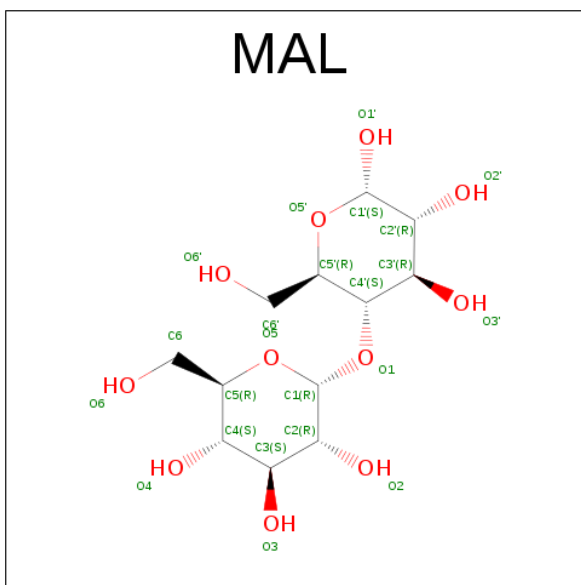
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Chain	Residue	Modelled	Actual	Comment	Reference
E	172	ALA	GLU	see remark 999	UNP A0A178SBV6
E	173	ALA	ASN	see remark 999	UNP A0A178SBV6
E	239	ALA	LYS	see remark 999	UNP A0A178SBV6
E	362	ALA	LYS	see remark 999	UNP A0A178SBV6
E	363	ALA	ASP	see remark 999	UNP A0A178SBV6
E	367	ASN	-	linker	UNP A0A178SBV6
E	368	ALA	-	linker	UNP A0A178SBV6
E	369	ALA	-	linker	UNP A0A178SBV6
E	370	ALA	-	linker	UNP A0A178SBV6
E	1220	MET	MET	linker	UNP Q8TAX9
F	82	ALA	ASP	see remark 999	UNP A0A178SBV6
F	83	ALA	LYS	see remark 999	UNP A0A178SBV6
F	172	ALA	GLU	see remark 999	UNP A0A178SBV6
F	173	ALA	ASN	see remark 999	UNP A0A178SBV6
F	239	ALA	LYS	see remark 999	UNP A0A178SBV6
F	362	ALA	LYS	see remark 999	UNP A0A178SBV6
F	363	ALA	ASP	see remark 999	UNP A0A178SBV6
F	367	ASN	-	linker	UNP A0A178SBV6
F	368	ALA	-	linker	UNP A0A178SBV6
F	369	ALA	-	linker	UNP A0A178SBV6
F	370	ALA	-	linker	UNP A0A178SBV6
F	1220	MET	MET	linker	UNP Q8TAX9
G	82	ALA	ASP	see remark 999	UNP A0A178SBV6
G	83	ALA	LYS	see remark 999	UNP A0A178SBV6
G	172	ALA	GLU	see remark 999	UNP A0A178SBV6
G	173	ALA	ASN	see remark 999	UNP A0A178SBV6
G	239	ALA	LYS	see remark 999	UNP A0A178SBV6
G	362	ALA	LYS	see remark 999	UNP A0A178SBV6
G	363	ALA	ASP	see remark 999	UNP A0A178SBV6
G	367	ASN	-	linker	UNP A0A178SBV6
G	368	ALA	-	linker	UNP A0A178SBV6
G	369	ALA	-	linker	UNP A0A178SBV6
G	370	ALA	-	linker	UNP A0A178SBV6
G	1220	MET	MET	linker	UNP Q8TAX9
H	82	ALA	ASP	see remark 999	UNP A0A178SBV6
H	83	ALA	LYS	see remark 999	UNP A0A178SBV6
H	172	ALA	GLU	see remark 999	UNP A0A178SBV6
H	173	ALA	ASN	see remark 999	UNP A0A178SBV6
H	239	ALA	LYS	see remark 999	UNP A0A178SBV6
H	362	ALA	LYS	see remark 999	UNP A0A178SBV6
H	363	ALA	ASP	see remark 999	UNP A0A178SBV6
H	367	ASN	-	linker	UNP A0A178SBV6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	368	ALA	-	linker	UNP A0A178SBV6
H	369	ALA	-	linker	UNP A0A178SBV6
H	370	ALA	-	linker	UNP A0A178SBV6
H	1220	MET	MET	linker	UNP Q8TAX9
I	82	ALA	ASP	see remark 999	UNP A0A178SBV6
I	83	ALA	LYS	see remark 999	UNP A0A178SBV6
I	172	ALA	GLU	see remark 999	UNP A0A178SBV6
I	173	ALA	ASN	see remark 999	UNP A0A178SBV6
I	239	ALA	LYS	see remark 999	UNP A0A178SBV6
I	362	ALA	LYS	see remark 999	UNP A0A178SBV6
I	363	ALA	ASP	see remark 999	UNP A0A178SBV6
I	367	ASN	-	linker	UNP A0A178SBV6
I	368	ALA	-	linker	UNP A0A178SBV6
I	369	ALA	-	linker	UNP A0A178SBV6
I	370	ALA	-	linker	UNP A0A178SBV6
I	1220	MET	MET	linker	UNP Q8TAX9
J	82	ALA	ASP	see remark 999	UNP A0A178SBV6
J	83	ALA	LYS	see remark 999	UNP A0A178SBV6
J	172	ALA	GLU	see remark 999	UNP A0A178SBV6
J	173	ALA	ASN	see remark 999	UNP A0A178SBV6
J	239	ALA	LYS	see remark 999	UNP A0A178SBV6
J	362	ALA	LYS	see remark 999	UNP A0A178SBV6
J	363	ALA	ASP	see remark 999	UNP A0A178SBV6
J	367	ASN	-	linker	UNP A0A178SBV6
J	368	ALA	-	linker	UNP A0A178SBV6
J	369	ALA	-	linker	UNP A0A178SBV6
J	370	ALA	-	linker	UNP A0A178SBV6
J	1220	MET	MET	linker	UNP Q8TAX9

- Molecule 2 is MALTOSE (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 23	C 12	O 11	0	0
2	B	1	Total 23	C 12	O 11	0	0
2	C	1	Total 23	C 12	O 11	0	0
2	D	1	Total 23	C 12	O 11	0	0
2	E	1	Total 23	C 12	O 11	0	0
2	F	1	Total 23	C 12	O 11	0	0
2	G	1	Total 23	C 12	O 11	0	0
2	H	1	Total 23	C 12	O 11	0	0
2	I	1	Total 23	C 12	O 11	0	0
2	J	1	Total 23	C 12	O 11	0	0

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

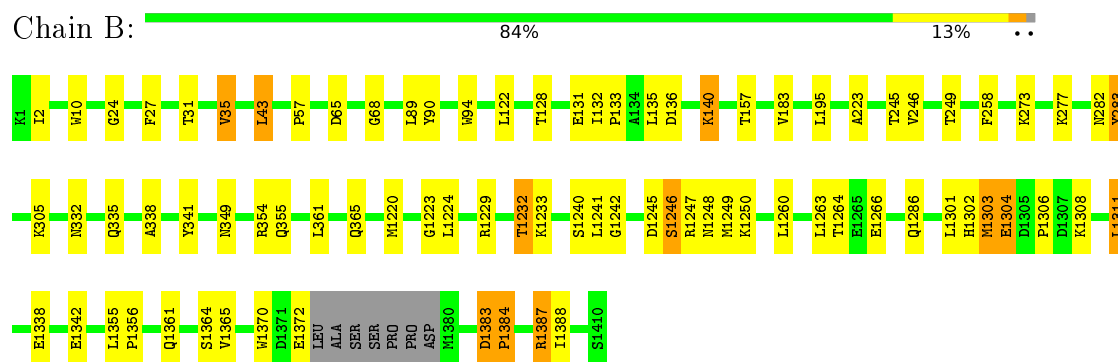| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
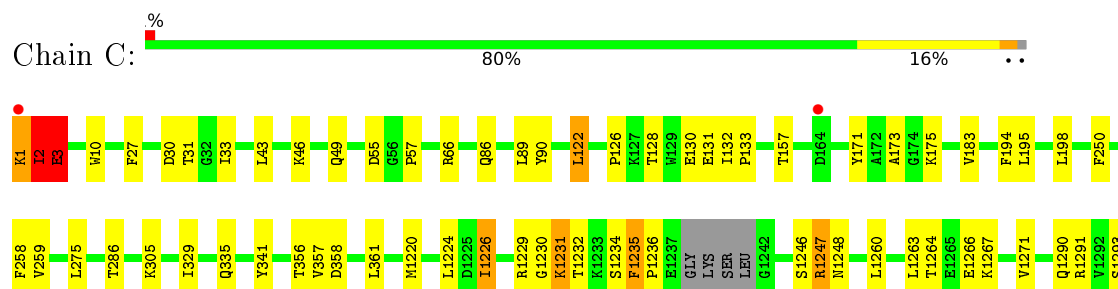
• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein
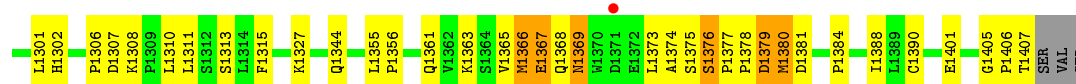

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein
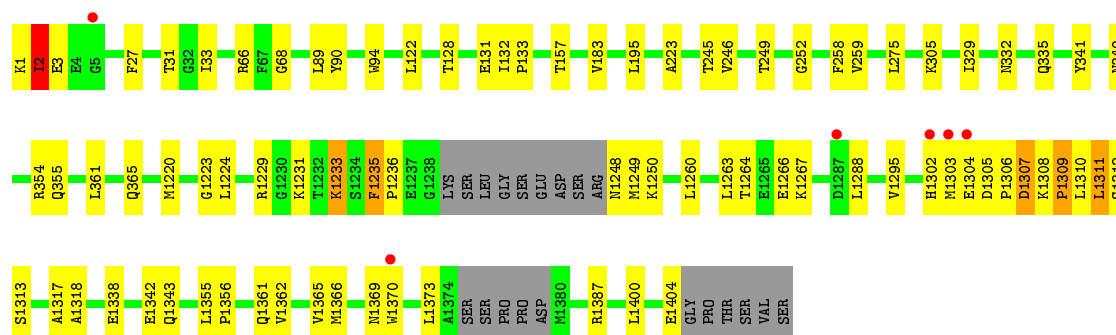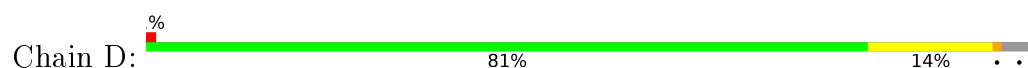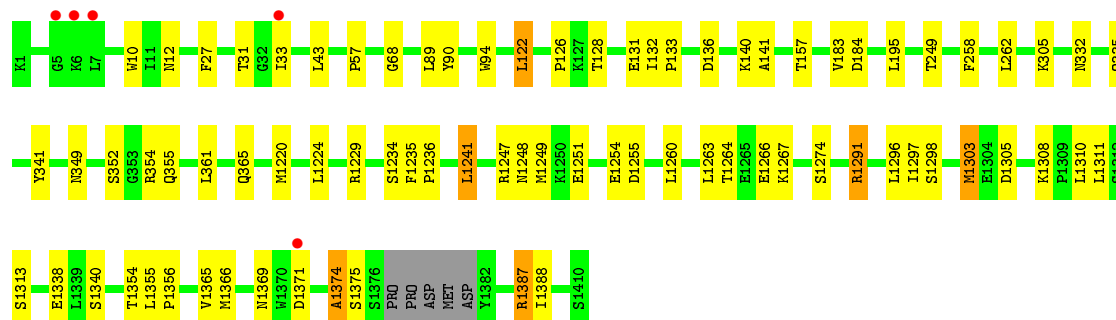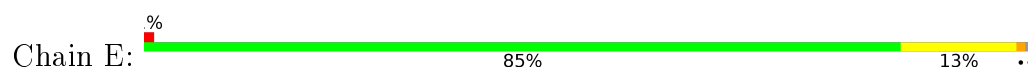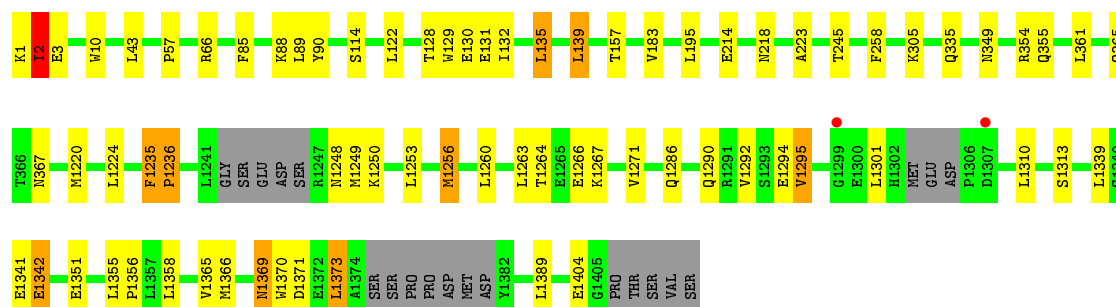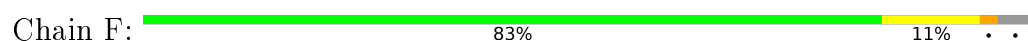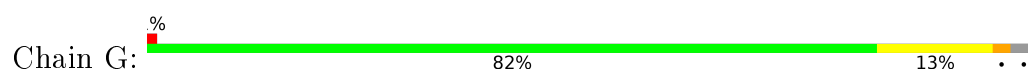

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

L1301 H1302 P1306 D1307 K1308 P1309 L1310 L1311 S1312 S1313 L1314 F1315 K1327 Q1344 L1355 P1356 Q1361 V1362 K1363 S1364 V1365 M1366 E1367 Q1368 N1369 W1370 D1371 E1372 L1373 A1374 S1375 S1376 P1377 P1378 D1379 M1380 D1381 P1384 I1388 L1389 C1390 E1401 G1405 P1406 T1407 SER VAL SER

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain D:

K1 I2 E3 E4 G5 F27 T31 G32 I33 R66 F67 G68 L89 Y90 W94 L122 T128 E131 I132 P133 T157 V183 L195 A223 T245 V246 T249 G252 F258 V259 L275 K305 I329 N332 Q335 Y341 N349

R354 Q355 L361 Q365 M1220 G1223 L1224 R1229 G1230 K1231 T1232 K1233 S1234 F1235 P1236 E1237 G1238 LYS SER LEU GLY SER GLU ASP SER ARG N1248 M1249 K1250 L1260 L1263 T1264 E1265 E1266 K1267 D1287 L1288 V1295 H1302 M1303 E1304 D1305 D1307 K1308 P1309 L1310 L1311 S1312

S1313 A1317 A1318 E1338 E1342 Q1343 L1355 P1356 Q1361 V1362 V1365 M1366 N1369 W1370 L1373 A1374 SER SER PRO PRO ASP M1380 R1387 L1400 E1404 GLY PRO THR SER VAL SER

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain E:

K1 G5 K6 L7 W10 I11 N12 F27 T31 G32 I33 L43 P57 G68 L89 Y90 W94 L122 P126 K127 T128 E131 I132 P133 D136 K140 A141 T157 V183 D184 L195 T249 F258 L262 K305 N332 Q335

Y341 N349 S352 G353 R354 Q355 L361 Q365 M1220 L1224 R1229 S1234 F1235 P1236 L1241 R1247 N1248 M1249 K1250 E1251 E1254 D1255 L1260 L1263 T1264 E1265 E1266 K1267 S1274 R1291 L1296 I1297 S1298 M1303 E1304 D1305 K1308 P1309 L1310 L1311 S1312

S1313 E1338 L1339 S1340 T1354 L1355 P1356 V1365 M1366 N1369 W1370 D1371 A1374 S1375 S1376 PRO PRO ASP MET ASP Y1382 R1387 I1388 S1410

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain F:

K1 I2 E3 W10 L43 P57 R66 F85 K88 L89 Y90 S114 L122 T128 W129 E130 E131 I132 L135 L139 T157 V183 L195 E214 N218 A223 T245 F258 K305 Q335 N349 R354 Q355 L361 Q365

T366 N367 M1220 L1224 F1235 P1236 L1241 GLY SER GLU ASP SER R1247 N1248 M1249 K1250 L1253 M1256 L1260 L1263 T1264 E1265 E1266 K1267 V1271 Q1286 V1292 S1293 E1294 V1295 G1299 E1300 L1301 H1302 MET GLU ASP P1306 D1307 L1310 S1313 L1339 S1340

E1341 E1342 E1351 L1355 P1356 L1357 L1358 V1365 M1366 N1369 W1370 D1371 E1372 L1373 A1374 SER SER PRO PRO ASP MET ASP Y1382 L1389 E1404 G1405 PRO THR SER VAL SER

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain G:

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein
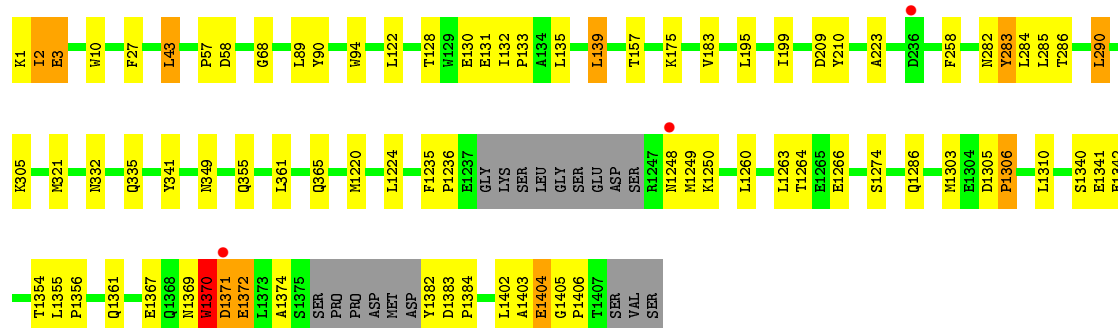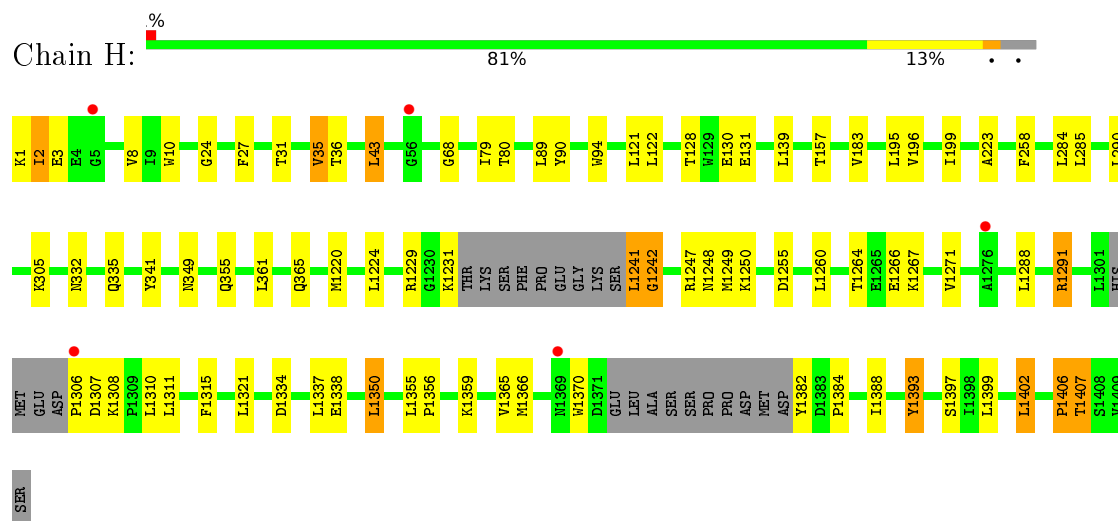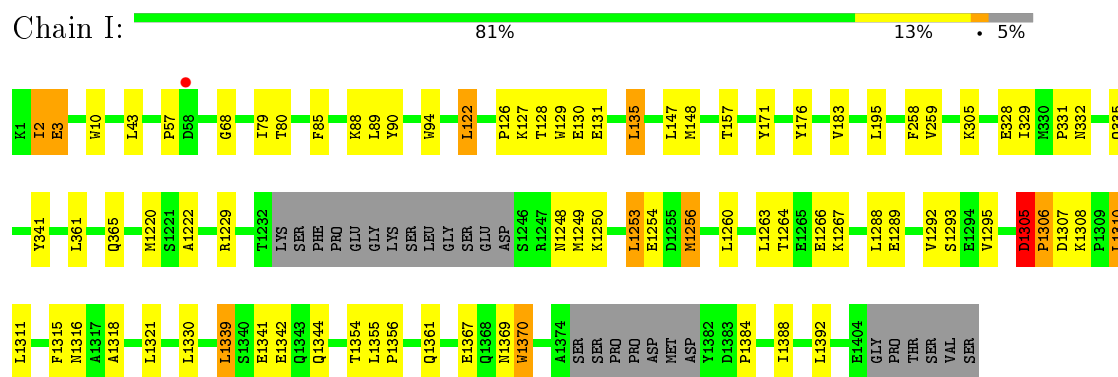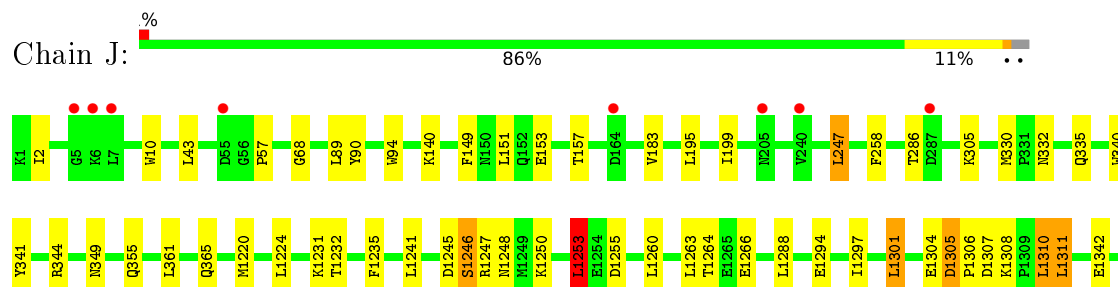
Chain H:

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain I:

• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain J:

T1354 L1355 P1356 Q1361 Q1368 N1369 TRP ASP GLU LEU ALA SER SER PRO PRO ASP MET D1381 R1387 V1394 S1408 VAL SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.60Å 274.57Å 174.02Å 90.00° 96.09° 90.00°	Depositor
Resolution (Å)	173.04 – 3.50 37.39 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (173.04-3.50) 99.8 (37.39-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.77 (at 3.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.248 0.214 , 0.217	Depositor DCC
R_{free} test set	5232 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	89.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 80.4	EDS
L-test for twinning[2]	$<|L|> = 0.45, <L^2> = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	39838	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.55	0/4149	0.79	5/5661 (0.1%)
1	B	0.53	0/4147	0.79	9/5659 (0.2%)
1	C	0.53	0/4157	0.80	5/5681 (0.1%)
1	D	0.50	0/4040	0.73	3/5519 (0.1%)
1	E	0.52	0/4161	0.78	7/5680 (0.1%)
1	F	0.52	0/4037	0.75	4/5518 (0.1%)
1	G	0.51	0/3968	0.76	11/5441 (0.2%)
1	H	0.52	0/3910	0.79	9/5356 (0.2%)
1	I	0.50	0/3874	0.72	3/5318 (0.1%)
1	J	0.52	0/3984	0.77	7/5461 (0.1%)
All	All	0.52	0/40427	0.77	63/55294 (0.1%)

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	89	LEU	CB-CG-CD2	10.84	129.42	111.00
1	C	89	LEU	CB-CG-CD2	10.65	129.10	111.00
1	A	89	LEU	CB-CG-CD2	10.52	128.88	111.00
1	A	65	ASP	CB-CG-OD2	10.29	127.56	118.30
1	B	65	ASP	CB-CG-OD2	10.11	127.40	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4066	0	3871	88	0
1	B	4064	0	3833	65	0
1	C	4070	0	3841	115	0
1	D	3959	0	3729	66	0
1	E	4077	0	3874	53	0
1	F	3956	0	3714	65	0
1	G	3885	0	3583	72	0
1	H	3832	0	3525	78	0
1	I	3795	0	3444	88	1
1	J	3902	0	3567	45	1
2	A	23	0	22	1	0
2	B	23	0	22	0	0
2	C	23	0	22	1	0
2	D	23	0	22	1	0
2	E	23	0	22	0	0
2	F	23	0	22	1	0
2	G	23	0	22	0	0
2	H	23	0	22	0	0
2	I	23	0	22	0	0
2	J	23	0	22	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
All	All	39838	0	37201	704	1

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 9.

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:I:259:VAL:CG2	1:I:329:ILE:HA	1.73	1.18
1:E:184:ASP:CB	1:E:365:GLN:OE1	1.96	1.14
1:H:1241:LEU:HD23	1:H:1242:GLY:H	1.07	1.12
1:D:2:ILE:HG22	1:D:3:GLU:H	1.03	1.12
1:C:1247:ARG:HH22	1:C:1327:LYS:HE3	1.01	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:171:TYR:OH	1:J:1231:LYS:O[2_444]	2.12	0.08

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	547/561 (98%)	504 (92%)	30 (6%)	13 (2%)	7	47
1	B	550/561 (98%)	510 (93%)	29 (5%)	11 (2%)	9	51
1	C	550/561 (98%)	517 (94%)	21 (4%)	12 (2%)	8	49
1	D	535/561 (95%)	505 (94%)	22 (4%)	8 (2%)	13	56
1	E	552/561 (98%)	520 (94%)	27 (5%)	5 (1%)	21	68
1	F	533/561 (95%)	511 (96%)	18 (3%)	4 (1%)	24	70
1	G	537/561 (96%)	513 (96%)	17 (3%)	7 (1%)	15	60
1	H	529/561 (94%)	504 (95%)	21 (4%)	4 (1%)	24	70
1	I	529/561 (94%)	509 (96%)	14 (3%)	6 (1%)	17	63
1	J	544/561 (97%)	521 (96%)	19 (4%)	4 (1%)	26	72
All	All	5406/5610 (96%)	5114 (95%)	218 (4%)	74 (1%)	14	58

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1226	ILE
1	A	1303	MET
1	A	1368	GLN
1	A	1370	TRP
1	A	1383	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	388/454 (86%)	385 (99%)	3 (1%)	86	95
1	B	384/454 (85%)	377 (98%)	7 (2%)	66	88
1	C	389/454 (86%)	383 (98%)	6 (2%)	72	90
1	D	372/454 (82%)	368 (99%)	4 (1%)	80	92
1	E	385/454 (85%)	381 (99%)	4 (1%)	82	93
1	F	372/454 (82%)	361 (97%)	11 (3%)	48	81
1	G	350/454 (77%)	345 (99%)	5 (1%)	74	91
1	H	347/454 (76%)	340 (98%)	7 (2%)	63	87
1	I	335/454 (74%)	329 (98%)	6 (2%)	66	88
1	J	351/454 (77%)	345 (98%)	6 (2%)	68	89
All	All	3673/4540 (81%)	3614 (98%)	59 (2%)	70	89

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	258	PHE
1	F	1369	ASN
1	J	365	GLN
1	F	354	ARG
1	F	1286	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	ASN
1	B	1368	GLN
1	D	325	GLN
1	A	1361	GLN
1	D	100	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	MAL	A	1501	-	24,24,24	0.76	0	35,35,35	1.66	7 (20%)
2	MAL	B	1501	-	24,24,24	0.52	0	35,35,35	1.17	3 (8%)
2	MAL	C	1501	-	24,24,24	0.50	0	35,35,35	1.15	3 (8%)
2	MAL	D	1501	-	24,24,24	0.54	0	35,35,35	0.99	1 (2%)
2	MAL	E	1501	-	24,24,24	0.53	0	35,35,35	1.49	5 (14%)
2	MAL	F	1501	-	24,24,24	0.57	0	35,35,35	1.00	3 (8%)
2	MAL	G	1501	-	24,24,24	0.66	0	35,35,35	1.38	6 (17%)
2	MAL	H	1501	-	24,24,24	0.52	0	35,35,35	1.44	5 (14%)
2	MAL	I	1501	-	24,24,24	0.70	0	35,35,35	1.05	2 (5%)
2	MAL	J	1501	-	24,24,24	0.54	0	35,35,35	1.22	4 (11%)

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	MAL	A	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	B	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	C	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	D	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	E	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	F	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	G	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	H	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	I	1501	-	-	0/8/48/48	0/2/2/2
2	MAL	J	1501	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1501	MAL	O2'-C2'-C3'	-3.31	102.91	110.36
2	A	1501	MAL	C1-O1-C4'	-3.04	109.91	118.00
2	B	1501	MAL	O3-C3-C4	-2.82	103.99	110.36
2	A	1501	MAL	O3-C3-C4	-2.75	104.15	110.36
2	G	1501	MAL	O3'-C3'-C2'	-2.70	104.26	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	MAL	1	0
2	C	1501	MAL	1	0
2	D	1501	MAL	1	0
2	F	1501	MAL	1	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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1405:GLY	C	1406:PRO	N	3.42

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	553/561 (98%)	-0.43	3 (0%)	91 | 88	36, 77, 141, 196	0
1	B	554/561 (98%)	-0.50	0	100 | 100	38, 75, 128, 171	0
1	C	554/561 (98%)	-0.41	3 (0%)	91 | 88	39, 82, 130, 181	0
1	D	541/561 (96%)	-0.28	6 (1%)	82 | 73	40, 79, 144, 200	0
1	E	556/561 (99%)	-0.48	5 (0%)	85 | 78	36, 76, 125, 175	0
1	F	541/561 (96%)	-0.37	2 (0%)	93 | 90	47, 86, 129, 193	0
1	G	543/561 (96%)	-0.27	3 (0%)	90 | 85	55, 104, 146, 204	0
1	H	537/561 (95%)	-0.09	5 (0%)	85 | 78	64, 112, 148, 184	0
1	I	535/561 (95%)	-0.15	1 (0%)	95 | 93	68, 118, 161, 205	0
1	J	548/561 (97%)	-0.18	8 (1%)	76 | 67	54, 120, 157, 202	0
All	All	5462/5610 (97%)	-0.32	36 (0%)	89 | 82	36, 93, 147, 205	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1371	ASP	4.0
1	D	1303	MET	3.3
1	J	205	ASN	3.2
1	A	1317	ALA	3.0
1	D	1302	HIS	3.0

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
2	MAL	C	1501	23/23	0.94	0.30	2.23	51,67,82,88	0
2	MAL	B	1501	23/23	0.97	0.23	1.58	46,52,62,66	0
2	MAL	H	1501	23/23	0.96	0.33	1.27	69,82,104,114	0
2	MAL	D	1501	23/23	0.97	0.26	1.15	39,48,67,76	0
2	MAL	A	1501	23/23	0.97	0.27	1.00	41,48,66,72	0
2	MAL	G	1501	23/23	0.97	0.24	0.86	53,60,67,84	0
2	MAL	I	1501	23/23	0.95	0.26	0.52	58,67,75,81	0
2	MAL	J	1501	23/23	0.96	0.22	0.23	76,93,107,116	0
2	MAL	E	1501	23/23	0.98	0.19	0.17	45,55,72,80	0
2	MAL	F	1501	23/23	0.98	0.22	0.03	36,43,59,70	0
3	NA	E	1502	1/1	0.92	0.18	-0.58	59,59,59,59	0
3	NA	B	1502	1/1	0.96	0.09	-2.92	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.